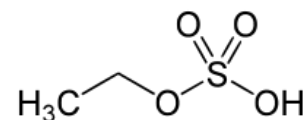
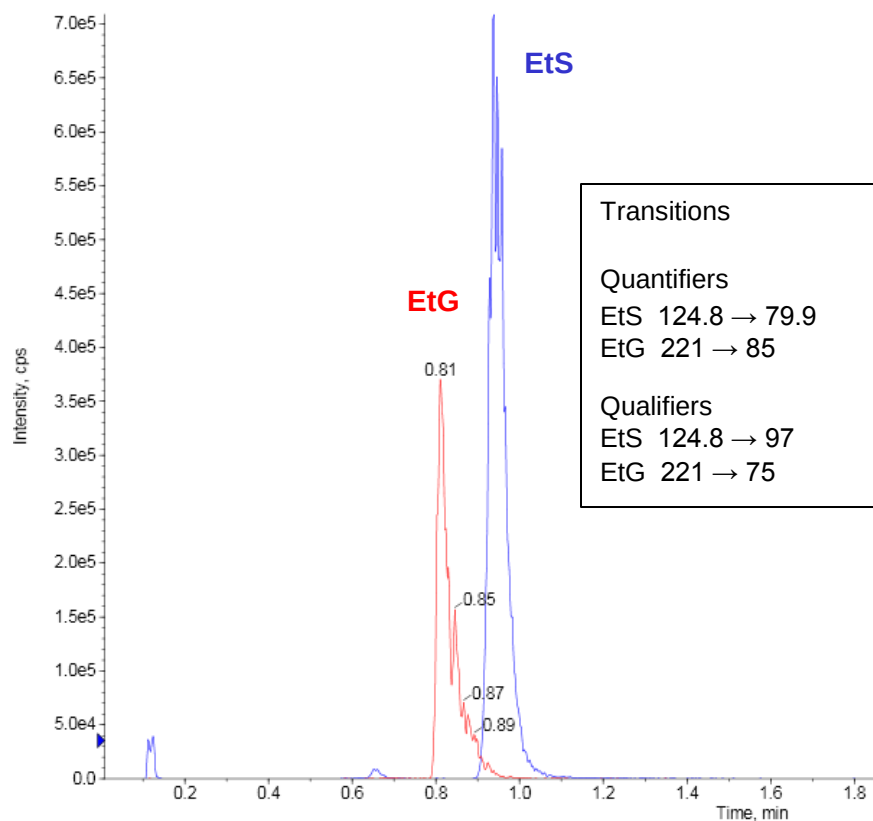


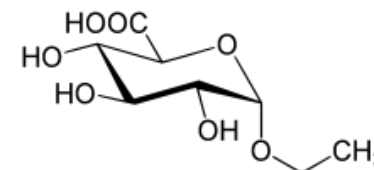


Alcohol Biomarkers by LC-MS/MS

Extracted ion chromatogram



Ethyl sulphate (EtS)



Ethyl glucuronide (EtG)

ACE Excel 1.7 C18 1.7µm, 100 x 2.1mm

Gradient analysis

A = 1mM ammonium fluoride

B = Acetonitrile

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

Flow rate: 0.4ml/min

Column temperature: 40°C

Injection volume: 1µl

AB SCIEX triple quad 5500

Negative ESI MRM

Source temperature: 750°C

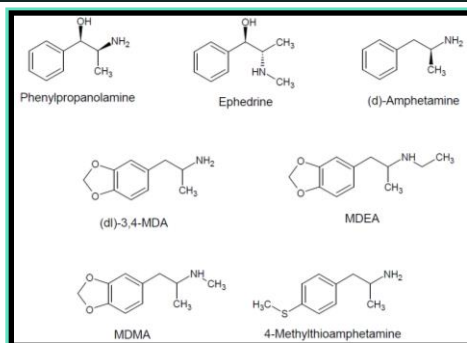
IonSpray voltage: -4500V

Fluoride counter-ion thought to enhance negative ESI response

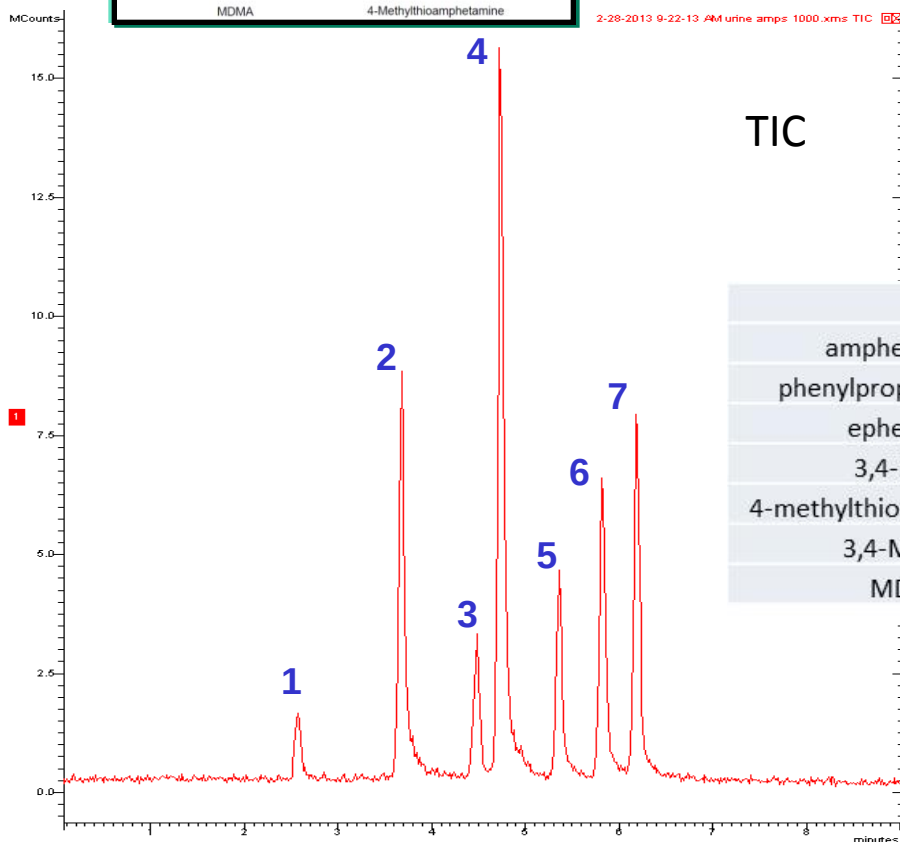
Detection limit ~ 1ng/ml in oral fluid



Amphetamines In Urine by LC-MS/MS



1. Phenylpropanolamine
2. (l)-Ephedrine
3. (dl)-3,4-MDA
4. (d)-Amphetamine
5. (dl)-3,4-MDMA
6. 4-methylthioamphetamine
7. (±)-MDEA



ACE Excel SuperC18, 3um, 75 x 2.1 mm
Gradient analysis

MP A: 5mM Ammonium Hydroxide, pH 10.8.
MP B: 5mM Ammonium Hydroxide, pH 10.8
in 1:9 v/v H₂O:MeOH.
0.6mL/min

T	%B
0	30
8	95

60C, 2uL.

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

Compound	Q1 Mass	Q3 Mass
(dl)-3,4-MDMA	193.7	163.0
Phenylpropanolamine	151.6	134.0
(d)-Amphetamine	135.8	90.9
(l)-Ephedrine	166.2	148.0
(dl)-3,4-MDA	179.7	163.0
(±)-MDEA	207.7	163.0
4-methylthioamphetamine	182.2	165.0



Opiates In Urine by LC-MS/MS

1. Morphine 3-β-D-glucuronide
2. Normorphine
3. Morphine 6-β-D-glucuronide
4. Morphine
5. 6-Acetylmorphine

	LOD (est)
Normorphine	100 ppb
Morphine	20 ppb
6-acetylmorphine	10 ppb
Morphine 3-β-DG	100ppb
Morphine 6-β-DG	100ppb

ACE Excel SuperC18, 3μm, 75 x 2.1 mm + guard
Gradient analysis

MP A: 5mM Ammonium Hydroxide, pH 10.8.
MP B: 5mM Ammonium Hydroxide, pH 10.8
in 1:9 v/v H₂O:MeOH.

0.6mL/min

T	%B
0	5
5	95

60C, 2μL.

Varian 320 Triple Quadrupole MS

Electrospray voltage: +5 kV

Inlet capillary voltage: 30 V

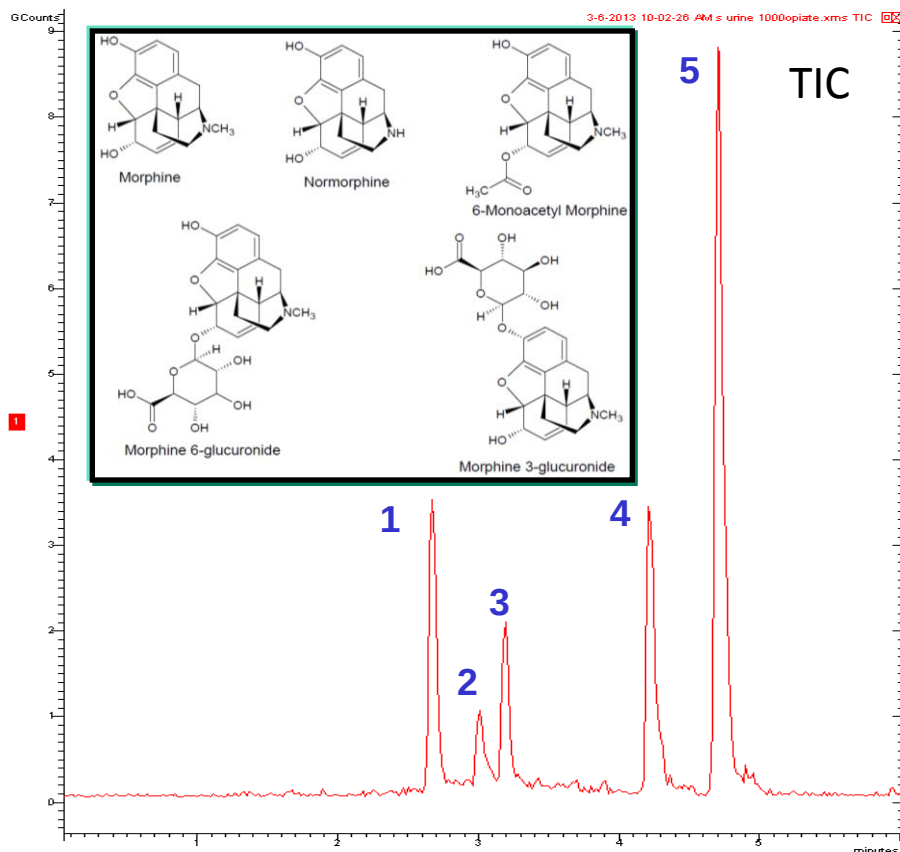
CID with argon at 1.5 mTorr; Collision cell
potential ranges from 5 to 17 V

Drying gas (nitrogen) temperature: 325 C

Nebulizing gas (nitrogen) pressure: 35 psi

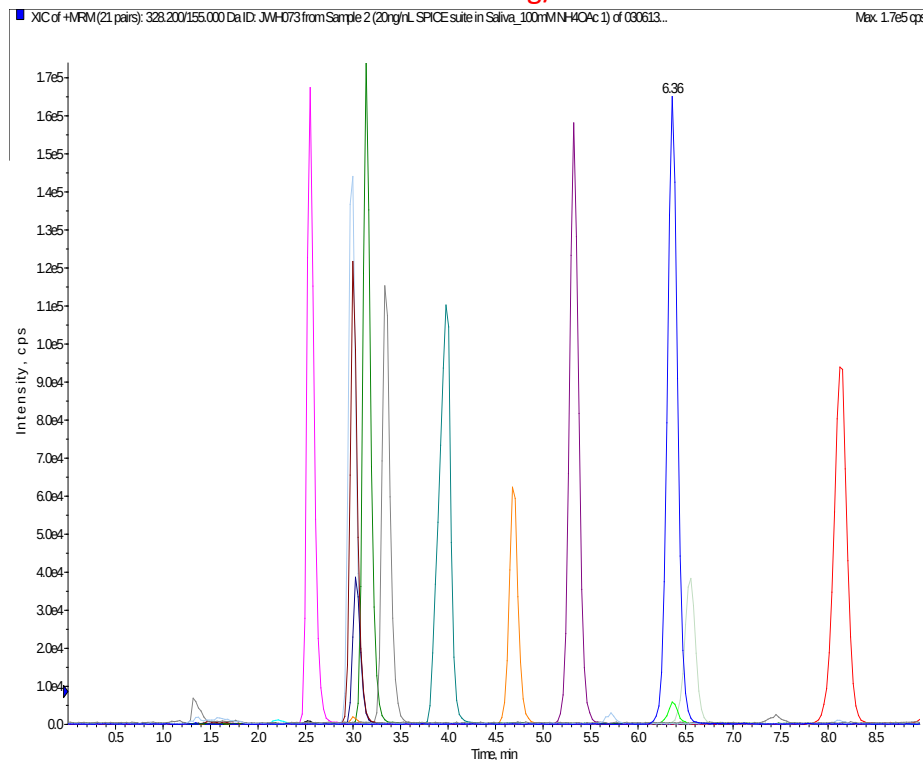
Extended Dynamic Range

Compound	Q1 Mass	Q3 Mass
morphine 3-β-D glucuronide	462.0	285.9
Normorphine	272.0	165.0
morphine 6-β-D glucuronide	462.0	285.9
6-acetylmorphine	328.0	164.9
morphine	286.0	200.9



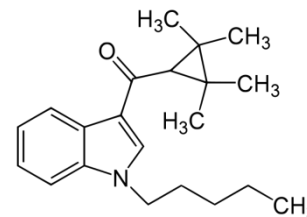
Synthetic Cannabinoids (SPICE) From Oral Fluid

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

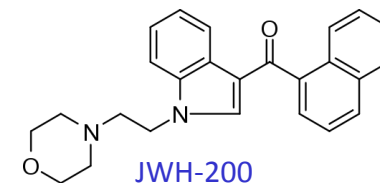


ACE Excel C18-AR 100x2.1mm, 2µm
Isocratic analysis
15:85 v/v A:B
A = 0.1% v/v formic acid (aq)
B = 0.1% v/v formic acid in MeOH
Ambient
0.3mL/min
Applied Biosystems / MDS Sciex 4000 Q-Trap
Positive mode Turbo Ionspray®

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



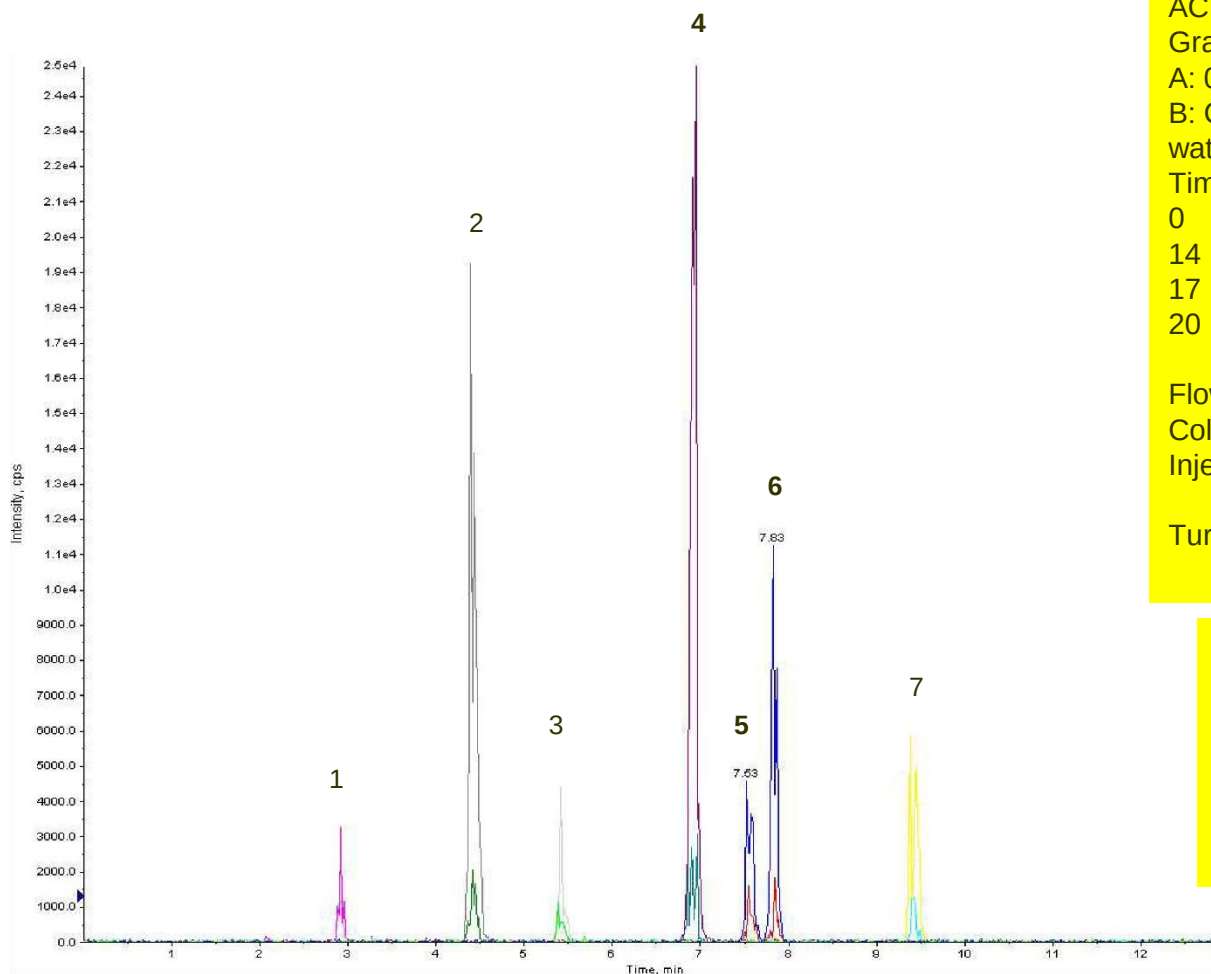
UR-144



JWH-200



Corticosteroids by LC-MS/MS



ACE C18-PFP, 3 μ m, 150 x 2.1mm
Gradient analysis

A: 0.1% formic acid in water

B: CH₃CN – 0.1% formic acid in water

Time (mins) %B

0 30

14 50

17 95

20 30

Flow rate: 0.3ml/min

Column temperature: 15°C

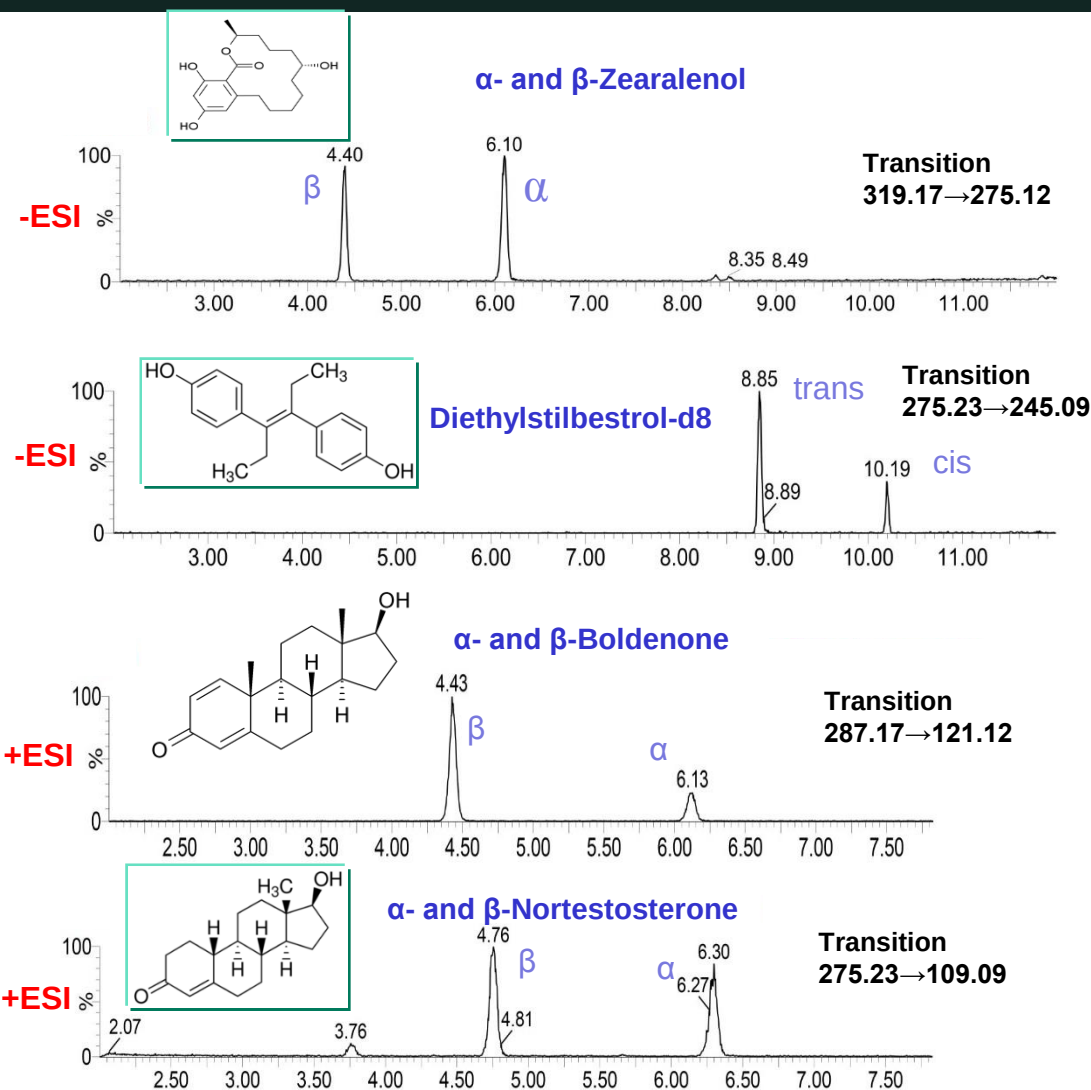
Injection volume: 25 μ l

Turbospray, MRM

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



Veterinary Steroids by LC-MS/MS



Also analysed in the same run (-ESI):

Talaranol and zearanol-d4

Talaranol and zearanol

Zearalenone

Hexestrol

Diethylstilbestrol

Dienestrol

ACE UltraCore SuperC18, 2.5 μ m, 100 x 2.1mm

Waters Acquity SDS system

Gradient analysis

A = 0.01mM amm. fluoride + 0.001% formic acid

B = Acetonitrile

Time (mins)	%B	Time (mins)	%B
0	25	7.5	35
0.5	25	10.5	60
7.0	35		

Flow rate: 0.5ml/min

Column temperature: 45°C

Positive or negative ESI

MRM data

Also analysed in the same run (+ESI):

Hydroxystanazolol

Hydroxystanazolol-d3

Methyltestosterone

Methyltestosterone-d3

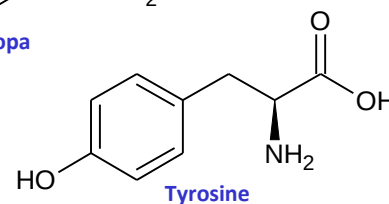
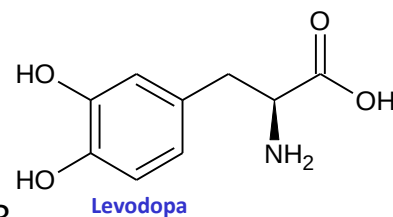
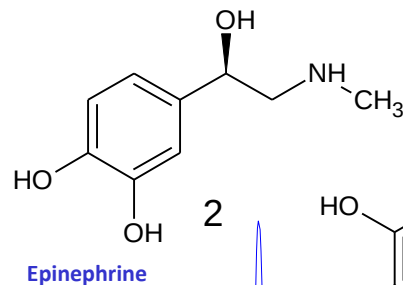
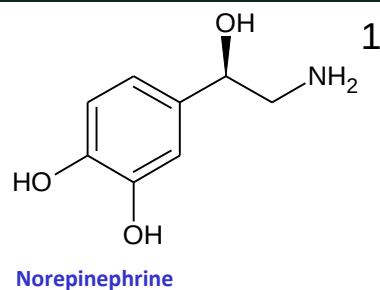
β -Nortestosterone-d3

β -Trenbolone

α -Trenbolone



Catecholamine Analysis



100% Aqueous

ACE C18-PFP, 5 μ m, 150 x 4.6 mm

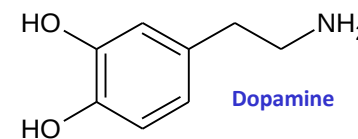
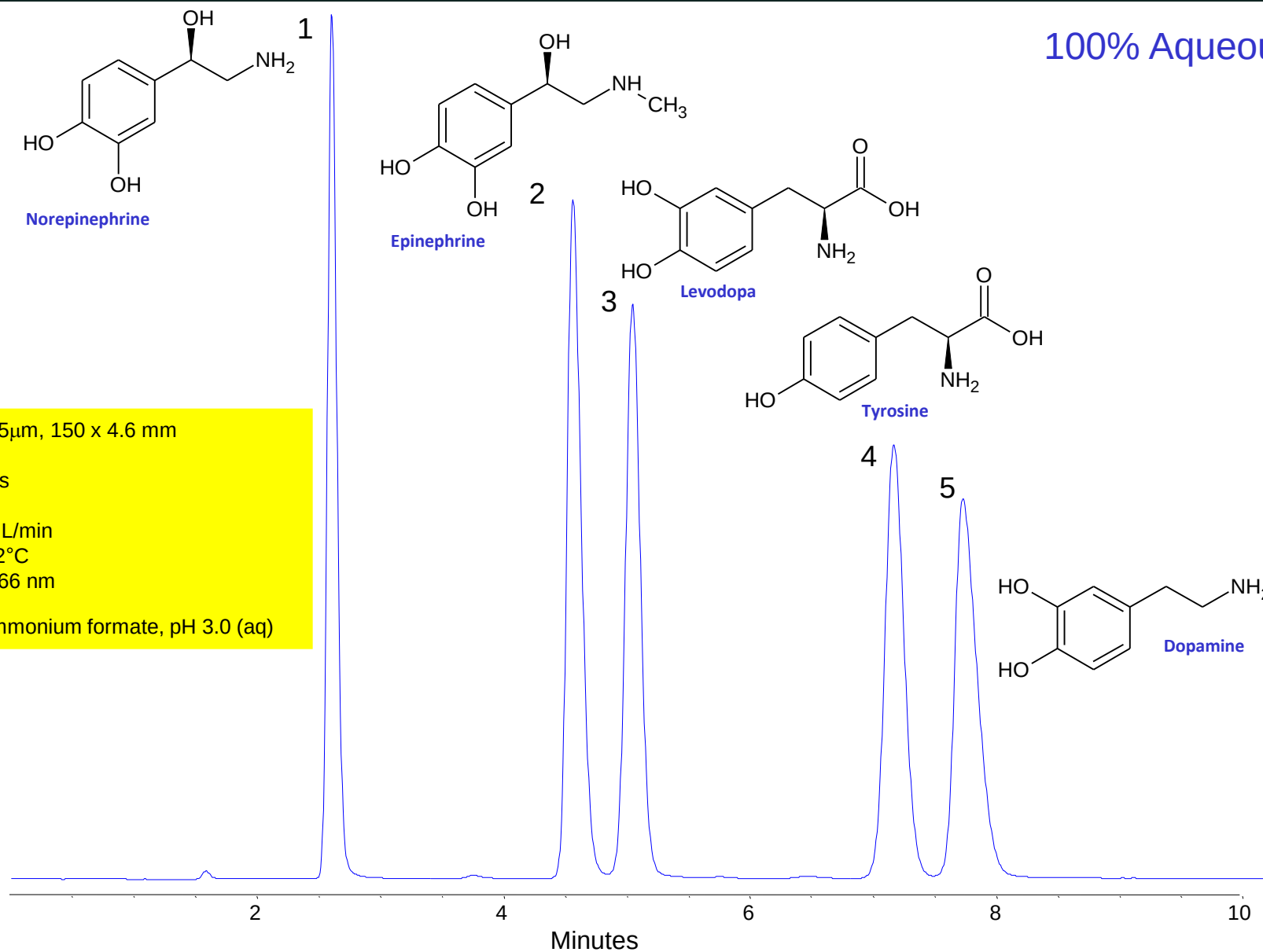
Isocratic analysis

Flow rate: 1.0 mL/min

Temperature: 22°C

Detection: UV 266 nm

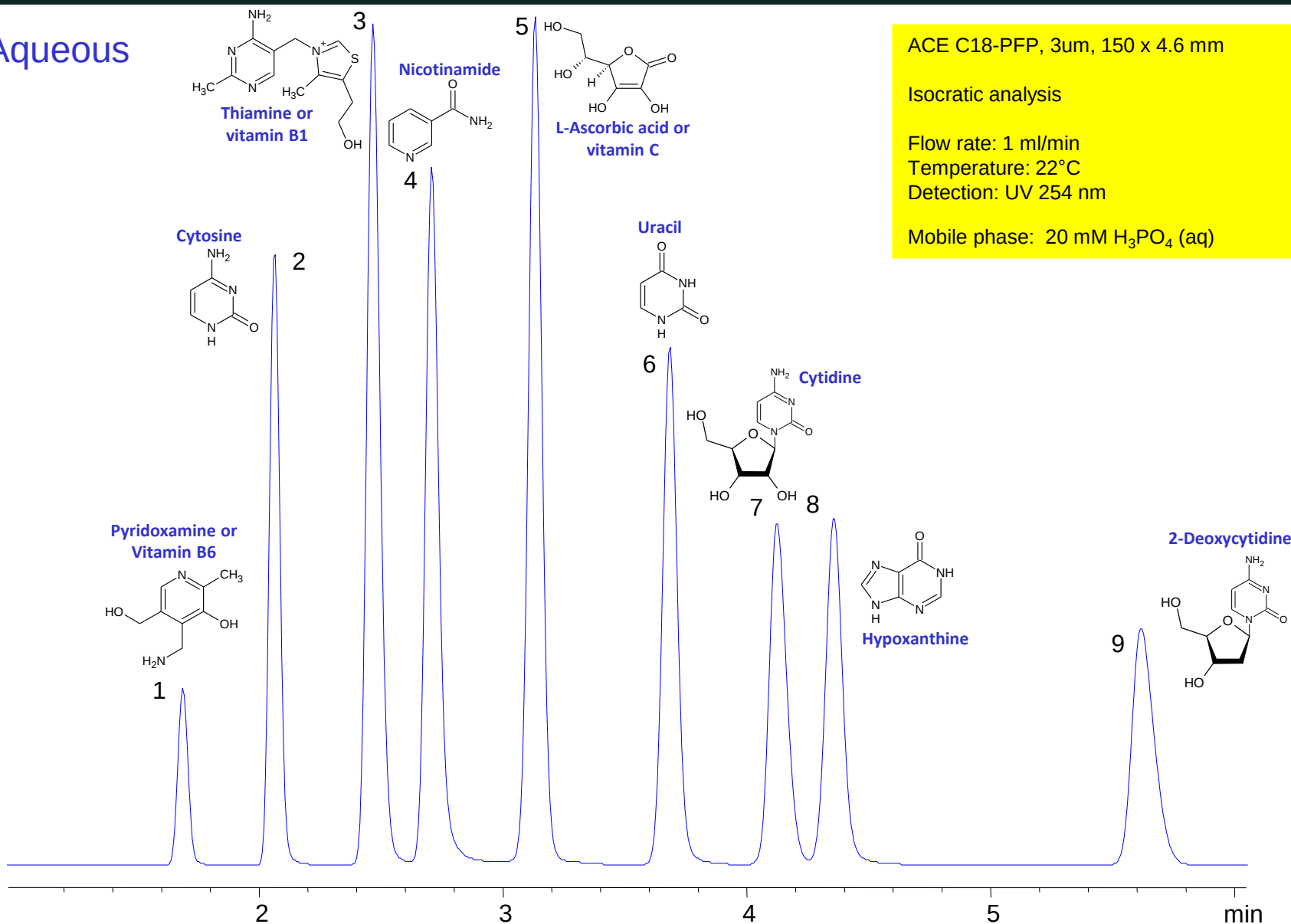
MP: 12.5mM Ammonium formate, pH 3.0 (aq)





Polar Analytes – Nucleosides & Vitamins

100% Aqueous





Separation of Sulphonamides

ACE Excel C18-PFP

3 μ m, 150 x 4.6mm

Gradient analysis

A = Water

B = Acetonitrile

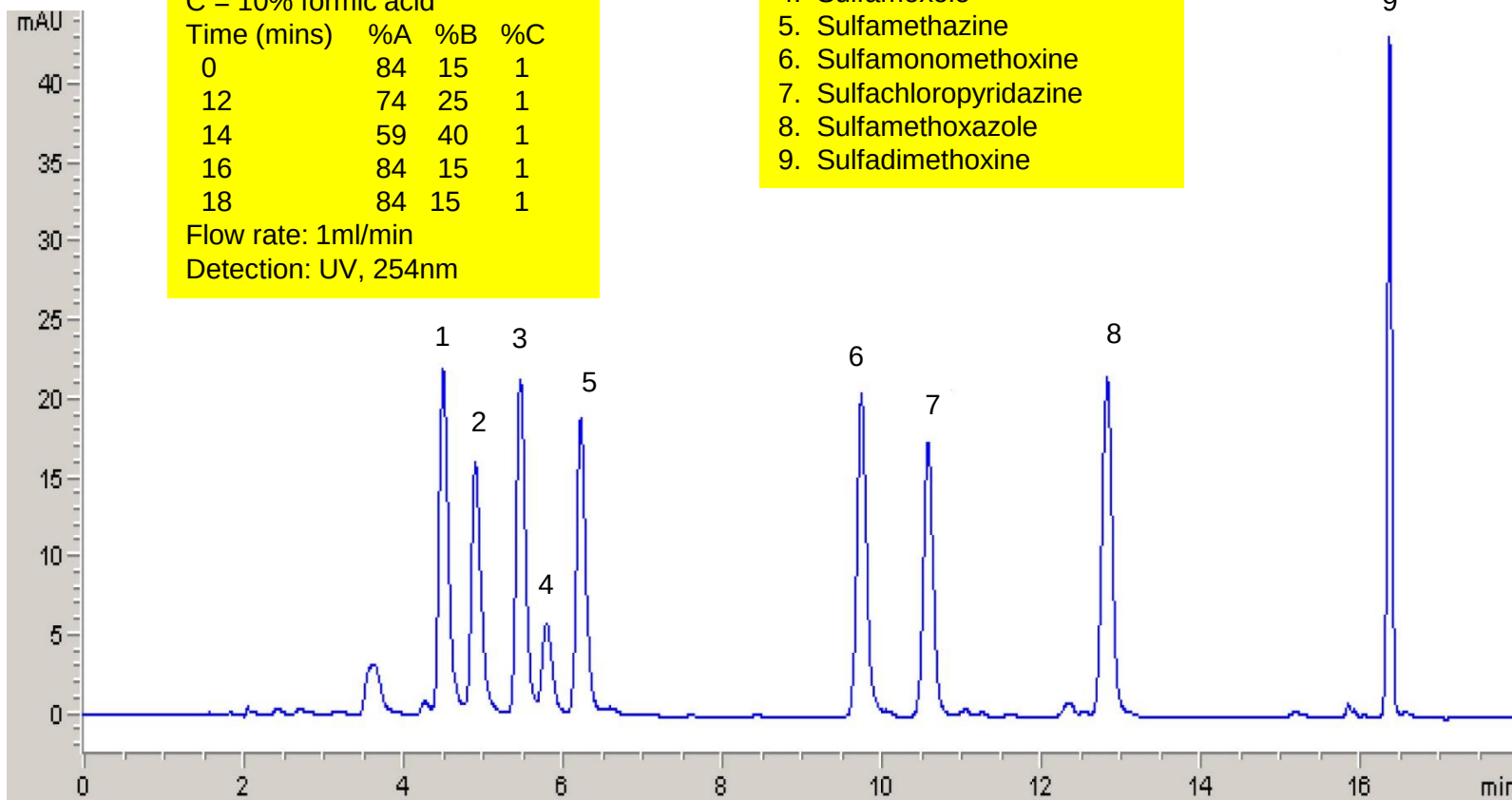
C = 10% formic acid

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: 1ml/min

Detection: UV, 254nm

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





Disease Biomarker Profiling

Nucleotide, Nucleoside & Nucleobase Analysis

Analytes

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

ACE C18 and ACE C18-PFP

3 μ m, 100 x 4.6 mm

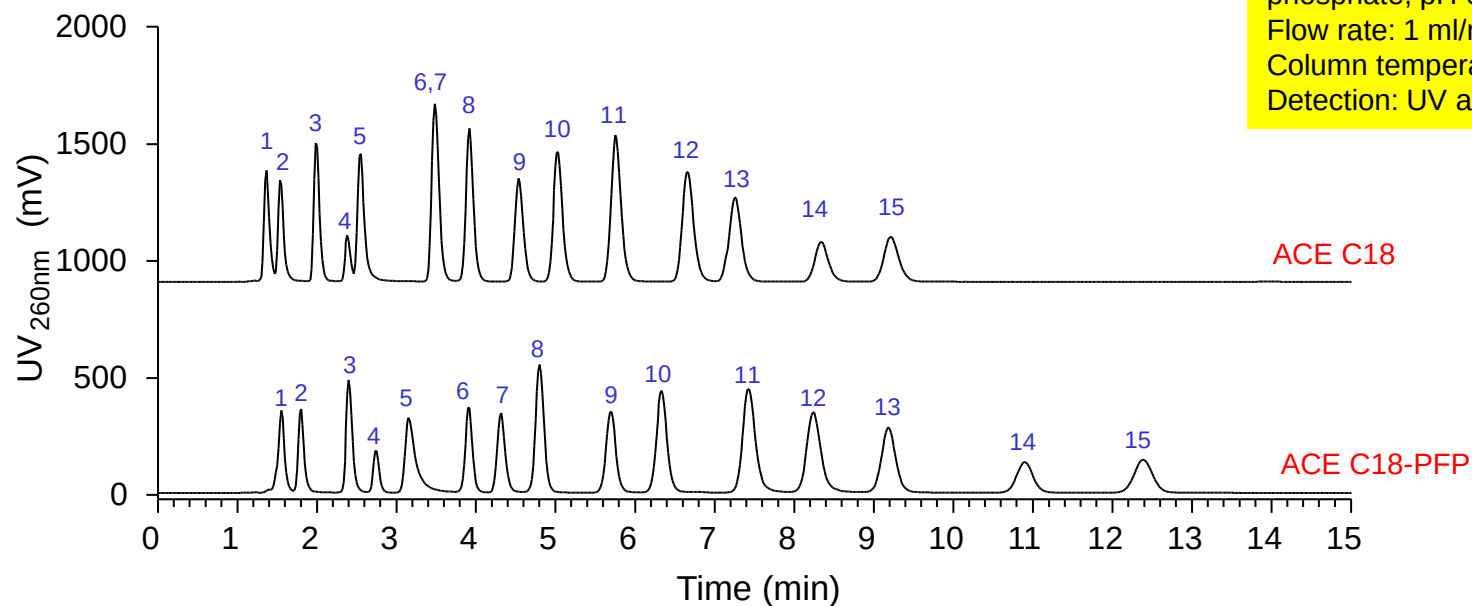
Isocratic analysis

Solvent = 12% methanol, 33 mM potassium phosphate, pH 6.2 with KOH

Flow rate: 1 ml/min

Column temperature: Ambient

Detection: UV at 260 nm





Disease Biomarker Profiling

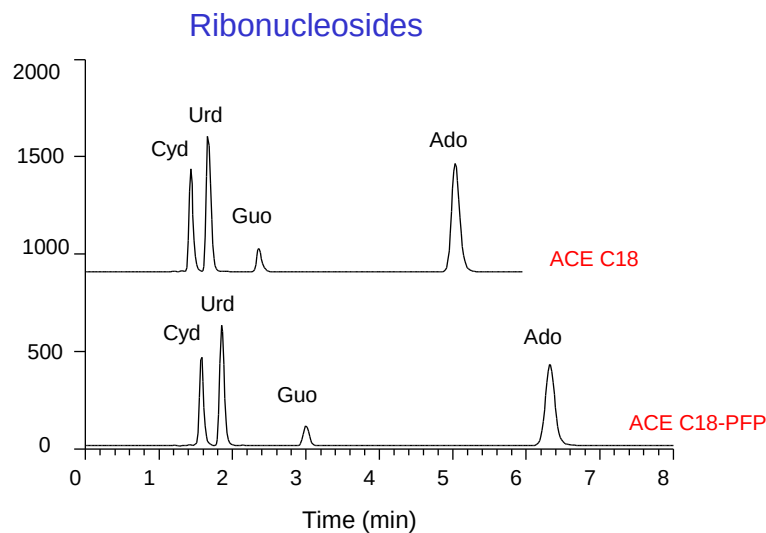
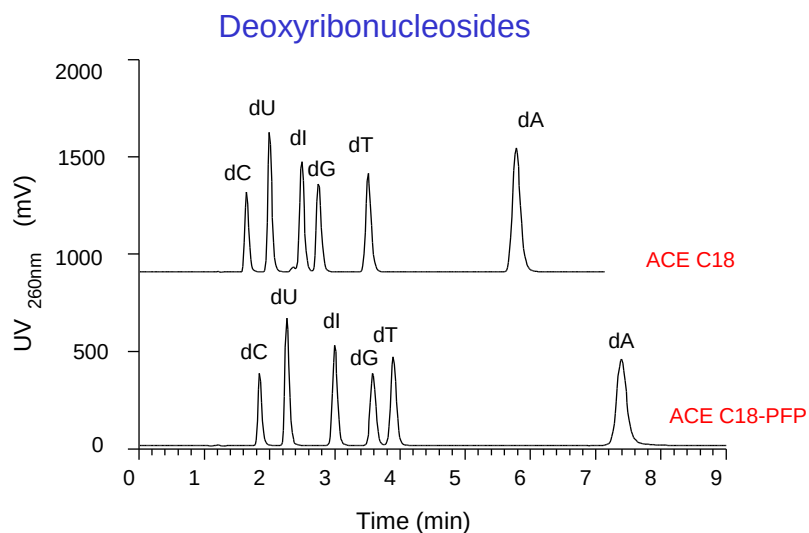
ACE C18 and ACE C18-PFP
3 μ m, 100 x 4.6 mm
Isocratic analysis
Mobile phase: 12% methanol, 33 mM
potassium phosphate, pH 6.2 with KOH
Flow rate: 1 ml/min
Column temperature: Ambient
Detection: UV at 260nm

Deoxyribonucleosides and Ribonucleosides

Key

dC deoxycytidine
dU deoxyuridine
dI deoxyinosine
dG deoxyguanosine
dT thymidine
dA deoxyadenosine

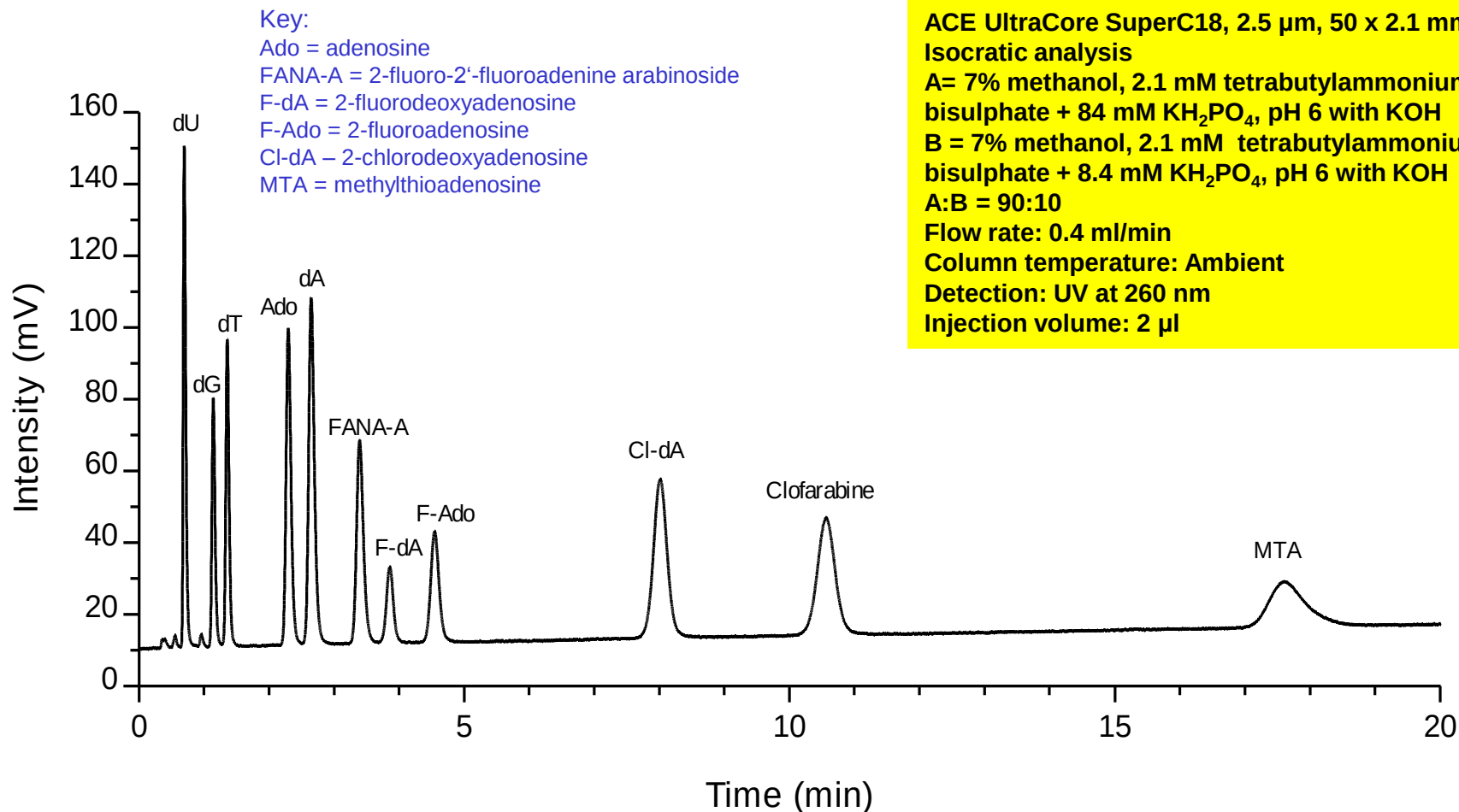
Cyd cytidine
Urd uridine
Guo guanosine
Ado adenosine





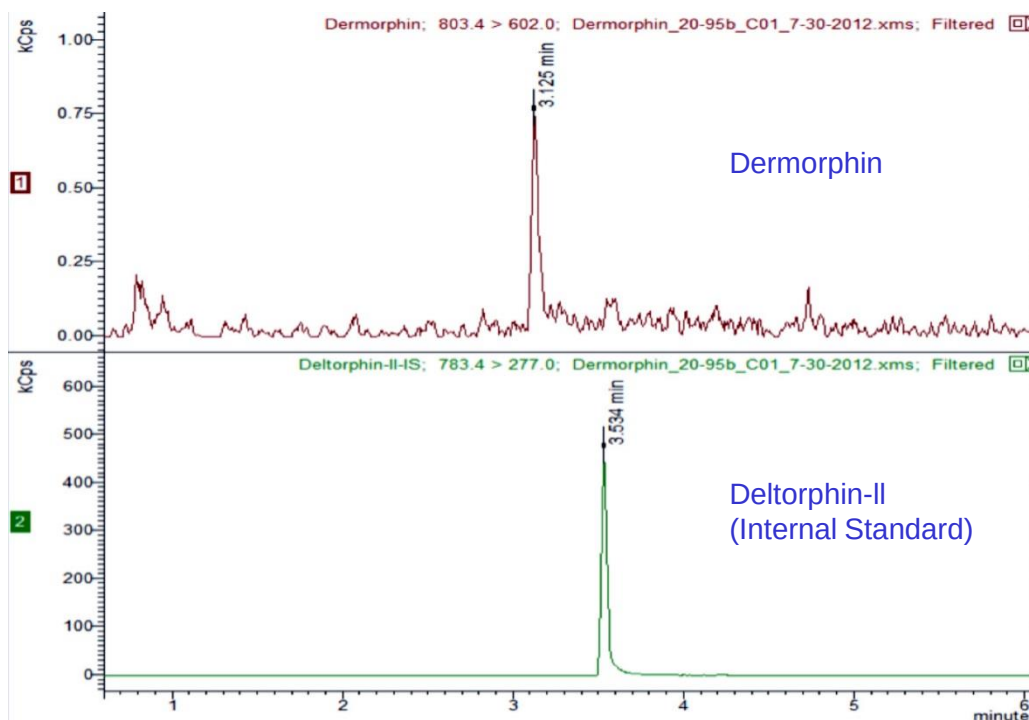
Biomarker Profiling

Deoxyribonucleosides



Dermorphin in Equine Urine by LC-MS/MS

MRM chromatogram of 0.05ng/ml dermorphin in equine urine



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

LLOQ = 0.05ng/ml

Transitions

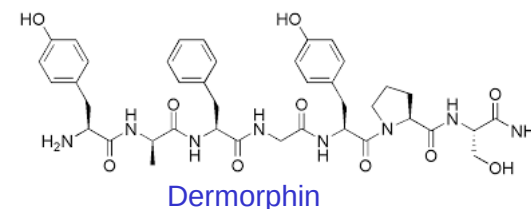
Dermorphin:

m/z 803.4 → 602 (quantifier ion)

m/z 803.4 → 202 (qualifier ion)

Deltorphin:

m/z 783 → 277



ACE 3 C18 (3μm, 100 x 2.1mm)

Gradient analysis

A = 0.2% formic acid in water

B = 0.2% formic acid in acetonitrile

T (mins)	%B	T (mins)	%B
0	5	8.5	95

0.2	5	8.51	5
-----	---	------	---

8	95	12.5	5
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Flow rate: 0.4ml/min

Injection volume: 40μl

Bruker EVOQ Elite triple quad MS

VIP heated-ESI temperature: 350°C

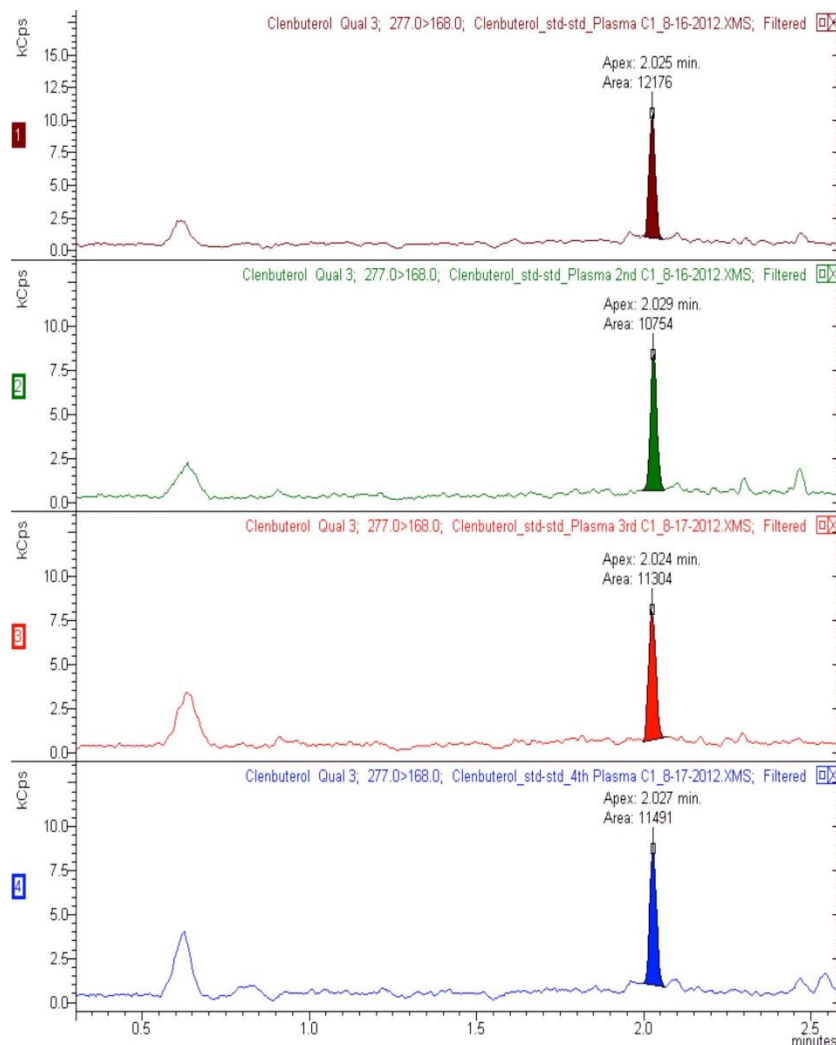
Cone gas temperature: 250°C

Spray voltage: +4000V

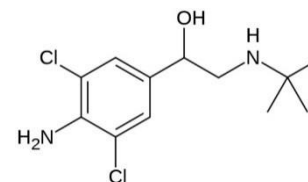


Clenbuterol in Equine Plasma by LC-MS/MS

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



Sustained high sensitivity performance under repeated exposure to horse plasma samples. Clenbuterol in crashed horse plasma injected by dilute and shoot method.



Clenbuterol

ACE 3 C18 (3 μ m, 100 x 2.1mm)

Gradient analysis

A = 0.2% formic acid in water

B = 0.2% formic acid in acetonitrile

T (mins)	%B	T (mins)	%B
0	10	2.8	10
0.3	10	4.5	10
2.5	95		

Flow rate: 0.45ml/min

Injection volume: 30 μ l

Bruker EVOQ Elite triple quad MS

VIP heated-ESI temperature: 300°C

Cone gas temperature: 300°C

Spray voltage: +3500V

Transitions:

Clenbuterol m/z 277.1 $\rightarrow$ 168

d9-Clenbuterol m/z 286.1 $\rightarrow$ 204

(Internal Standard)