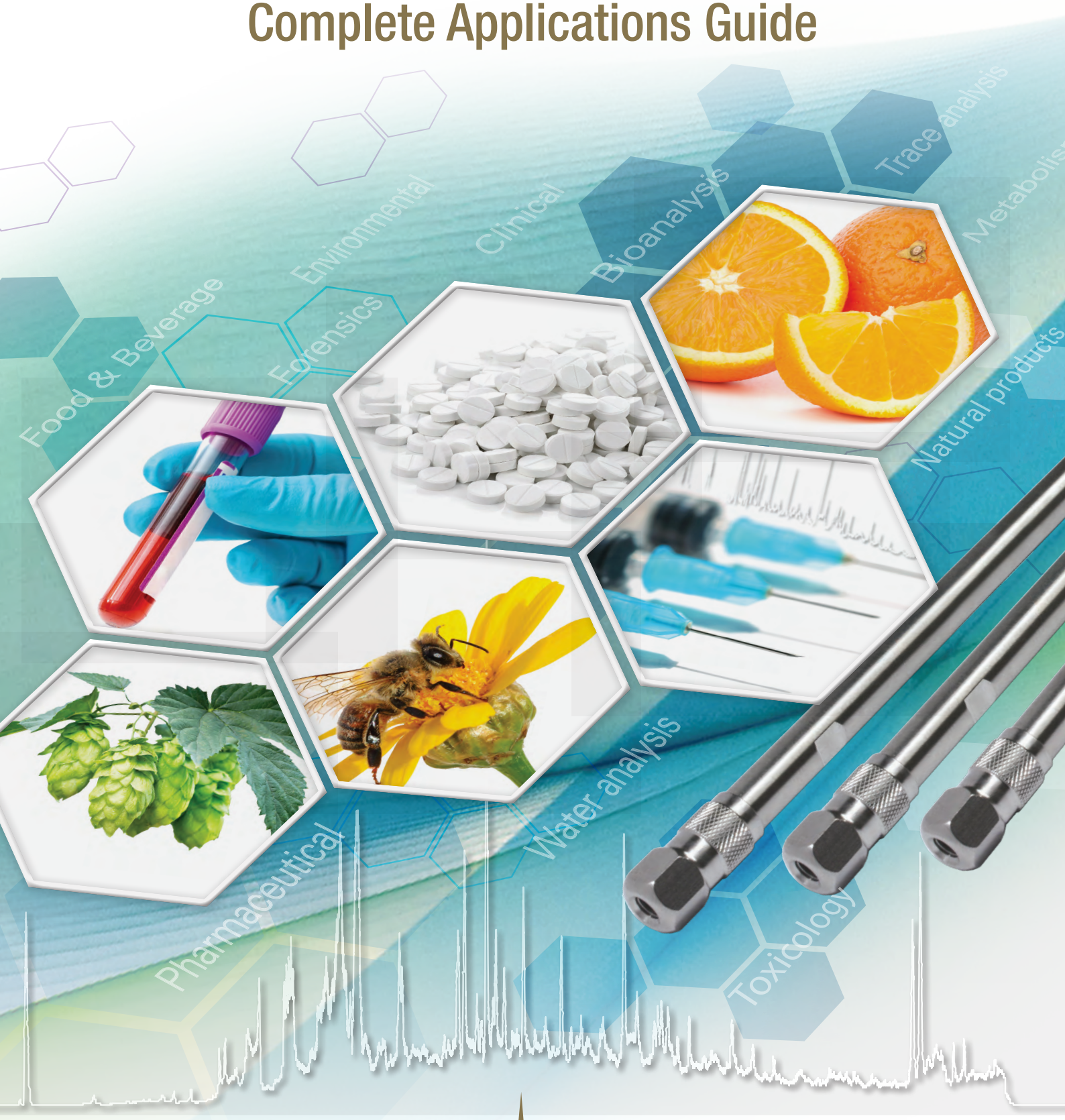
ACE®

UHPLC and HPLC Columns

Complete Applications Guide



ACE®
UHPLC and HPLC Columns

ACE Ultra-Inert, Base Deactivated HPLC and UHPLC columns give you the choices you need to achieve successful separations

Preface

This ACE UHPLC/HPLC Applications Guide contains over 300 applications including pharmaceutical, environmental, food, beverage, clinical, forensics and bioanalysis separations. The chromatograms were produced by Advanced Chromatography Technologies and by satisfied ACE customers throughout the world.

The purpose of this guide is to assist chromatographers with the selection of the best UHPLC/HPLC column and conditions for their methods, by providing good examples of successful separations.

The information in this guide is provided for reference purposes only and Advanced Chromatography Technologies assumes no risk or liabilities that may result from its use by others. Furthermore, Advanced Chromatography Technologies makes no representations or warranties that the information provided in this guide will address any particular need or purpose of any user of the Application Guide.



Send us your application and receive a FREE ACE UHPLC/HPLC column

Send us your ACE UHPLC/HPLC application and help us extend our applications database. Your proven method will enable your chromatography colleagues to benefit and if we select your application for publication we'll send you a **FREE** ACE UHPLC/HPLC column.

To submit your application contact your local ACE distributor or email us at: info@ace-hplc.com

ACE performance guarantee

If ACE does not outperform the column you are currently using, simply contact us for a full refund and keep the ACE column FREE OF CHARGE.

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Explore Selectivity

2 and 3 column kits available for the **same price** as a single column

ACE Method Development Kits

Not sure which ACE phase to select for your application?
ACE Method Development Kits offer up to 3 columns for the same price as a single column.

For additional advice on the best kit to choose see page 5 or **email: info@ace-hplc.com**



Can't find the application you need?

Contact us today at info@ace-hplc.com and our technical experts will assist you, free of charge, to find the application that meets your needs.

We are continually updating our applications database and have many more applications available.

ACE Portfolio Specifications

Choices you need to achieve successful separations

15 PHASES

C18 | C18-AR | C18-PFP | C18-Amide | CN-ES | SuperC18 | SuperPhenylHexyl | AQ | C8 | C4 | Phenyl | Amino | CN | C18-HL | Silica | *

8 PARTICLE SIZES

Six fully porous particles: 1.7 µm | 2 µm | 3 µm | 5 µm | 10 µm | 15 µm | and two superficially porous particles: 2.5 µm | 5 µm

12 STANDARD COLUMN IDs

0.075 mm | 0.10 mm | 0.30 mm | 0.50 mm | 1.0 mm | 2.1 mm | 3.0 mm | 4.0 mm | 4.6 mm | 10.0 mm |21.2 mm | 30.0 mm

3 PORE SIZES

90 Å | 100 Å | 300 Å

11 STANDARD COLUMN LENGTHS

20 mm | 30 mm | 35 mm | 50 mm | 75 mm |100 mm | 125 mm | 150 mm | 200 mm | 250 mm | 300 mm

*New phases - launching soon.

Phase	USP Listing	Functional Group	Endcapped	Particle Size (µm)	Pore Size (Å)	Surface Area (m^2/g)	Carbon Load (%)	pH Range	100% AQ Compatible
UltraCore SuperC18 (solid core)	L1	Octadecyl encapsulated	Encapsulated	2.5 5	95	95	7.0 5.4	1.5 – 11.0	-
UltraCore SuperPhenylHexyl (solid core)	L11	Phenyl Hexyl encapsulated	Encapsulated	2.5 5	95	95	4.6 3.6	1.5 – 11.0	-
C18	L1	Octadecyl	Yes	1.7, 2, 3, 5, 10	100	300	15.5	2 – 8	-
C18-AR	L1	Octadecyl with integral phenyl	Yes	1.7, 2, 3, 5, 10	100	100	15.5	2 – 8	Yes
C18-PFP	L1	Octadecyl with integral PFP	Yes	1.7, 2, 3, 5, 10	100	100	14.3	2 – 8	Yes
SuperC18	L1	Octadecyl encapsulated	Encapsulated	1.7, 2, 3, 5, 10	90	90	14.8	1.5 – 11.5	-
C18-Amide	L1 / L60	Polar embedded amide	Yes	1.7, 2, 3, 5, 10	100	100	17.0	2 – 8	Yes
CN-ES	L10	Cyano with extended alkyl spacer	Yes	1.7, 2, 3, 5, 10	100	100	12.6	2 – 8	Yes
NH_2	L8	Proprietary aminopropyl	Proprietary	1.7, 3, 5	100	100	4.0	2 – 7	Yes
C18-HL	L1	Octadecyl	Yes	3, 5, 10, 15	90	90	20	2 – 8	-
C8	L7	Octyl	Yes	2, 3, 5, 10	100	300	9.0	2 – 8	-
C4	L26	Butyl	Yes	2, 3, 5, 10	100	300	5.5	2 – 8	-
CN	L10	Cyano	Yes	2, 3, 5, 10	100	300	5.5	2 – 7	-
Ph	L11	Phenyl	Yes	2, 3, 5, 10	100	300	9.5	2 – 8	-
AQ	L1	Proprietary	Yes	2, 3, 5, 10	100	100	14	2 – 8	Yes
SIL	L3	Unbonded	No	2, 3, 5, 10	100	100	N/A	2 – 7	-
C18-300	L1	Octadecyl	Yes	3, 5, 10	300	100	9.0	2 – 8	-
C8-300	L7	Octyl	Yes	3, 5, 10	300	100	5.0	2 – 8	-
C4-300	L26	Butyl	Yes	3, 5, 10	300	100	2.6	2 – 8	-
CN-300	L10	Cyano	Yes	3, 5, 10	300	100	2.6	2 – 7	-
Ph-300	L11	Phenyl	Yes	3, 5, 10	300	100	5.3	2 – 8	-

ACE Method Development Kits

Intelligent Solutions for Method Development

- **Highly cost effective - ACE Method Development Kits are available for the same price as a single column!**
- **1.7 µm to 5 µm particle size kits available**
- **4 different ACE Method Development Kits available from microbore (0.5 mm id) through to analytical 4.6 mm id) dimensions for rapid, systematic method development.**
- **Each kit contains carefully selected ACE phases which enable the power of selectivity to be fully exploited.**
- **Each ACE phase provides different selectivity due to differing interactions.**

		Bonded Phase	Separation Mechanism and Relative Strength[1]				
			Hydrophobic Binding	π-π Interaction	Dipole-Dipole	Hydrogen Bonding	Shape Selectivity
1	**ACE Advanced Method Development Kit** (see page 6)	ACE C18	****	-	-	*	**
		ACE C18-AR	****	*** (donor)	*	**	***
		ACE C18-PFP	****	*** (acceptor)	****	***	****
2	**ACE Extended Method Development Kit** (see page 8)	ACE SuperC18	****	-	-	-	**
		ACE C18-Amide	****	-	**	****	**/***
		ACE CN-ES	***	*	***	**	*
3	**ACE UltraCore Method Development Kit** (see page 10)	ACE UltraCore SuperC18	***	-	-	-	**
		ACE UltraCore SuperPhenylHexyl	**	*** (donor)	*	**	***
4	**ACE Bioanalytical 300 Å Method Development Kit** (see page 11)	ACE C18-300	**	-	-	*	*
		ACE C4-300	*	-	-	-	-
		ACE Phenyl-300	*	** (donor)	*	**	**

[1] Approximate value – determined by semi-quantitative mechanism weightings and/or by reference to other ACE phases using >100 characterising analytes.

FREE Method Development Support!

- Not sure which ACE phase or kit will work best for your application?
- FREE Application Support and FREE Method Development Service
- Trust your method development to our experts and free up time for your other projects!
- Contact our expert method development team via **info@ace-hplc.com** or contact your local distributor

Learn More: www.ace-hplc.com



Explore Selectivity
2 and 3 column kits available for the **same price** as a single column

ACE Advanced Method Development Kit

- **Contains ACE C18, ACE C18-AR and ACE C18-PFP phases**
- **Ideal starting point for routine method development**
- **Available from microbore (0.5 mm id) through to analytical (4.6 mm id) dimensions**
- **Particularly recommended for compounds containing aromatic rings**

Phase	Functional Group	Endcapped	Particle Size (µm)	Pore Size (Å)	Surface Area (m^2/g)	Carbon Load (%)	Recommended pH Range	100% Aqueous Compatible	USP Listing
ACE C18	Octadecyl (C18)	Yes	1.7, 2, 3, 5, 10	100	300	15.5	2.0-8.0[a]	No	L1
ACE C18-AR	C18 with integral Phenyl	Yes	1.7, 2, 3, 5, 10	100	300	15.5	2.0-8.0[a]	Yes	L1
ACE C18-PFP	C18 with integral PFP	Yes	1.7, 2, 3, 5, 10	100	300	14.3	2.0-8.0[a]	Yes	L1

[a] For optimum column lifetime, a pH range of 2-8 is recommended. To increase column lifetime at higher pH, organic buffers, low buffer concentrations, high % organic solvent and low temperatures must be considered. Further information is contained within "A Guide to HPLC and LC/MS Buffer Selection" by John Dolan – please contact your distributor to request your FREE copy or visit www.ace-hplc.com

ACE C18

ACE C18 remains the "go-to" column of choice for HPLC and UHPLC separations. With an excellent reputation for performance, reproducibility and lifetime, ACE C18 provides a rugged, reproducible starting point for method development.

Recommended Applications

- Analytes differing in hydrophobicity
- Polar, moderately polar and non-polar analytes
- Uncharged acids and bases
- Ionized acids or bases using ion-pairing
- Ideal starting point for method development

ACE C18-AR

ACE C18-AR combines the excellent performance and advantages of the ACE C18 phase with the added selectivity of an integral phenyl group.

Recommended Applications

- Analytes with π-bonding and conjugated systems
- Analytes with electron delocalization and electron withdrawing groups, such as halogens, nitro groups, ketones, esters and acids
- Analytes with different dipole moments
- Analytes differing in hydrophobicity
- Stereoisomers, steroids, substituted aromatics and sulphur containing compounds
- Fully wettable - 100% aqueous buffer compatible
- Applications where C18 does not provide adequate separation
- Applications where conventional phenyl phases provide insufficient retention, poor stability, or significant bleed.

ACE C18-PFP

ACE C18-PFP brings together the stability, reproducibility and low bleed of the ACE C18 phase with the additional selectivity of an integral pentafluorophenyl (PFP) group.

Recommended Applications

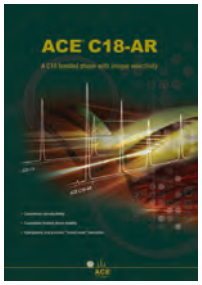
- Analytes with π-bonding
- Analytes with electron donating groups, such as phenols, aromatic ethers and amines
- Analytes with proton donor groups
- Analytes with different dipole moments
- Analytes differing in hydrophobicity
- Stuctural isomers, steroids, substituted aromatics and taxanes
- Fully wettable - 100% aqueous buffer compatible
- Applications where C18 does not provide adequate separation
- Applications where conventional PFP phases provide insufficient retention, poor stability or significant bleed.

Additional Information

Product bulletins containing further details on the ACE C18, C18-AR and C18-PFP columns contained within the Advanced ACE Method Development Kit are available to download at **www.ace-hplc.com** Alternatively, please contact our technical support team via **info@ace-hplc.com** or contact your local distributor.

Learn More: www.ace-hplc.com







ACE Advanced Method Development UHPLC/HPLC Column Kits

(Contains 3 columns: ACE C18, ACE C18-AR and ACE C18-PFP of specified dimensions)

	(UHPLC/HPLC hardware format with 1000 bar/15000 psi pressure limit)			
Column Dimensions	**1.7 µm**	**2 µm**	**3 µm**	**5 µm**
2.1 x 20 mm	MDKA-17-0202U	MDKA-2-0202U	MDKA-3-0202U	MDKA-5-0202U
2.1 x 30 mm	MDKA-17-0302U	MDKA-2-0302U	MDKA-3-0302U	MDKA-5-0302U
2.1 x 35 mm	MDKA-17-3502U	MDKA-2-3502U	MDKA-3-3502U	MDKA-5-3502U
2.1 x 50 mm	MDKA-17-0502U	MDKA-2-0502U	MDKA-3-0502U	MDKA-5-0502U
2.1 x 75 mm	MDKA-17-7502U	MDKA-2-7502U	MDKA-3-7502U	MDKA-5-7502U
2.1 x 100 mm	MDKA-17-1002U	MDKA-2-1002U	MDKA-3-1002U	MDKA-5-1002U
2.1 x 125 mm	-	MDKA-2-1202U	MDKA-3-1202U	MDKA-5-1202U
2.1 x 150 mm	-	MDKA-2-1502U	MDKA-3-1502U	MDKA-5-1502U
2.1 x 250 mm	-	-	MDKA-3-2502U	MDKA-5-2502U
3.0 x 20 mm	MDKA-17-0203U	MDKA-2-0203U	MDKA-3-0203U	MDKA-5-0203U
3.0 x 30 mm	MDKA-17-0303U	MDKA-2-0303U	MDKA-3-0303U	MDKA-5-0303U
3.0 x 35 mm	MDKA-17-3503U	MDKA-2-3503U	MDKA-3-3503U	MDKA-5-3503U
3.0 x 50 mm	MDKA-17-0503U	MDKA-2-0503U	MDKA-3-0503U	MDKA-5-0503U
3.0 x 75 mm	MDKA-17-7503U	MDKA-2-7503U	MDKA-3-7503U	MDKA-5-7503U
3.0 x 100 mm	MDKA-17-1003U	MDKA-2-1003U	MDKA-3-1003U	MDKA-5-1003U
3.0 x 125 mm	-	MDKA-2-1203U	MDKA-3-1203U	MDKA-5-1203U
3.0 x 150 mm	-	MDKA-2-1503U	MDKA-3-1503U	MDKA-5-1503U
3.0 x 250 mm	-	-	MDKA-3-2503U	MDKA-5-2503U
4.6 x 20 mm	-	MDKA-2-0246U	MDKA-3-0246U	MDKA-5-0246U
4.6 x 30 mm	-	MDKA-2-0346U	MDKA-3-0346U	MDKA-5-0346U
4.6 x 35 mm	-	MDKA-2-3546U	MDKA-3-3546U	MDKA-5-3546U
4.6 x 50 mm	-	MDKA-2-0546U	MDKA-3-0546U	MDKA-5-0546U
4.6 x 75 mm	-	MDKA-2-7546U	MDKA-3-7546U	MDKA-5-7546U
4.6 x 100 mm	-	MDKA-2-1046U	MDKA-3-1046U	MDKA-5-1046U
4.6 x 125 mm	-	MDKA-2-1246U	MDKA-3-1246U	MDKA-5-1246U
4.6 x 150 mm	-	MDKA-2-1546U	MDKA-3-1546U	MDKA-5-1546U
4.6 x 250 mm	-	-	MDKA-3-2546U	MDKA-5-2546U

ACE Advanced Method Development Microbore HPLC Column Kits

(Contains 3 columns: ACE C18, ACE C18-AR and ACE C18-PFP of specified dimensions)

	(HPLC hardware format with 400 bar/6000 psi recommended pressure limit)					
	2 µm		**3 µm**		**5 µm**	
Column Dimensions	**1/16" port**	**1/32" port**	**1/16" port**	**1/32" port**	**1/16" port**	**1/32" port**
0.5 x 30 mm	MDKA-2-03005	MDKA-2-03005S	MDKA-3-03005	MDKA-3-03005S	MDKA-5-03005	MDKA-5-03005S
0.5 x 50 mm	MDKA-2-05005	MDKA-2-05005S	MDKA-3-05005	MDKA-3-05005S	MDKA-5-05005	MDKA-5-05005S
0.5 x 75 mm	MDKA-2-75005	MDKA-2-75005S	MDKA-3-75005	MDKA-3-75005S	MDKA-5-75005	MDKA-5-75005S
0.5 x 100 mm	MDKA-2-10005	MDKA-2-10005S	MDKA-3-10005	MDKA-3-10005S	MDKA-5-10005	MDKA-5-10005S
0.5 x 125 mm	MDKA-2-12005	MDKA-2-12005S	MDKA-3-12005	MDKA-3-12005S	MDKA-5-12005	MDKA-5-12005S
0.5 x 150 mm	MDKA-2-15005	MDKA-2-15005S	MDKA-3-15005	MDKA-3-15005S	MDKA-5-15005	MDKA-5-15005S
0.5 x 250 mm	-	-	-	-	MDKA-5-25005	MDKA-5-25005S
1.0 x 30 mm	MDKA-2-0301	MDKA-2-0301S	MDKA-3-0301	MDKA-3-0301S	MDKA-5-0301	MDKA-5-0301S
1.0 x 50 mm	MDKA-2-0501	MDKA-2-0501S	MDKA-3-0501	MDKA-3-0501S	MDKA-5-0501	MDKA-5-0501S
1.0 x 75 mm	MDKA-2-7501	MDKA-2-7501S	MDKA-3-7501	MDKA-3-7501S	MDKA-5-7501	MDKA-5-7501S
1.0 x 100 mm	MDKA-2-1001	MDKA-2-1001S	MDKA-3-1001	MDKA-3-1001S	MDKA-5-1001	MDKA-5-1001S
1.0 x 125 mm	MDKA-2-1201	MDKA-2-1201S	MDKA-3-1201	MDKA-3-1201S	MDKA-5-1201	MDKA-5-1201S
1.0 x 150 mm	MDKA-2-1501	MDKA-2-1501S	MDKA-3-1501	MDKA-3-1501S	MDKA-5-1501	MDKA-5-1501S
1.0 x 250 mm	-	-	-	-	MDKA-5-2501	MDKA-5-2501S

Important Note: ACE microbore columns (1.0 mm id and 0.5 mm id) are available with either standard 1/16" (10-32 thread) connections or 1/32" (6-40 thread) connections. For use with Eksigent micro and nano LC systems, order columns with 1/32" connections and use either ACE 6-40 fittings (part number ACE-MC3210, 10 pack) or Eksigent 6-40 fittings (part number 5019621).

For 1/16" HPLC column connections up to 6000 psi, PEEK™ 1/16" fingertight fittings (part number ACE-CC10, 10 pack) are recommended. For 1/32" microbore HPLC column connections up to 6000 psi, PEEK™ 1/32" (6-40 thread) fingertight fittings (part number ACE-MC3210, 10 pack) are recommended. For 1/16" UHPLC column connections up to 25000 psi, reuseable 1/16" fittings (part number EXL-CC10, 10 pack) are recommended. To further extend UHPLC and HPLC column lifetimes, ACE pre-column filters are recommended. For further details please contact your distributor or visit www.ace-hplc.com

Explore Selectivity
2 and 3 column kits available for the **same price** as a single column

ACE Extended Method Development Kit

- **Contains ACE SuperC18, ACE C18-Amide and ACE CN-ES phases**
- **Use ACE SuperC18 to exploit selectivity changes at low, intermediate and high pH**
- **Available from microbore (0.5 mm id) through to analytical (4.6 mm id) dimensions**
- **ACE C18-Amide and ACE CN-ES phases both offer alternative selectivity, especially for polar molecules**

Phase	Functional wGroup	Endcapped	Particle Size (µm)	Pore Size (Å)	Surface Area (m^2/g)	Carbon Load (%)	Recommended pH Range	100% Aqueous Compatible	USP Listing
ACE SuperC18	Octadecyl (C18)	Encapsulated bonding	1.7, 2, 3, 5, 10	90	400	14.8	1.5-11.5[a]	No	L1
ACE C18-Amide	C18 with integral amide polar group	Yes	1.7, 2, 3, 5, 10	100	300	16.4	2.0-8.0[b]	Yes	L1/L60
ACE CN-ES	CN with proprietary extended alkyl spacer	Yes	1.7, 2, 3, 5, 10	100	300	12.6	2.0-8.0[b]	Yes	L10

[a] ACE SuperC18 is designed for use with LC/MS compatible buffers. Further information is contained within "ACE SuperC18 - A Guide to Buffer Selection" – please contact your distributor to request your FREE copy or visit www.ace-hplc.com.

[b] For optimum column lifetime, a pH range of 2-8 is recommended. To increase column lifetime at higher pH, organic buffers, low buffer concentrations, high % organic solvent and low temperatures must be considered. Further information is contained within "A Guide to HPLC and LC/MS Buffer Selection" by John Dolan – please contact your distributor to request your FREE copy or visit www.ace-hplc.com

ACE SuperC18

ACE SuperC18 is a uniquely bonded, EBT™* endcapped C18 phase which offers unprecedented inertness, excellent efficiency and uncompromising durability over an extended pH range of 1.5 – 11.5.

Recommended Applications

- Analytes differing in hydrophobicity
- Polar, moderately polar and non-polar analytes
- Uncharged acids and bases
- Ionized acids or bases using ion-pairing
- Recommended starting point for developing methods at intermediate and high pH to exploit selectivity changes

ACE C18-Amide

ACE C18-Amide is a uniquely designed polar-embedded phase that offers enhanced retention and resolution of polar acidic, phenolic and hydroxy-substituted analytes. The extended spacer ligand technology provides extended column lifetime.

Recommended Applications

- Small water soluble analytes and polar molecules - especially acidic species
- Analytes with H bond donors, acids, bases and phenolic compounds
- Small peptides
- Analytes differing in hydrophobicity
- Fully wettable - 100% aqueous buffer compatible
- Applications where C18 does not provide adequate separation
- Applications where conventional amide/ polar embedded phases provide insufficient retention, poor stability, or significant bleed

ACE CN-ES

ACE CN-ES is a unique phase having an extended alkyl chain with a terminal cyano group. It provides C18 levels of retention and stability compared to commercial cyano propyl phases which typically exhibit low retentivity and poor stability.

Recommended Applications

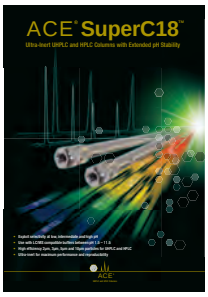
- Mixtures of very polar, polar and non-polar analytes
- Analytes with double and triple bonds
- Analytes differing in hydrophobicity
- Suitable for NP and RP separations
- Fully wettable - 100% aqueous buffer compatible
- Applications where a typical C18 column does not provide adequate separation
- Applications where traditional CN bonded phases provide insufficient retention, poor stability or significant bleed
- An orthogonal phase for method development

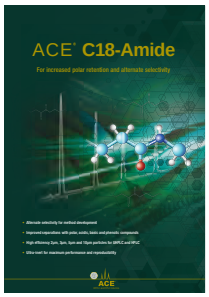
*Encapsulated Bonding Technology

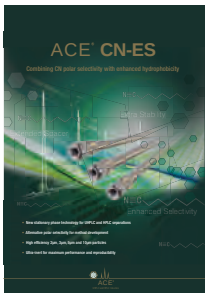
Additional information

Product bulletins containing further details on the ACE SuperC18, C18-Amide and CN-ES columns contained within the Extended ACE Method Development Kit are available to download at **www.ace-hplc.com** Alternatively, please contact our technical support team via **info@ace-hplc.com** or contact your local distributor.

Learn More: www.ace-hplc.com







ACE Extended Method Development UHPLC/HPLC Column Kits

(Contains 3 columns: ACE SuperC18, ACE C18-Amide and ACE CN-ES of specified dimensions)

	(UHPLC/HPLC hardware format with 1000 bar/15000 psi pressure limit)			
Column Dimensions	**1.7 µm**	**2 µm**	**3 µm**	**5 µm**
2.1 x 20 mm	MDKE-17-0202U	MDKE-2-0202U	MDKE-3-0202U	MDKE-5-0202U
2.1 x 30 mm	MDKE-17-0302U	MDKE-2-0302U	MDKE-3-0302U	MDKE-5-0302U
2.1 x 35 mm	MDKE-17-3502U	MDKE-2-3502U	MDKE-3-3502U	MDKE-5-3502U
2.1 x 50 mm	MDKE-17-0502U	MDKE-2-0502U	MDKE-3-0502U	MDKE-5-0502U
2.1 x 75 mm	MDKE-17-7502U	MDKE-2-7502U	MDKE-3-7502U	MDKE-5-7502U
2.1 x 100 mm	MDKE-17-1002U	MDKE-2-1002U	MDKE-3-1002U	MDKE-5-1002U
2.1 x 125 mm	-	MDKE-2-1202U	MDKE-3-1202U	MDKE-5-1202U
2.1 x 150 mm	-	MDKE-2-1502U	MDKE-3-1502U	MDKE-5-1502U
2.1 x 250 mm	-	-	MDKE-3-2502U	MDKE-5-2502U
3.0 x 20 mm	MDKE-17-0203U	MDKE-2-0203U	MDKE-3-0203U	MDKE-5-0203U
3.0 x 30 mm	MDKE-17-0303U	MDKE-2-0303U	MDKE-3-0303U	MDKE-5-0303U
3.0 x 35 mm	MDKE-17-3503U	MDKE-2-3503U	MDKE-3-3503U	MDKE-5-3503U
3.0 x 50 mm	MDKE-17-0503U	MDKE-2-0503U	MDKE-3-0503U	MDKE-5-0503U
3.0 x 75 mm	MDKE-17-7503U	MDKE-2-7503U	MDKE-3-7503U	MDKE-5-7503U
3.0 x 100 mm	MDKE-17-1003U	MDKE-2-1003U	MDKE-3-1003U	MDKE-5-1003U
3.0 x 125 mm	-	MDKE-2-1203U	MDKE-3-1203U	MDKE-5-1203U
3.0 x 150 mm	-	MDKE-2-1503U	MDKE-3-1503U	MDKE-5-1503U
3.0 x 250 mm	-	-	MDKE-3-2503U	MDKE-5-2503U
4.6 x 20 mm	-	MDKE-2-0246U	MDKE-3-0246U	MDKE-5-0246U
4.6 x 30 mm	-	MDKE-2-0346U	MDKE-3-0346U	MDKE-5-0346U
4.6 x 3 mm	-	MDKE-2-3546U	MDKE-3-3546U	MDKE-5-3546U
4.6 x 50 mm	-	MDKE-2-0546U	MDKE-3-0546U	MDKE-5-0546U
4.6 x 75 mm	-	MDKE-2-7546U	MDKE-3-7546U	MDKE-5-7546U
4.6 x 100 mm	-	MDKE-2-1046U	MDKE-3-1046U	MDKE-5-1046U
4.6 x 125 mm	-	MDKE-2-1246U	MDKE-3-1246U	MDKE-5-1246U
4.6 x 150 mm	-	MDKE-2-1546U	MDKE-3-1546U	MDKE-5-1546U
4.6 x 250 mm	-	-	MDKE-3-2546U	MDKE-5-2546U

ACE Extended Method Development Microbore HPLC Column Kits

(Contains 3 columns: ACE SuperC18, ACE C18-Amide and ACE CN-ES of specified dimensions)

	(HPLC hardware format with 400 bar/6000 psi recommended pressure limit)					
	2 µm		**3 µm**		**5 µm**	
Column Dimensions	**1/16" port**	**1/32" port**	**1/16" port**	**1/32" port**	**1/16" port**	**1/32" port**
0.5 x 30 mm	MDKE-2-03005	MDKE-2-03005S	MDKE-3-03005	MDKE-3-03005S	MDKE-5-03005	MDKE-5-03005S
0.5 x 50 mm	MDKE-2-05005	MDKE-2-05005S	MDKE-3-05005	MDKE-3-05005S	MDKE-5-05005	MDKE-5-05005S
0.5 x 75 mm	MDKE-2-75005	MDKE-2-75005S	MDKE-3-75005	MDKE-3-75005S	MDKE-5-75005	MDKE-5-75005S
0.5 x 100 mm	MDKE-2-10005	MDKE-2-10005S	MDKE-3-10005	MDKE-3-10005S	MDKE-5-10005	MDKE-5-10005S
0.5 x 125 mm	MDKE-2-12005	MDKE-2-12005S	MDKE-3-12005	MDKE-3-12005S	MDKE-5-12005	MDKE-5-12005S
0.5 x 150 mm	MDKE-2-15005	MDKE-2-15005S	MDKE-3-15005	MDKE-3-15005S	MDKE-5-15005	MDKE-5-15005S
0.5 x 250 mm	-	-	-	-	MDKE-5-25005	MDKE-5-25005S
1.0 x 30 mm	MDKE-2-0301	MDKE-2-0301S	MDKE-3-0301	MDKE-3-0301S	MDKE-5-0301	MDKE-5-0301S
1.0 x 50 mm	MDKE-2-0501	MDKE-2-0501S	MDKE-3-0501	MDKE-3-0501S	MDKE-5-0501	MDKE-5-0501S
1.0 x 75 mm	MDKE-2-7501	MDKE-2-7501S	MDKE-3-7501	MDKE-3-7501S	MDKE-5-7501	MDKE-5-7501S
1.0 x 100 mm	MDKE-2-1001	MDKE-2-1001S	MDKE-3-1001	MDKE-3-1001S	MDKE-5-1001	MDKE-5-1001S
1.0 x 125 mm	MDKE-2-1201	MDKE-2-1201S	MDKE-3-1201	MDKE-3-1201S	MDKE-5-1201	MDKE-5-1201S
1.0 x 150 mm	MDKE-2-1501	MDKE-2-1501S	MDKE-3-1501	MDKE-3-1501S	MDKE-5-1501	MDKE-5-1501S
1.0 x 250 mm	-	-	-	-	MDKE-5-2501	MDKE-5-2501S

IMPORTANT NOTE: ACE microbore columns (1.0 mm id and 0.5 mm id) are available with either standard 1/16" (10-32 thread) connections or 1/32" (6-40 thread) connections. For use with Eksigent micro and nano LC systems, order columns with 1/32" connections and use either ACE 6-40 fittings (part number ACE-MC3210, 10 pack) or Eksigent 6-40 fittings (part number 5019621).

For 1/16" HPLC column connections up to 6000 psi, PEEK™ 1/16" fingertight fittings (part number ACE-CC10, 10 pack) are recommended. For 1/32" microbore HPLC column connections up to 6000 psi, PEEK™ 1/32" (6-40 thread) fingertight fittings (part number ACE-MC3210, 10 pack) are recommended. For 1/16" UHPLC column connections up to 25000psi, reuseable 1/16" fittings (part number EXL-CC10, 10 pack) are recommended. To further extend UHPLC and HPLC column lifetimes, ACE pre-column filters are recommended. For further details please contact your distributor or visit www.ace-hplc.com



ACE UltraCore Method Development Kit

- **Contains ACE UltraCore SuperC18 and SuperPhenylHexyl phases**
- **Use to exploit selectivity changes at low, intermediate and high pH**
- **Available from microbore (0.5 mm id) through to analytical (4.6 mm id) dimensions**
- **Ultra inert core-shell particles and Encapsulated Bonding Technology (EBT™) provide excellent peak shape**

Phase	Functional Group	Particle Size (µm)	Pore Size (Å)	Surface Area (m^2/g)	Carbon Load (%)	Maximum pH Range	USP Listing
ACE UltraCore 2.5 SuperC18	Octadecyl encapsulated	2.5	95	130	7.0	1.5-11.0[a]	L1
ACE UltraCore 2.5 SuperPhenylHexyl	Phenyl-Hexyl encapsulated	2.5	95	130	4.6	1.5-11.0[a]	L11
ACE UltraCore 5 SuperC18	Octadecyl encapsulated	5	95	100	5.4	1.5-11.0[a]	L1
ACE UltraCore 5 SuperPhenylHexyl	Phenyl-Hexyl encapsulated	5	95	100	3.6	1.5-11.0[a]	L11

[a] ACE UltraCore columns are designed for use with LC/MS compatible buffers. Further information is contained within "ACE UltraCore – A Guide to Buffer Selection" - please contact your distributor to request your FREE copy or visit www.ace-hplc.com.

ACE UltraCore Method Development UHPLC/HPLC Column Kits

(Contains 2 columns: ACE UltraCore SuperC18 and ACE UltraCore SuperPhenylHexyl of specified dimensions)

(UHPLC/HPLC hardware format with 1000 bar/15000 psi pressure limit)		
Column Dimensions	**2.5 µm**	**5 µm**
2.1 x 20 mm	MDKU-25-0202U	MDKU-5-0202U
2.1 x 30 mm	MDKU-25-0302U	MDKU-5-0302U
2.1 x 35 mm	MDKU-25-3502U	MDKU-5-3502U
2.1 x 50 mm	MDKU-25-0502U	MDKU-5-0502U
2.1 x 75 mm	MDKU-25-7502U	MDKU-5-7502U
2.1 x 100 mm	MDKU-25-1002U	MDKU-5-1002U
2.1 x 125 mm	MDKU-25-1202U	MDKU-5-1202U
2.1 x 150 mm	MDKU-25-1502U	MDKU-5-1502U
2.1 x 250 mm	-	MDKU-5-2502U
3.0 x 20 mm	MDKU-25-0203U	MDKU-5-0203U
3.0 x 30 mm	MDKU-25-0303U	MDKU-5-0303U
3.0 x 35 mm	MDKU-25-3503U	MDKU-5-3503U
3.0 x 50 mm	MDKU-25-0503U	MDKU-5-0503U
3.0 x 75 mm	MDKU-25-7503U	MDKU-5-7503U

(UHPLC/HPLC hardware format with 1000 bar/15000 psi pressure limit)		
Column Dimensions	**2.5 µm**	**5 µm**
3.0 x 100 mm	MDKU-25-1003U	MDKU-5-1003U
3.0 x 125 mm	MDKU-25-1203U	MDKU-5-1203U
3.0 x 150 mm	MDKU-25-1503U	MDKU-5-1503U
3.0 x 250 mm	-	MDKU-5-2503U
4.6 x 20 mm	MDKU-25-0246U	MDKU-5-0246U
4.6 x 30 mm	MDKU-25-0346U	MDKU-5-0346U
4.6 x 35 mm	MDKU-25-3546U	MDKU-5-3546U
4.6 x 50 mm	MDKU-25-0546U	MDKU-5-0546U
4.6 x 75 mm	MDKU-25-7546U	MDKU-5-7546U
4.6 x 100 mm	MDKU-25-1046U	MDKU-5-1046U
4.6 x 125 mm	MDKU-25-1246U	MDKU-5-1246U
4.6 x 150 mm	MDKU-25-1546U	MDKU-5-1546U
4.6 x 250 mm	-	MDKU-5-2546U

ACE UltraCore Method Development Microbore HPLC Column Kits

(Contains 2 columns: ACE UltraCore SuperC18 and ACE UltraCore SuperPhenylHexyl of specified dimensions)

(HPLC hardware format with 400 bar/6000 psi recommended pressure limit)				
	2.5 µm		**5 µm**	
Column Dimensions	**1/16" port**	**1/32" port**	**1/16" port**	**1/32" port**
0.5 x 30 mm	MDKU-25-03005	MDKU-25-03005S	MDKU-5-03005	MDKU-5-03005S
0.5 x 50 mm	MDKU-25-05005	MDKU-25-05005S	MDKU-5-05005	MDKU-5-05005S
0.5 x 75 mm	MDKU-25-75005	MDKU-25-75005S	MDKU-5-75005	MDKU-5-75005S
0.5 x 100 mm	MDKU-25-10005	MDKU-25-10005S	MDKU-5-10005	MDKU-5-10005S
0.5 x 125 mm	MDKU-25-12005	MDKU-25-12005S	MDKU-5-12005	MDKU-5-12005S
0.5 x 150 mm	MDKU-25-15005	MDKU-25-15005S	MDKU-5-15005	MDKU-5-15005S
0.5 x 250 mm	-	-	MDKU-5-25005	MDKU-5-25005S
1.0 x 30 mm	MDKU-25-0301	MDKU-25-0301S	MDKU-5-0301	MDKU-5-0301S
1.0 x 50 mm	MDKU-25-0501	MDKU-25-0501S	MDKU-5-0501	MDKU-5-0501S
1.0 x 75 mm	MDKU-25-7501	MDKU-25-7501S	MDKU-5-7501	MDKU-5-7501S
1.0 x 100 mm	MDKU-25-1001	MDKU-25-1001S	MDKU-5-1001	MDKU-5-1001S
1.0 x 125 mm	MDKU-25-1201	MDKU-25-1201S	MDKU-5-1201	MDKU-5-1201S
1.0 x 150 mm	MDKU-25-1501	MDKU-25-1501S	MDKU-5-1501	MDKU-5-1501S
1.0 x 250 mm	-	-	MDKU-5-2501	MDKU-5-2501S

ACE Bioanalytical 300 Å Method Development Kit

Explore Selectivity
2 and 3 column kits available for the **same price** as a single column

- **Contains ACE C18-300, ACE C4-300 and ACE Phenyl-300 phases**
- **Ideal starting point for protein and peptide method development**
- **Available from microbore (0.5 mm id) through to analytical (4.6 mm id) dimensions**
- **Ultra-inert 300 Å phases provide excellent peak shape and reproducibility**

Phase	Functional Group	Particle Size (µm)	Pore Size (Å)	Surface Area (m^2/g)	Carbon Load (%)	Recommended pH Range	USP Listing
ACE C18-300	Octadecyl (C18)	3, 5, 10	300	100	9.0	2.0-8.0	L1
ACE C4-300	Butyl (C4)	3, 5, 10	300	100	2.6	2.0-8.0	L26
ACE Phenyl-300	Phenyl	3, 5, 10	300	100	5.3	2.0-8.0	L11

ACE Bioanalytical 300 Å Method Development HPLC Column Kits

(Contains 3 columns: ACE C18-300, ACE C4-300 and ACE Phenyl-300 of specified dimensions)

(HPLC hardware format with 275 bar/4000 psi pressure limit)		
Column Dimensions	**3 µm**	**5 µm**
2.1 x 20 mm	MDKB-3-0202	MDKB-5-0202
2.1 x 30 mm	MDKB-3-0302	MDKB-5-0302
2.1 x 35 mm	MDKB-3-3502	MDKB-5-3502
2.1 x 50 mm	MDKB-3-0502	MDKB-5-0502
2.1 x 75 mm	MDKB-3-7502	MDKB-5-7502
2.1 x 100 mm	MDKB-3-1002	MDKB-5-1002
2.1 x 125 mm	MDKB-3-1202	MDKB-5-1202
2.1 x 150 mm	MDKB-3-1502	MDKB-5-1502
2.1 x 250 mm	-	MDKB-5-2502
3.0 x 20 mm	MDKB-3-0203	MDKB-5-0203
3.0 x 30 mm	MDKB-3-0303	MDKB-5-0303
3.0 x 35 mm	MDKB-3-3503	MDKB-5-3503
3.0 x 50 mm	MDKB-3-0503	MDKB-5-0503
3.0 x 75 mm	MDKB-3-7503	MDKB-5-7503

(HPLC hardware format with 275 bar/4000 psi pressure limit)		
Column Dimensions	**3 µm**	**5 µm**
3.0 x 100 mm	MDKB-3-1003	MDKB-5-1003
3.0 x 125 mm	MDKB-3-1203	MDKB-5-1203
3.0 x 150 mm	MDKB-3-1503	MDKB-5-1503
3.0 x 250 mm	-	MDKB-5-2503
4.6 x 20 mm	MDKB-3-0246	MDKB-5-0246
4.6 x 30 mm	MDKB-3-0346	MDKB-5-0346
4.6 x 35 mm	MDKB-3-3546	MDKB-5-3546
4.6 x 50 mm	MDKB-3-0546	MDKB-5-0546
4.6 x 75 mm	MDKB-3-7546	MDKB-5-7546
4.6 x 100 mm	MDKB-3-1046	MDKB-5-1046
4.6 x 125 mm	MDKB-3-1246	MDKB-5-1246
4.6 x 150 mm	MDKB-3-1546	MDKB-5-1546
4.6 x 250 mm	-	MDKB-5-2546

Note: 4.0 mm id ACE Bioanalytical 300 Å Method Development Kits also available – please enquire

ACE Bioanalytical 300 Å Method Development Microbore HPLC Column Kits

(Contains 3 columns: ACE C18-300, ACE C4-300 and ACE Phenyl-300 of specified dimensions)

(HPLC hardware format with 275 bar/4000 psi recommended pressure limit)				
	3 µm		**5 µm**	
Column Dimensions	**1/16" port**	**1/32" port**	**1/16" port**	**1/32" port**
0.5 x 30 mm	MDKB-3-03005	MDKB-3-03005S	MDKB-5-03005	MDKB-5-03005S
0.5 x 50 mm	MDKB-3-05005	MDKB-3-05005S	MDKB-5-05005	MDKB-5-05005S
0.5 x 75 mm	MDKB-3-75005	MDKB-3-75005S	MDKB-5-75005	MDKB-5-75005S
0.5 x 100 mm	MDKB-3-10005	MDKB-3-10005S	MDKB-5-10005	MDKB-5-10005S
0.5 x 125 mm	MDKB-3-12005	MDKB-3-12005S	MDKB-5-12005	MDKB-5-12005S
0.5 x 150 mm	MDKB-3-15005	MDKB-3-15005S	MDKB-5-15005	MDKB-5-15005S
0.5 x 250 mm	-	-	MDKB-5-25005	MDKB-5-25005S
1.0 x 30 mm	MDKB-3-0301	MDKB-3-0301S	MDKB-5-0301	MDKB-5-0301S
1.0 x 50 mm	MDKB-3-0501	MDKB-3-0501S	MDKB-5-0501	MDKB-5-0501S
1.0 x 75 mm	MDKB-3-7501	MDKB-3-7501S	MDKB-5-7501	MDKB-5-7501S
1.0 x 100 mm	MDKB-3-1001	MDKB-3-1001S	MDKB-5-1001	MDKB-5-1001S
1.0 x 125 mm	MDKB-3-1201	MDKB-3-1201S	MDKB-5-1201	MDKB-5-1201S
1.0 x 150 mm	MDKB-3-1501	MDKB-3-1501S	MDKB-5-1501	MDKB-5-1501S
1.0 x 250 mm	-	-	MDKB-5-2501	MDKB-5-2501S

IMPORTANT NOTE: ACE microbore columns (1.0 mm id and 0.5 mm id) are available with either standard 1/16" (10-32 thread) connections or 1/32" (6-40 thread) connections. For use with Eksigent micro and nano LC systems, order columns with 1/32" connections and use either ACE 6-40 fittings (part number ACE-MC3210, 10 pack) or Eksigent 6-40 fittings (part number 5019621).

For 1/16" HPLC column connections up to 6000 psi, PEEK™ 1/16" fingertight fittings (part number ACE-CC10, 10 pack) are recommended. For 1/32" microbore HPLC column connections up to 6000 psi, PEEK™ 1/32" (6-40 thread) fingertight fittings (part number ACE-MC3210, 10 pack) are recommended. For 1/16" UHPLC column connections up to 25000psi, reuseable 1/16" fittings (part number EXL-CC10, 10 pack) are recommended. To further extend UHPLC and HPLC column lifetimes, ACE pre-column filters are recommended. For further details please contact your distributor or visit www.ace-hplc.com



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

email: info@ace-hplc.com



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Garlic Analysis (I)	77			✓			
Garlic Analysis (II)	77			✓			
Ginkgo Biloba – Ultra Resolution	78			✓	✓		
Ginseng Extract	79			✓			
Ginsenosides from Chinese Medicine by UHPLC-MS/MS	78			✓	✓	✓	
Gliotoxin from *Aspergillus Fumigatus* Liquid Culture	80	✓		✓			
Glyphosate and Related Compounds as FMOC Derivatives (Gradient)	80		✓				
Glyphosate and Related Compounds as FMOC Derivatives (Isocratic)	80		✓				
Green Tea Extract	80			✓			
Green Tea Metabolite Profiling by LC-MS	81			✓		✓	
Hair Dye Restricted Components (I)	82						✓
Hair Dye Restricted Components (II)	82						✓
Halogenated Positional Isomer Separations	82						✓
Hepcidin-25 and Truncated Isoforms by LC-HRMS	83	✓				✓	
Herbicide – Benfluralin	83		✓	✓			
Herbicide Impurity Profile	84		✓	✓			

Application Index

	Page Number	Clinical, Forensics & Bioanalysis	Environmental	Food & Beverage	Pharmaceutical	LC-MS	Other
Herbicide – Trifluralin	83		✓	✓			
Hippuric Acid	84	✓		✓			
Human Urine Metabolite Profiling by LC-MS	85	✓				✓	
Combined Hypertension Therapy Drugs	86				✓		
Hydroxychloroquine in Whole (EDTA) Blood by LC-MS/MS	86	✓			✓	✓	
Ibuprofen and Related Impurities	87	✓			✓		
Ibuprofen in Combination with Antihistamine and Decongestant	87	✓			✓		
Illegal Dyes in Spices	88			✓			
Insulin Analogues in Clinical and Post-Mortem Analyses	88	✓				✓	
Insulins	89	✓		✓			
Isoflavones	89			✓			
Isoflavones in Red Clover and Soy Extract	89			✓			
Itraconazole and Hydroxyitraconazole in Human Whole Blood by LC-MS/MS	90	✓			✓	✓	
Lansoprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl	91				✓		
Lapatinib Anticancer Drug in Human Plasma by LC-MS/MS	91	✓			✓	✓	
Lidocaine in Saliva by LC-MS/MS	92	✓			✓	✓	
Lincosamide Antibiotics	92	✓			✓		
Lipid Classes Separation from *Drosophila Melanogaster*	93	✓				✓	
Liquorice Extracts Fingerprint	93			✓			
Local Anaesthetics	94				✓		
15-Hydroxy Lubiprostone in Human Plasma	94	✓			✓	✓	
Lubricant Additives: ADPA/OPNA Antioxidants	95		✓				
Lurbinectedin in Plasma by LC-MS/MS	95	✓			✓	✓	
Malachite Green	96			✓			
Maleic and Fumaric Acids	96						✓
MDMA (Ecstasy) and PMA (Dr Death) Separation	96	✓					
Melamine using Ion-Pairing Reagent	96			✓			
Metabolomic Analysis of Extracted Jurkat T Cells by LC-HRMS	97	✓				✓	
Metabolomic Biomarkers in Ethylmalonic Encephalopathy	97	✓				✓	
Metabolomics and Biochemical Genetics - Acylglycines	98	✓				✓	
Metabolomics – C4 & C5 Hydroxy and Dicarboxylic Acids	98	✓				✓	
Metabolomics – C4 Hydroxy Acids	99	✓				✓	
Metabolomics – C6 & C7 Hydroxy and Dicarboxylic Acids	99	✓				✓	
Methotrexate in K_3EDTA Human Plasma by LC-MS/MS	100	✓			✓	✓	
17α-Methyltestosterone in Freshwater Tilapia Aquaculture	100	✓					
mGluR5 PET Tracer by Radio HPLC Analysis	101	✓					
Microbial Extract by LC-MS	101	✓				✓	
Microcystins from Blue/Green Algae in Drinking Water	102	✓	✓	✓		✓	
Milk Proteins	102	✓		✓			
Mycotoxins/Aflatoxins from Peppers	103			✓			
Mycotoxins by LC-MS/MS	103			✓		✓	
Naphthalenes (Substituted)	104						✓
Neonicotinoids in Honey by LC-MS/MS	104			✓		✓	

Application Index

	Page Number	Clinical, Forensics & Bioanalysis	Environmental	Food & Beverage	Pharmaceutical	LC-MS	Other
Neurotransmitters and Metabolites from Rat Brain by LC-MS/MS	105	✓				✓	
Nitroanilines (I)	106				✓		
Nitroanilines (II)	106				✓		
Nitrofuran Metabolites by LC-MS/MS	106			✓	✓	✓	
Nitrosamines European Toy Standard Method by LC-MS/MS	107		✓			✓	
Non-Steroidal Anti-Inflammatory Drugs by LC-MS/MS	108	✓			✓	✓	
Non-Steroidal Anti-Inflammatory Drugs – Fast Analysis	108	✓			✓		
Non-Steroidal Anti-Inflammatory Drugs (I)	107	✓			✓		
Non-Steroidal Anti-Inflammatory Drugs (II)	107	✓			✓		
Non-Steroidal Anti-Inflammatory Drugs (III)	108	✓			✓		
Nucleic Acids / Disease Biomarker Profiling (I)	109	✓					
Nucleic Acids / Disease Biomarker Profiling (II)	109	✓					
Nucleosides and Vitamins	109			✓			
Ochratoxin A	110			✓			
Olanzapine in Human Plasma by LC-MS/MS	110	✓			✓	✓	
Omeprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl	110				✓		
Opiates from Drugs of Abuse Screen (#AN2190)	111	✓			✓	✓	
Opiates in Urine by LC-MS/MS	111	✓			✓	✓	
Organic Acids	112			✓			
Organic Acids – Fast Separation	112			✓			
Organophosphorus Flame Retardants in Water by LC-MS/MS	113		✓	✓		✓	
Organophosphorus (Isomeric) Flame Retardants in Water	113		✓	✓		✓	
Organotin Compounds	114		✓			✓	
OTC Gastric Drugs	114				✓		
Oxymetazoline in Nasal Spray Formulation	115				✓		
Oxysterols by LC-MS/MS	114	✓				✓	
Paclitaxel	115				✓		
Paeonia Lactiflora Extract HPLC Fingerprint	115	✓					
Paraben Preservatives	116			✓	✓		
Paracetamol and Related Compounds	116				✓		
Paracetamol and Related Substances – Enhanced Resolution	117				✓		
Paracetamol and Related Substances – Fast Analysis (I)	116				✓		
Paracetamol and Related Substances – Phase Selectivity	117				✓		
Paralytic Shellfish Poisoning (PSP) Toxins	118	✓	✓	✓			
Parotoid Macrogland Secretions from South American Toads	118	✓					
Paroxetine and Desfluoro Analogue	119				✓		
Peptides – Selectivity Changes with Bonded Phase and Mobile Phase	120	✓					
Peptides – Varying pH	119	✓					
Peptide Test Mix	119	✓					
Perfluorinated Compounds in Water by LC-MS/MS	122		✓	✓		✓	
Perfluoro Acids by LC-MS/MS	121		✓	✓		✓	
Perfluoroalkyl Substances by Ion-Pairing LC-MS/MS	121		✓	✓		✓	
250 Pesticide Screen by LC-MS/MS	123		✓	✓		✓	

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	Page Number	Clinical, Forensics & Bioanalysis	Environmental	Food & Beverage	Pharmaceutical	LC-MS	Other
300 Pesticide Screen by LC-MS/MS	127		✓	✓		✓	
Pesticides by LC-MS/MS	132		✓	✓		✓	
Pesticides in Water	132		✓	✓			
Pharmaceutically Relevant Compounds (II)	133				✓		
Pharmaceutically Relevant Compounds (III)	133				✓		
Pharmaceutically Relevant Compounds (IV)	133				✓		
Pharmaceutically Relevant Compounds (V)	134				✓		
Pharmaceutically Relevant Mixture (I) – Different Selectivity Using pH	134				✓		
Pharmaceutically Relevant Mixture (II) – Different Selectivity Using pH	135				✓		
Phenelzine in Human Plasma by LC-MS/MS	135	✓				✓	
Phenol and Phenoxy Acid Herbicides	136		✓	✓			
Phenolic Acids	136			✓			
Phenolic Compounds from Red Grape Seed Extract	137			✓			
Phenolic Compounds in Ground Water & Landfill Leachates	136		✓				
Phenols in Purple Coneflower *(Echinacea Purpurea)*	137			✓			
Phosphatidylethanol Biomarker Analysis by UHPLC-MS/MS	138	✓				✓	
Phytoestrogens from Hop Extract by LC-MS/MS	138			✓		✓	
Pilocarpine	139				✓		
Plant Hormones Involved in Abiotic Stresses	139	✓	✓			✓	
[^{14}C]Pomalidomide and Metabolites in Human Plasma and Urine	141	✓				✓	
Polar Compounds Separation	140						✓
Polyamines	140	✓					
Polycyclic Tetracarboxylic Acids	140		✓			✓	
Polyethylene Glycol 1000	141		✓			✓	
Porphyrins in Oral Bacteria by LC-MS/MS	142	✓				✓	
Pravastatin and Isomers by LC-MS/MS	142	✓			✓	✓	
Pravastatin in Cell Lysate Samples by LC-MS/MS	143	✓				✓	
Prednisolone, Prednisone, Cortisol and Cortisone in Serum by LC-MS/MS	144	✓			✓	✓	
Preservatives (I)	144			✓			
Preservatives (II)	144			✓			
Pristinamycin Components in Plasma by LC-MS/MS	145	✓			✓	✓	
Proanthocyanidins from Cinnamon Bark Extract	145	✓		✓			
Procaine and p-Aminobenzoic Acid Separation	146				✓		
Propolis Phenolic Acids Applied to Human Skin	146	✓				✓	
Prostaglandins using LC-MS/MS	147	✓				✓	
Protein Test Mix	147	✓					
Proton Pump Inhibitors (PPIs)	147				✓		
Psychoactive Substances in 'Synthacaine' by LC-UV	148	✓			✓		
Quinidine, Quinine and their Hydroderivatives Separation	148	✓			✓		
Ranitidine Hydrochloride and Related Impurities	149	✓			✓		
Recombinant hGMCSF Purified from *Escherichia Coli*	149	✓					
Rifamycin Anti-tubercular Antibiotics in Human Plasma	150	✓				✓	
Sennosides in Traditional Chinese Medicine	151			✓	✓		

Application Index

	Page Number	Clinical, Forensics & Bioanalysis	Environmental	Food & Beverage	Pharmaceutical	LC-MS	Other
Snake Venom from *Crotalus Durissus Terrificus*	151	✓					
Sotalol	151				✓		
Stability Indicating Method for HIV Injection Treatment	152				✓		
Statins – Atorvastatin	154	✓			✓		
Statins – Fluvastatin	154	✓			✓		
Statins in Lactone and Hydroxy Acid Forms by HPLC-UV	153				✓		
Statins – Pravastatin	155	✓			✓		
Statins – Simvastatin	155	✓			✓		
Steroid Hormones (Endogenous) by LC-MS/MS	155	✓				✓	
Steroid Mixture Separation	156	✓			✓		
Steroids Separation using Enhanced Polar Selectivity	157	✓			✓		
Steroids UHPLC-UV Analysis and Comparison	156				✓		
Steroids (Veterinary) by LC-MS/MS	157	✓			✓	✓	
St John's Wort	158			✓			
Substituted Methoxybenzene Isomers	159						✓
Sugars – Cola vs Diet Cola	159			✓			
Sugars – Disaccharides	159			✓			
Sugars – Lactulose	159			✓	✓		
Sugars – Maple Syrup	160			✓			
Sugars – Monosaccharides	160			✓			
Sugars – Orange Juice	161			✓			
Sugars Separation	161			✓			
Sulfonamides	161	✓		✓	✓		
Sulfurous Analytes Separation Comparison	162						✓
Sumatriptan and Promethazine by LC-MS/MS	162	✓			✓	✓	
Sunscreen Agents	163						✓
Synthetic Cannabinoids (SPICE) from Oral Fluid	164	✓			✓	✓	
Taxol in Fungal Extract by LC-MS/MS	165	✓				✓	
Telithromycin Analysis	165	✓			✓		
Terfenadine and Fexofenadine in Rat Plasma	166	✓			✓	✓	
Testosterone	166	✓				✓	
Tetracyclines	166				✓		
Thyroid Hormones by LC-MS/MS (I)	167	✓				✓	
Tocopherols	168	✓		✓			
Tocopherols Mixture Separation	167	✓		✓			
Toxins from *Amanita Phalloides* Mushrooms by LC-HRMS	168			✓		✓	
Tricyclic Antidepressants	168	✓			✓		
Tricyclic Antidepressants (Gradient)	169	✓			✓		
Tricyclic Antidepressants (Isocratic)	169	✓			✓		
Tricyclic Antidepressants (Isocratic Rapid Analysis)	170	✓			✓		
Triple API Pharmaceutical and Related Substances using Ultra Resolution	171				✓		
Tyrosine, Tryptophan and Tramadol by HPLC with Fluorescence Detection	172	✓					
USP Monograph – 17α-Ethinylestradiol	172				✓		

Application Index

	Page Number	Clinical, Forensics & Bioanalysis	Environmental	Food & Beverage	Pharmaceutical	LC-MS	Other
USP Monograph – Amlodipine Besylate	172				✓		
USP Monograph – Budesonide	173				✓		
USP Monograph – Doxepin	173				✓		
USP Monograph – Estradiol	173				✓		
USP Monograph – Glimepiride	173				✓		
USP Monograph – Guaifenesin	174				✓		
USP Monograph – Hydrocortisone	174				✓		
USP Monograph – Hydroquinone	174				✓		
USP Monograph – Indomethacin	174				✓		
USP Monograph – Metronidazole	175				✓		
USP Monograph – Naproxen	175				✓		
USP Monograph – Paracetamol/Aspirin/Caffeine	175				✓		
Vanilla Flavourings – Natural and Artificial	176			✓			
Vanillins	177			✓			
Vanillins – Fast Analysis	177			✓			
1,25-Dihydroxyvitamins D2 and D3 in Serum by LC-MS/MS	179	✓				✓	
25-Hydroxy Vitamin D in Serum by LC-MS/MS	178	✓		✓		✓	
Vitamin D2/D3	178	✓		✓			
Vitamins – Fat Soluble	180	✓		✓			
Vitamins – Water Soluble (Gradient I)	180	✓		✓			
Vitamins – Water Soluble (Gradient II)	180			✓			
Vitamins – Water Soluble (Gradient III)	181			✓			
Vitamins – Water Soluble (Gradient IV)	181			✓			
Vitamins – Water Soluble (Isocratic I)	182			✓			
Vitamins – Water Soluble (Isocratic II)	182			✓			
Vitamins in Fruit Juice by Fast LC-MS	182			✓		✓	
Vitamins in Green Vegetables by LC-MS/MS - Water Soluble	183			✓		✓	
Vitamins and Polar Molecules - Water Soluble	184			✓			
Water Soluble Artificial Colours	184			✓			
Whey Proteins from Whole Milk	184	✓		✓		✓	
Wine Acid Analysis	185			✓			

For further applications

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

Acylcarnitines by LC-MS/MS

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

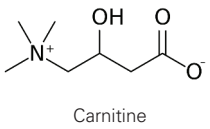
Gradient:

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

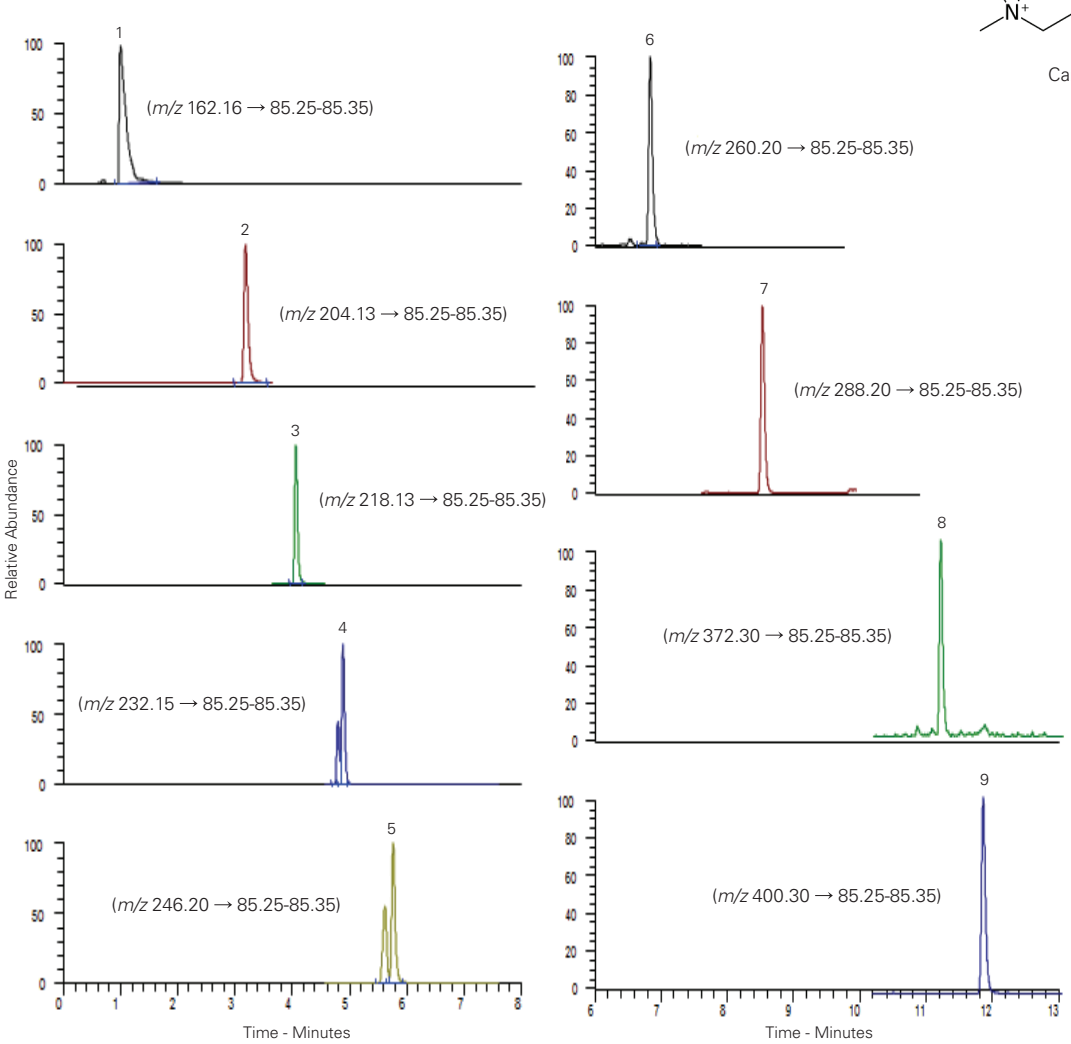
Flow Rate: 0.3 mL/min
Sample: Dried serum extract
Detection: Positive mode ESI

Analytes

1. Carnitine
2. Acetylcarnitine
3. Propionylcarnitine
4. Butyrylcarnitine & Isobutyrylcarnitine
5. Isovalerylcarnitine & 2-Methylbutyrylcarnitine
6. Hexanoylcarnitine
7. Octanoylcarnitine
8. Myristoylcarnitine
9. Palmitoylcarnitine



Carnitine



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Additives and Intense Sweeteners

Application #AN2950

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.0 mm
Part Number: ACE-121-2504
Mobile Phase: A: H_2O
B: MeCN
C: 1% TFA in H_20

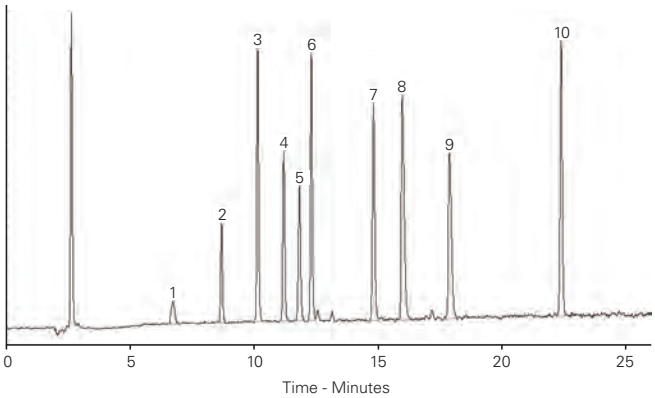
Gradient:

Time (mins)	%A	%B	%C
0	88	2	10
25	50	40	10
30	30	60	10
35	88	2	10

Flow Rate: 1.0 mL/min
Temperature: 30 °C
Detection: ELSD

Analytes

1. Acesulfame K
2. Theobromine
3. Theophylline
4. Cyclamate
5. Saccharin
6. Caffeine
7. Sucralose
8. Quinine sulphate
9. Aspartame
10. Neohesperidin dihydrochalcone



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Alcohol Biomarkers by UHPLC-MS/MS

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

Gradient:

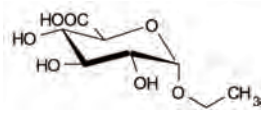
Time (mins)	%B
0.0	0
0.5	20
1.5	20
2.0	100
4.0	100
4.5	0

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

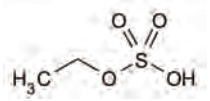
Fluoride counter-ion thought to enhance negative ESI response
Detection limit ~ 1 ng/mL in oral fluid

Analytes

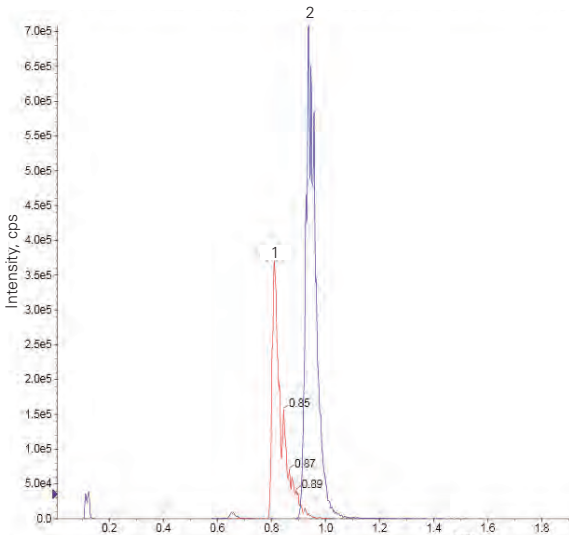
1. Ethyl glucuronide (EtG)
2. Ethyl sulphate (EtS)



Ethyl glucuronide (EtG)



Ethyl sulphate (EtS)



Transitions

Quantifiers
EtS *m/z* 124.8 → 79.9
EtG *m/z* 221 → 85

Qualifiers
EtS *m/z* 124.8 → 97
EtG *m/z* 221 → 75

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Alternative Selectivity Provided by ACE CN-ES

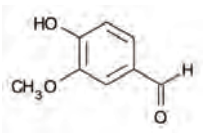
Application #AN2450

Conditions

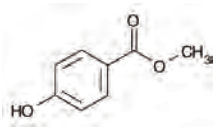
Column:	ACE Excel 3 CN-ES ACE Excel 3 CN ACE Excel 3 C18
Dimensions:	50 x 2.1 mm
Part Number:	EXL-1113-0502U (ACE Excel 3 CN-ES), EXL-114-0502U (ACE Excel 3 CN), EXL-111-0502U (ACE Excel 3 C18)
Mobile Phase:	A: 0.1% formic acid in H_2O B: 0.1% formic acid in MeOH/H_2O (90:10 v/v)
Gradient:	**Time (mins) %B** 0 3 5 100
Flow Rate:	0.6 mL/min
Injection:	1 µL
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

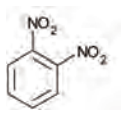
1. Metronidazole
2. Benzyl alcohol
3. Hydrochlorothiazide
4. Vanillin
5. Methyl paraben
6. 1,2-Dinitrobenzene



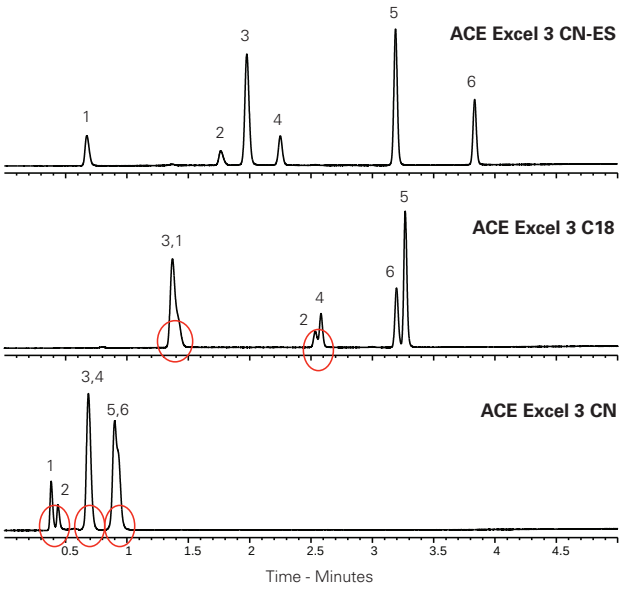
Vanillin

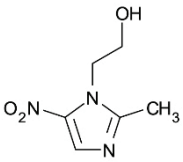


Methyl paraben

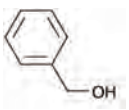


1,2-Dinitrobenzene

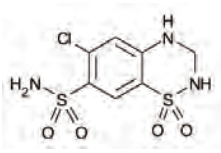




Metronidazole



Benzyl alcohol



Hydrochlorothiazide

Amino Acid Profile of Edible Stink Bugs by LC-MS

Application #AN3530

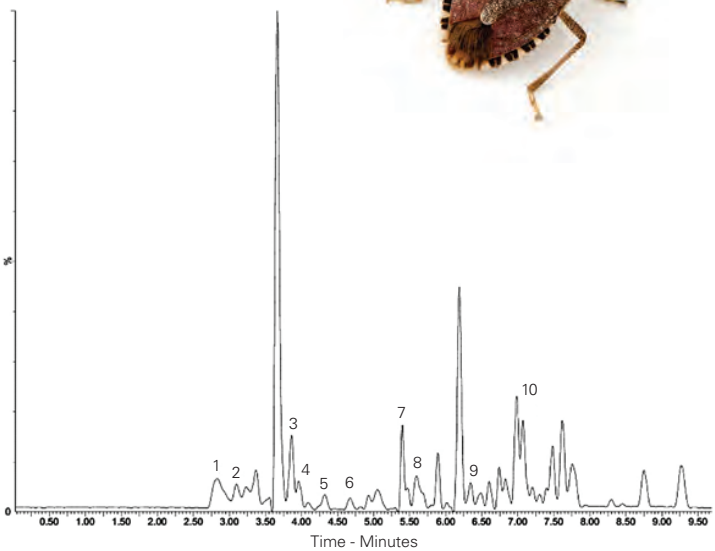
Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: 0.01% formic acid in H_2O B: 0.01% formic acid in MeCN
Gradient:	**Time (mins) %B** 0.0 5 3.0 30 6.0 30 7.5 80 10.5 80 13.0 100 18.0 100 20.0 5 22.0 5
Flow Rate:	0.7 mL/min
Injection:	1 µL
Detection:	Waters QToF-MS ESI in positive ion mode Scan range: *m/z* 100-700
Sample:	Profile of edible stink bugs (*Encosternum delegorguei* Spinola) after acid hydrolysis of extracted proteins

Analytes

1. Arginine
2. Isoleucine
3. Leucine
4. Proline
5. Valine
6. Methionine
7. Hydroxyproline
8. Tyrosine
9. Lysine
10. Phenylalanine





Musundire R, Osuga IM, Cheseto X, Irungu J, Torto B (2016) Aflatoxin Contamination Detected in Nutrient and Anti-Oxidant Rich Edible Stink Bug Stored in Recycled Grain Containers. PLoS ONE 11(1): e0145914. doi:10.1371/journal.pone.0145914

Amino Acid Enantiomer Separation of Seawater Samples

Application #AN3880

This method enables the quantification of free, dissolved combined, particulate and total amino acid enantiomers from seawater. After hydrolysis, hydrolysates are evaporated, dissolved in borate buffer (pH 10) and centrifuged to remove flocculates. Samples are derivatised with OPA/IBDC (N-isobutyryL-D-cysteine) and SMC (S-methyL-L-cysteine) added as internal standard. Enantiomer elution order can be reversed by using IBLC (N-isobutyryL-L-cysteine)

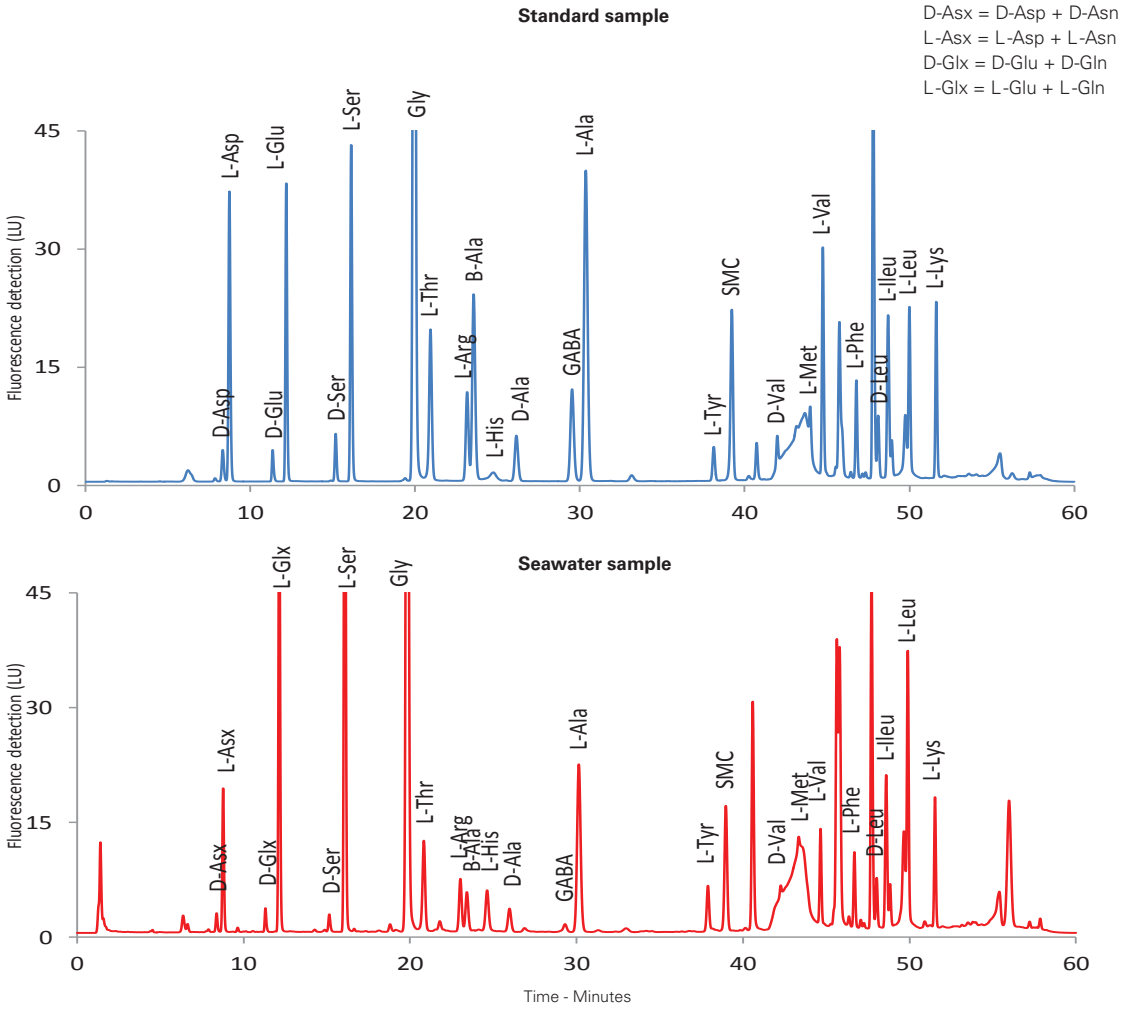
Conditions

Column: ACE UltraCore 5 SuperC18
Dimensions: 250 x 3.0 mm
Part Number: CORE-5A-2503U
Mobile Phase: A: 95% 40 mM KH_2PO_4 pH 6.15 in H_2O + MeOH/MeCN (93:7 v/v)
B: 62% MeOH/MeCN (93:7 v/v) + 38% A

Gradient:

Time (mins)	%B
0.0	0
13.0	27
33.0	36
38.0	58
54.0	92
55.0	100
57.5	0
60.0	0

Flow Rate: 0.7 mL/min
Temperature: 45 °C
Detection: Fluorescence, λ_{ex} 330 nm λ_{em} 450 nm



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Amino Acids and Biogenic Amines in Wine and Beer

Application #AN2800

Conditions

Column: ACE 5 C18-HL
Dimensions: 250 x 4.6 mm
Part Number: ACE-321-2546
Mobile Phase: A: 25 mM acetate buffer (pH 5.8)
B: MeCN/MeOH (80:20 v/v)

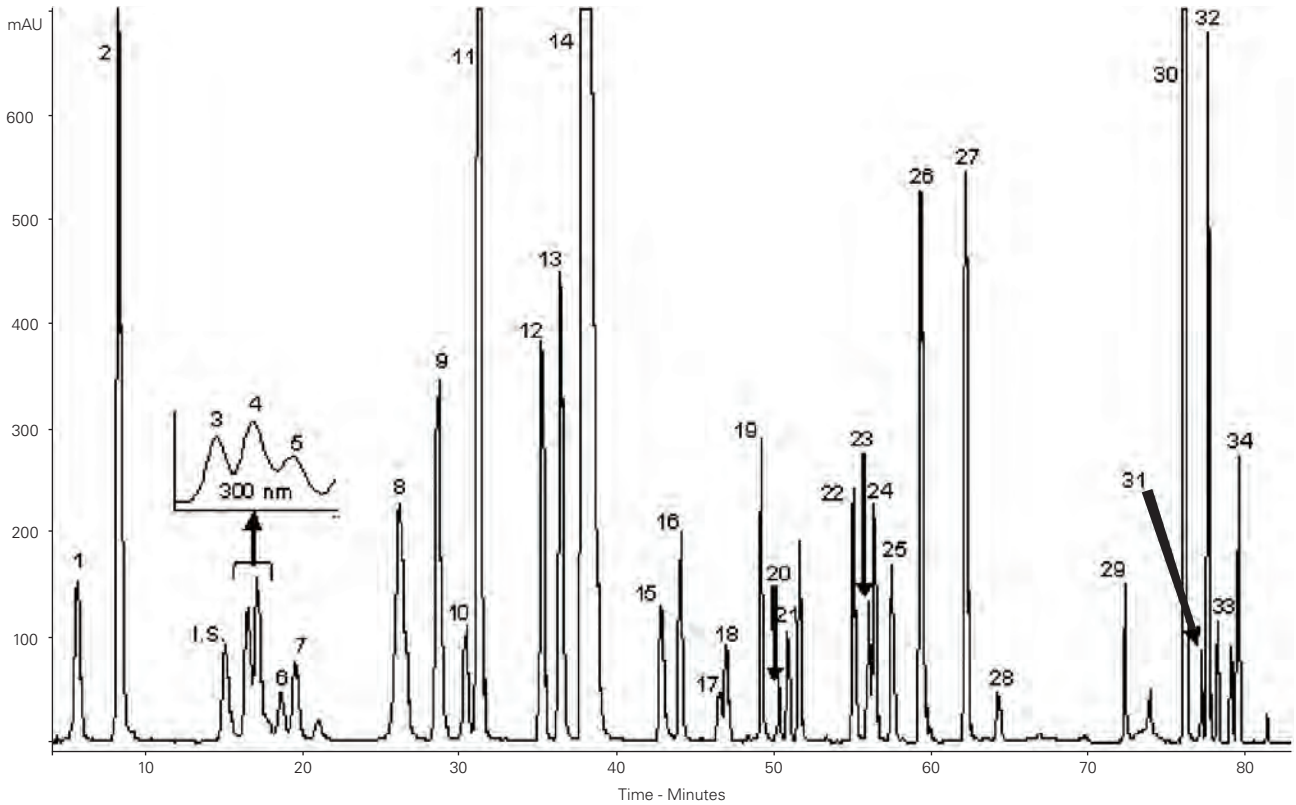
Gradient:

Time (mins)	%B
0.0	45
20.0	60
30.5	17
33.5	17
65.0	40
73.0	72
78.0	82
82.0	100
85.0	100

Flow Rate: 0.8 mL/min
Injection: 20 µL
Temperature: 16 °C
Detection: DAD, 269, 280 and 300 nm
Sample: Derivatisation with diethyl ethoxymethylmalonate

Analytes

1. Aspartic acid
2. Glutamic acid
3. Asparagine
4. Serine
5. Hydroxyproline
6. Glutamine
7. Histidine
8. Glycine
9. Threonine
10. β-Alanine
11. Arginine
12. α-Alanine
13. GABA
14. Proline
15. Histamine
16. Tyrosine
17. Ammonium ion
18. Agmatine
19. Valine
20. Methionine
21. Cysteine
22. Isoleucine
23. Tryptophan
24. Leucine
25. Phenylalanine
26. Ornithine
27. Lysine
28. Spermidine
29. Tyramine
30. Putrescine
31. Tryptamine
32. Cadaverine
33. Phenylethylamine
34. Isoamylamine
I.S. L-2-Aminoadipic acid



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

Amino Acids in Extracellular Matrix

Application #AN4410

Conditions

Column: ACE 3 AQ
Dimensions: 150 x 0.5 mm
Part Number: ACE-116-15005
Mobile Phase: A: 0.1% (v/v) formic acid in H_2O
B: 0.1% (v/v) formic acid in MeCN

Gradient:

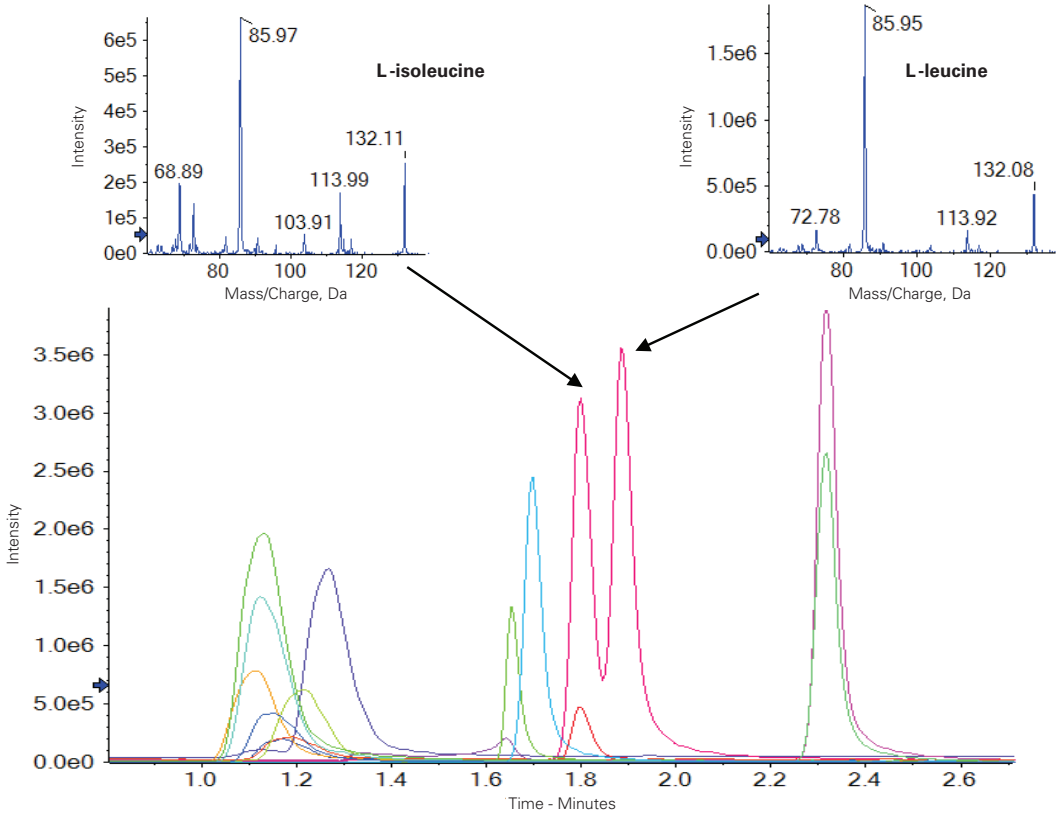
Time (mins)	%B
0	2
5	20

Flow Rate: 20 µL/min
Injection: 2 µL
Detection: SCIEX QTRAP 6500 LC-MS/MS system
IonDrive Turbo V source
Positive ion MRM mode
Sample: Standard solution containing 2.5 µmol/mL each amino acid (1.25 µmol/mL cysteine).
0.5 pmol on-column (except for cysteine, 0.25 pmol on-column).
Method also applied to analysis of cell supernatant from purified peripheral blood mononuclear cells (PBMCs)

Peak	Analyte	Rt (mins)	MRM Transition (*m/z*)	LOD (fmol)	PBMC cell conc. (fmol/µL)
1	Lys	1.094	147.1 → 84	5	305
2	His	1.111	156.1 →110	5	23
3	Arg	1.117	175.2 → 70	2.5	220
4	Gly	1.129	76.1 → 30	<1000	<LOD
5	Cys	1.140	241.2 → 152.1	1.25	36
6	Asp	1.155	134.1 → 74	10	26
7	Ser	1.156	106.1 → 60	50	21
8	Ala	1.189	90.1 → 44	<1000	<LOD
9	Glu	1.208	148.1 → 84	5	55
10	Pro	1.262	116.1 → 70	2.5	96
11	Val	1.630	118.1 → 55	25	105
12	Met	1.645	150.2 → 104	1	3
13	Tyr	1.669	182.2 → 165.2	1	97
14	Ile	1.773	132.1 → 86, 69	2.5	329
15	Leu	1.858	132.1 → 86	2.5	338
16	Phe	2.273	166.1 → 103	1	100
17	Thr	2.275	120.1 → 103.2	1	97

MRM transitions and limits of detection (LODs) for 17 free amino acids and their concentrations measured in diluted PBMC cell supernatant

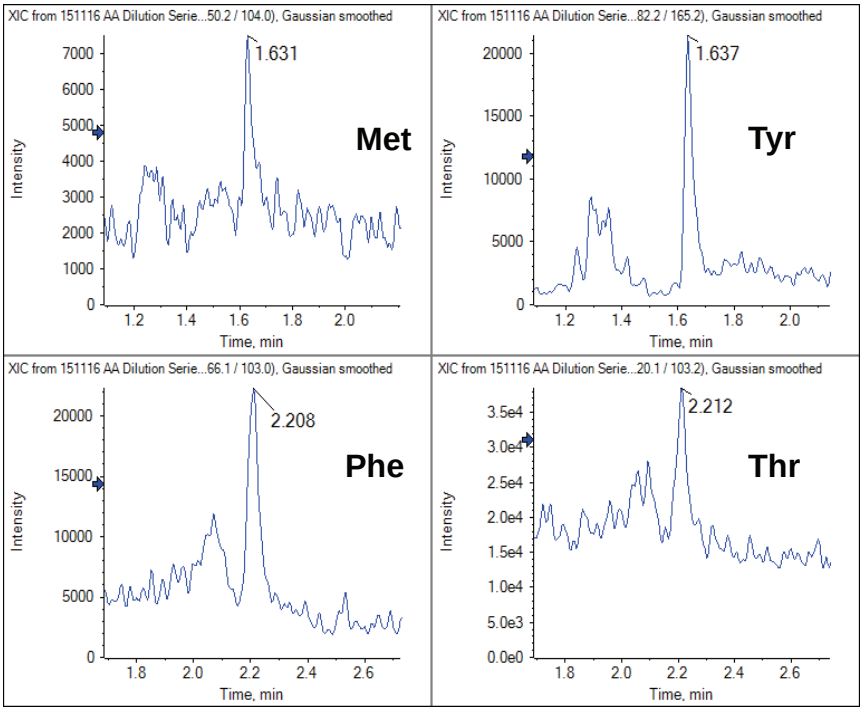
Full scan linear ion trap MS/MS data can distinguish isobaric amino acids L-isoleucine and L-leucine.



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Amino Acids in Extracellular Matrix (*Continued*)

MRM extracted ion chromatograms for four amino acids each at 1 fmol on-column



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Amino Acids Derivatised with Dabsyl Chloride

Conditions

Column: ACE 3 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-111-1503
Mobile Phase: A: 10 mM KH_2PO_4 buffer (pH 6.55)
B: MeCN/2-Propanol (70:30 v/v)

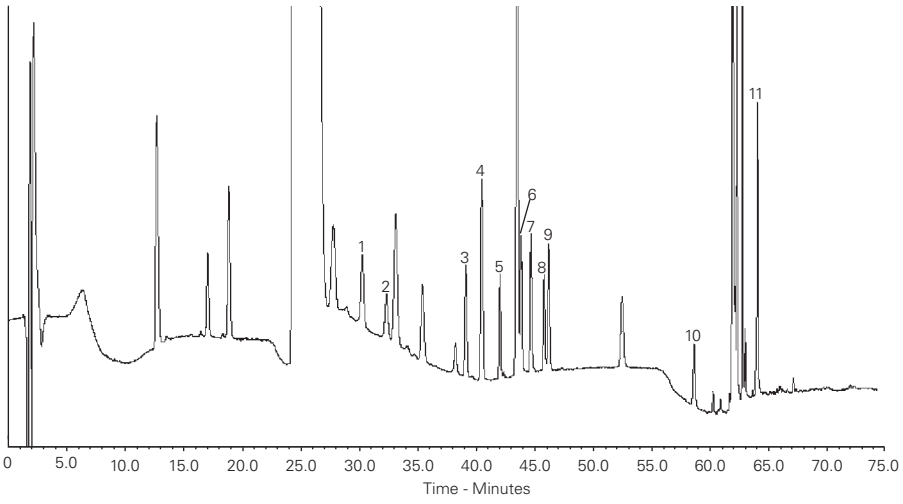
Gradient:

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 (PDA detector)

Analytes

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 in Peas *(Pisum Sativum)* by HPLC-HRAM-MS

Application #AN2660

Conditions

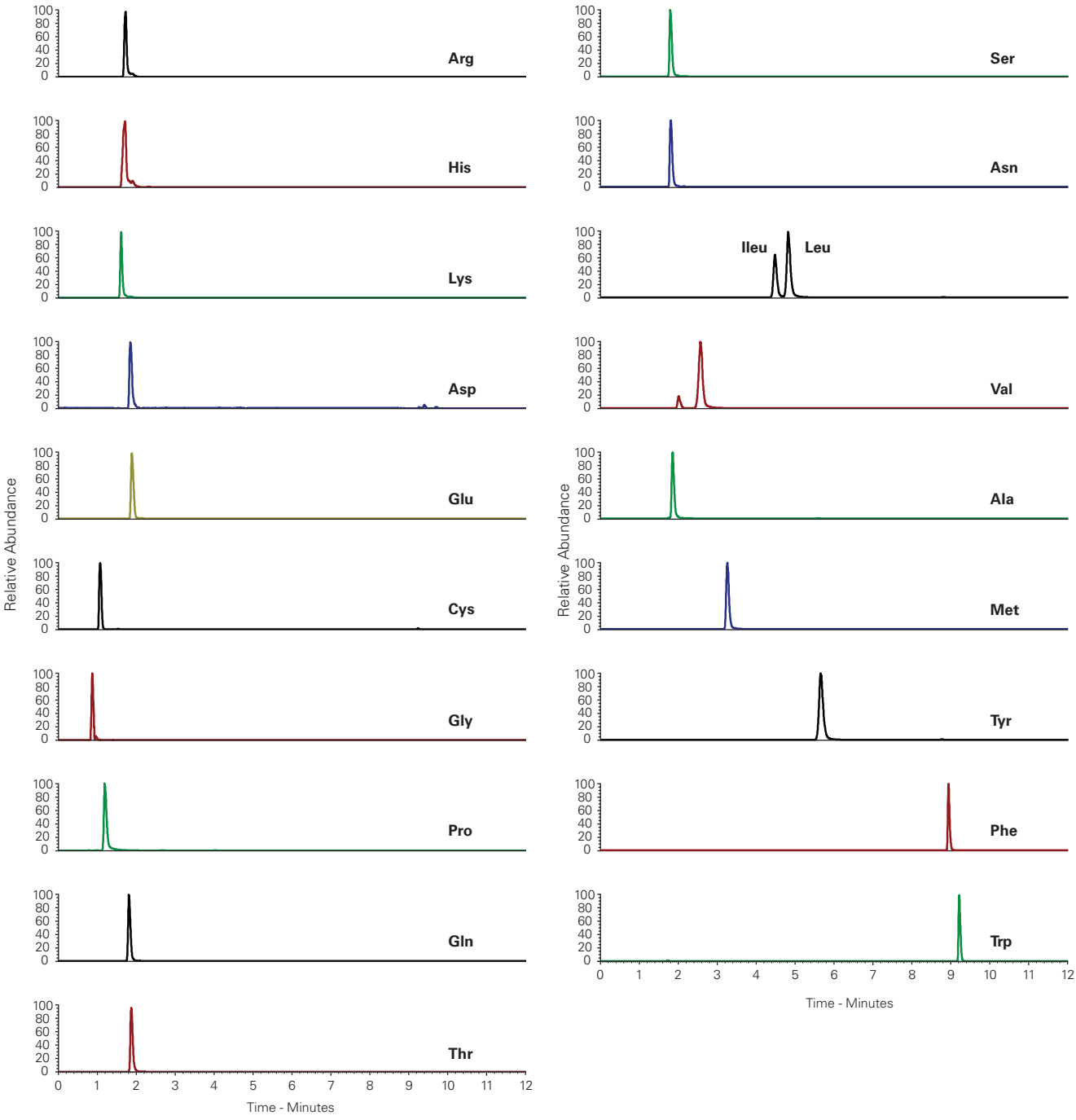
Column: ACE 3 AQ
Dimensions: 150 x 3.0 mm
Part Number: ACE-116-1503
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

Gradient:

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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Aminoglycosides in Eggs

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)

Gradient:

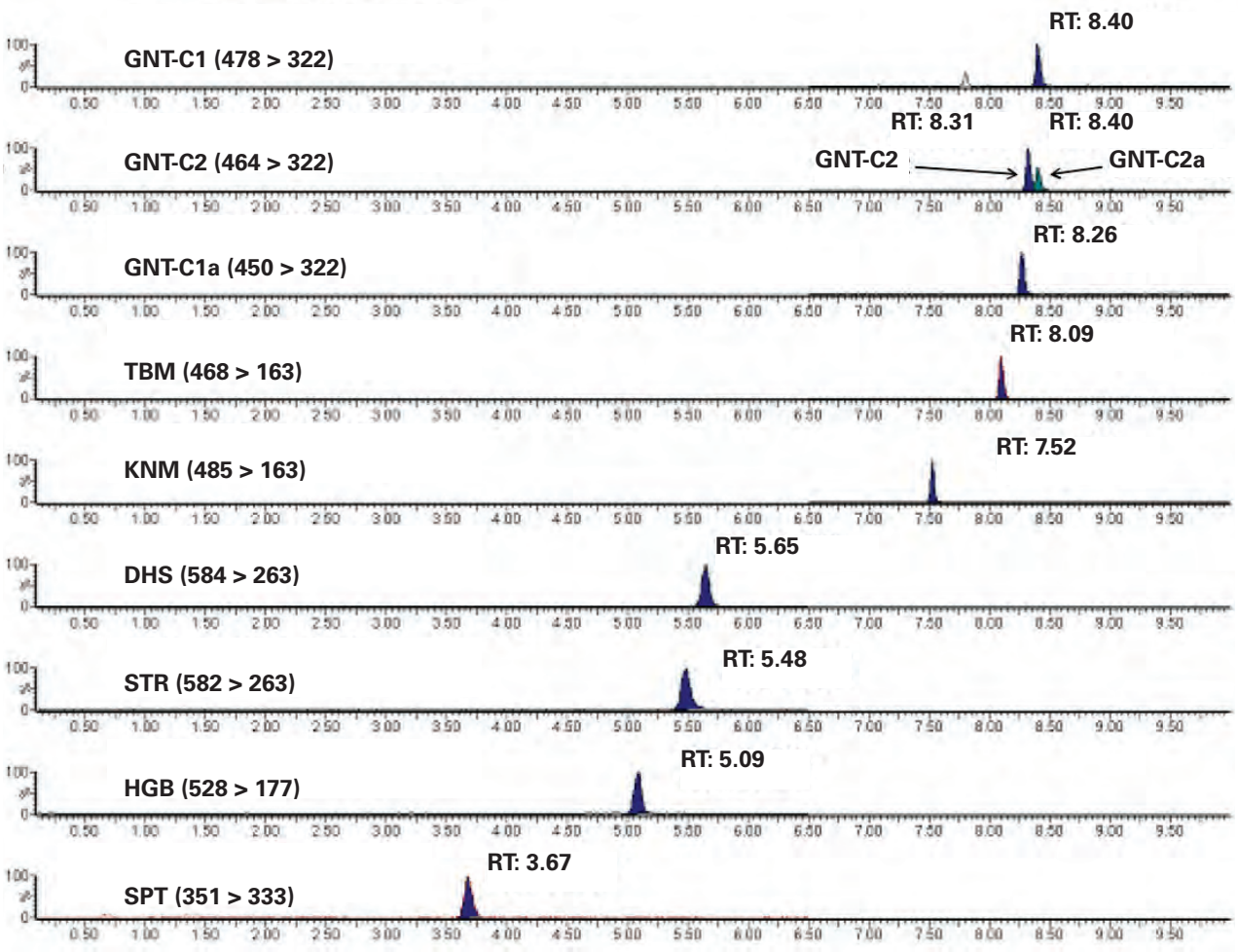
Time (mins)	%B	Curve
0.0	5.0	-
2.0	15.0	6
4.5	19.0	6
5.5	19.5	8
6.0	22.0	6
7.0	35.0	6
9.0	48.0	8
9.5	5.0	6

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)

Analytes

GNT Gentamicin
TBM Tobramycin
KNM Kanamycin
DHS Dihydrostreptomycin
STR Streptomycin
HGB Higromycin-B
SPT Spectinomycin





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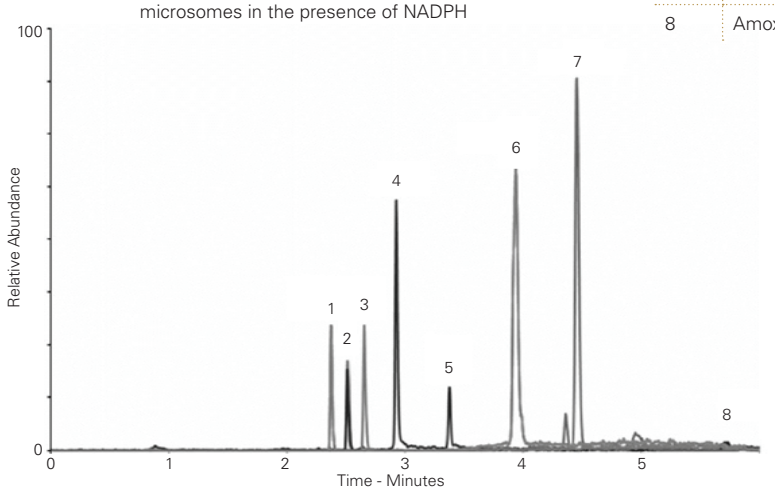
Amoxicillin Metabolites in Human Liver Microsomes

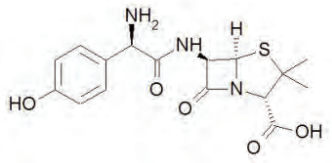
Application #AN4400

Conditions

Column: ACE 5 C18-300
Dimensions: 150 x 4.6 mm
Part Number: ACE-221-1546
Mobile Phase: 0.1% (v/v) formic acid in H_2O/MeCN (35:65 v/v)
Flow Rate: 0.4 mL/min
Injection: 15 µL
Temperature: 21 °C
Detection: Agilent 6410 triple quad MS
ESI in positive ion mode
Full scan MS and MS/MS data obtained
Sample: *In vitro* incubation of amoxicillin with human liver microsomes in the presence of NADPH

Peak	Analyte	[M+H]+	Elemental Composition	Metabolic Reaction
1	M1	382	$C_{16}H_{20}N_3O_6S$	Hydroxylation
2	M2	379	$C_{17}H_{19}N_2O_7S$	Oxidative deamination
3	M3	382	$C_{16}H_{20}N_3O_6S$	Oxidation of aliphatic chain
4	M4	380	$C_{16}H_{18}N_3O_6S$	Oxidation of aliphatic chain
5	M5	396	$C_{16}H_{20}N_3O_7S$	Oxidation of aliphatic chain
6	M6	322	$C_{15}H_{19}N_3O_3S$	Decarboxylation
7	M7	542	$C_{25}H_{28}N_3O_{11}S$	Glucuronidation
8	Amoxicillin	366	$C_{16}H_{20}N_3O_5S$	





Amoxicillin

Szultka M, Krzeminski R, Jackowski M, Buszewski B. (2014) Identification of in vitro Metabolites of Amoxicillin in Human Liver Microsomes by LC-ESI/MS, Chromatographia, 77 , 1027-1035. doi 10.1007/s10337-014-2648-2

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Amphetamines from Drugs of Abuse Screen (#AN2190)

Application #AN2350

Conditions

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

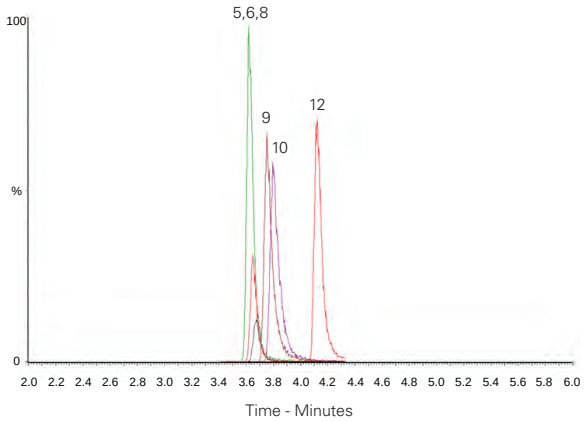
Gradient:

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

Flow Rate: 0.3 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: MS Quattro Premier XE triple quad
MRM, positive and negative ESI mode
Desolvation temperature: 450 °C
Ion source temperature: 150 °C
Collision gas pressure: 3.5 x10^{-3} mbar

Analytes

5. Amphetamine-d5
(*m/z* 141.0 → 123.9)
6. Amphetamine
(*m/z* 136.0 → 118.9)
8. MDA
(*m/z* 180.1 → 105.0)
9. MDMA
(*m/z* 194.1 → 163.0)
10. Methamphetamine
(*m/z* 150.0 → 90.9)
12. MDEA
(*m/z* 208.2 → 163.0)



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Amphetamines in Urine by LC-MS/MS

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)

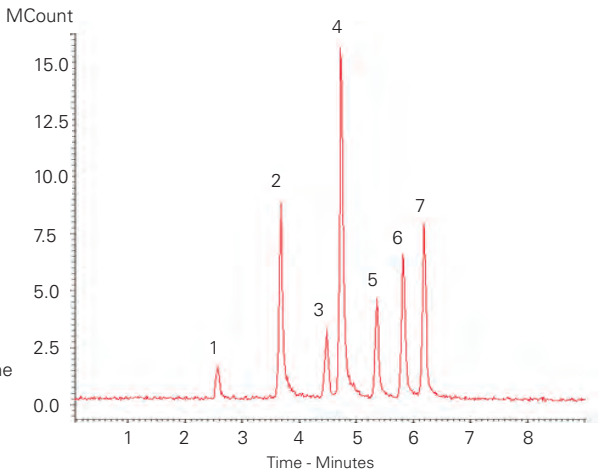
Gradient:

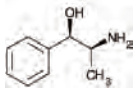
Time (mins)	%B
0	30
8	95

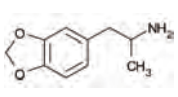
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: Varian 320 Triple Quadrupole MS
Electrospray voltage: +5 kV
Inlet capillary voltage: 30 V
CID with argon at 1.5 mTorr
Collision cell potential ranges from 5 to 17 V
Drying gas (nitrogen) temperature: 325 °C
Nebulizing gas (nitrogen)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

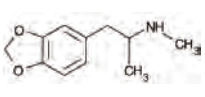
Analytes

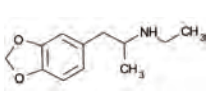
1. Phenylpropanolamine
LOD (est) 4 ppb
(*m/z* 151.6 → 134.0)
2. (l)-Ephedrine
LOD (est) 2 ppb
(*m/z* 166.2 → 148.0)
3. (dl)-3,4-MDA
LOD (est) 30 ppb
(*m/z* 179.7 → 163.0)
4. (d)-Amphetamine
LOD (est) 4 ppb
(*m/z* 135.8 → 90.9)
5. (dl)-3,4-MDMA
LOD (est) 2 ppb
(*m/z* 193.7 → 163.0)
6. 4-Methylthioamphetamine
LOD (est) 10 ppb
(*m/z* 182.2 → 165.0)
7. (±)-MDEA
LOD (est) 1 ppb
(*m/z* 207.7 → 165.0)

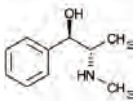


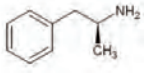

Phenylpropanolamine

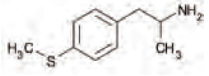

(dl)-3,4-MDA


(dl)-3,4-MDMA


(±)-MDEA


(l)-Ephedrine


(d)-Amphetamine


4-Methylthioamphetamine

Anabolic Steroids from Horse Urine by LC-MS/MS

Application #AN2360

Conditions

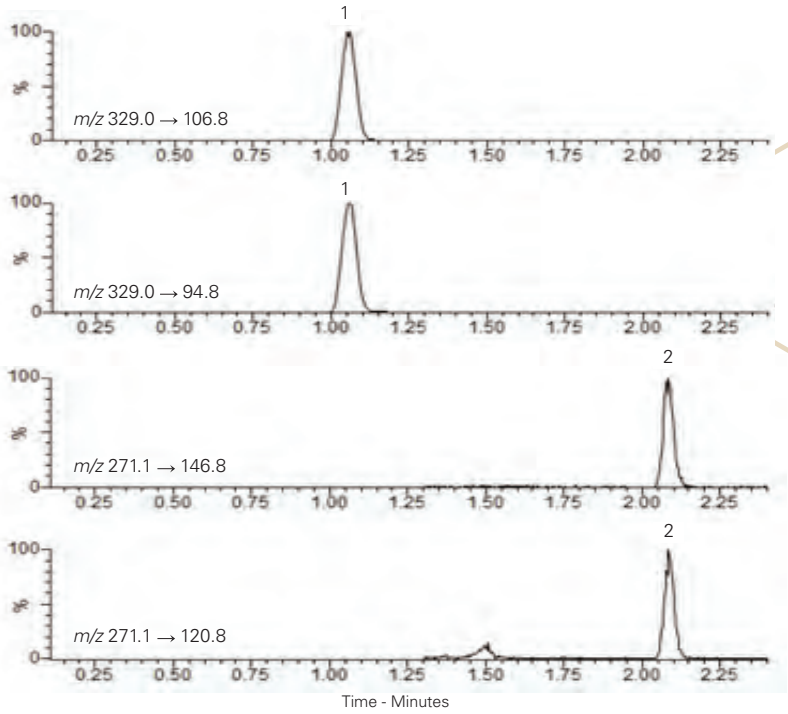
Column:	ACE Excel 2 C18
Dimensions:	50 x 2.1 mm
Part Number:	EXL-101-0502U
Mobile Phase:	A: 2 mM ammonium acetate, 0.1% formic acid in H_2O
	B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

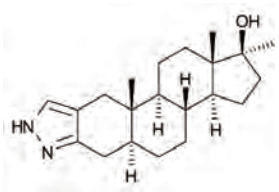
Gradient:	**Time (mins)**	**%B**
	0.00	75
	0.25	75
	1.50	90
	1.51	100
	3.50	100
	3.51	75
	4.00	75

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

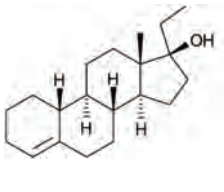
Analytes

1. Stanozolol
2. Ethylestrenol





Stanozolol



Ethylestrenol

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Analgesic Rapid Separation

Application #AN1370

Conditions

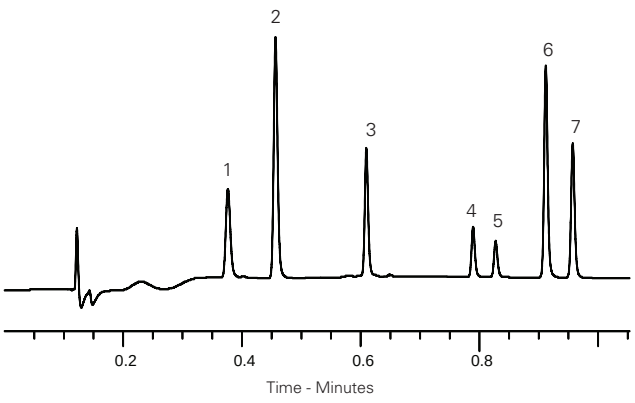
Column:	ACE Excel 2 SuperC18
Dimensions:	50 x 2.1 mm
Part Number:	EXL-1011-0502U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

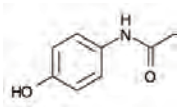
Gradient:	**Time (mins)**	**%B**
	0.0	5
	1.0	100
	1.5	100
	1.6	5
	3.1	5

Flow Rate:	1.2 mL/min
Injection:	0.5 µL
Temperature:	50 °C
Detection:	UV, 214 nm

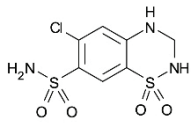
Analytes

1. Paracetamol
2. Hydrochlorothiazide
3. Aspirin
4. Bendroflumethiazide
5. Ketoprofen
6. Flurbiprofen
7. Ibuprofen

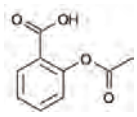




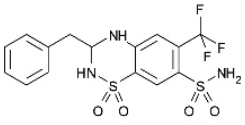
Paracetamol



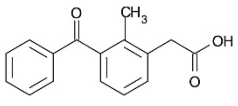
Hydrochlorothiazide



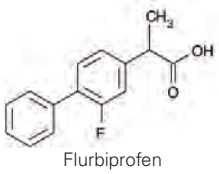
Aspirin



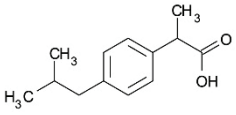
Bendroflumethiazide



Ketoprofen



Flurbiprofen



Ibuprofen

Analgesic Separation

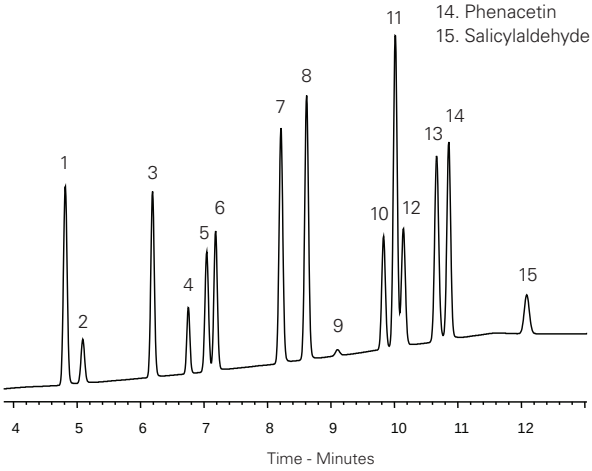
Application #AN2490

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 MeCN	
Gradient:	**Time (mins)**	**%B**
	0	5
	9	35
	14	35
Flow Rate:	1 mL/min	
Temperature:	40 °C	
Detection:	UV, 240 nm	

Analytes

1. 4-Acetamidophenol
2. 4-Aminobenzoic acid
3. 4-Hydroxybenzoic acid
4. Caffeine
5. 2-Acetamidophenol
6. 3-Hydroxybenzoic acid
7. Salicylamide
8. Acetanilide
9. Phenol
10. Acetylsalicylic acid
11. Benzoic acid
12. Sorbic acid
13. Salicylic acid
14. Phenacetin
15. Salicylaldehyde



For additional column dimensions

Please enquire
email: info@ace-hplc.com

Analgesics / Cough & Cold Medicine Ingredients

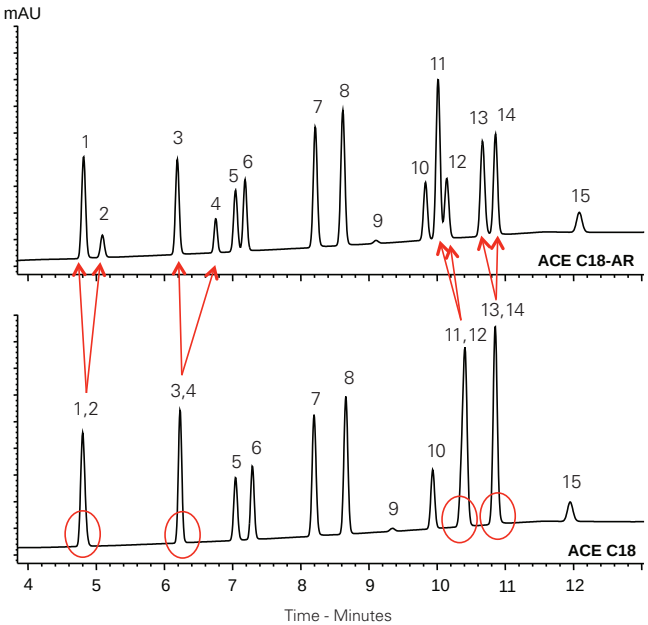
Application #AN1930

Conditions

Column:	ACE 3 C18-AR	
	ACE 3 C18	
Dimensions:	150 x 4.6 mm	
Part Numbers:	ACE-119-1546	
	ACE-111-1546	
Mobile Phase:	A: 0.1% formic acid in H_2O	
	B: 0.1% formic acid in MeCN	
Gradient:	**Time (mins)**	**%B**
	0	5
	9	35
	14	35
	15	5
Flow Rate:	1 mL/min	
Temperature:	40 °C	
Detection:	UV, 240 nm	

Analytes

1. Paracetamol
2. 4-Aminobenzoic acid
3. 4-Hydroxybenzoic acid
4. Caffeine
5. 2-Acetamidophenol
6. 3-Hydroxybenzoic acid
7. Salicylic acid
8. Acetanilide
9. Phenol
10. Aspirin
11. Benzoic acid
12. Sorbic acid
13. Salicylic acid
14. Phenacetin
15. Salicylaldehyde





Andrographis Paniculata Fingerprint Profile by RRLC-TOF-MS

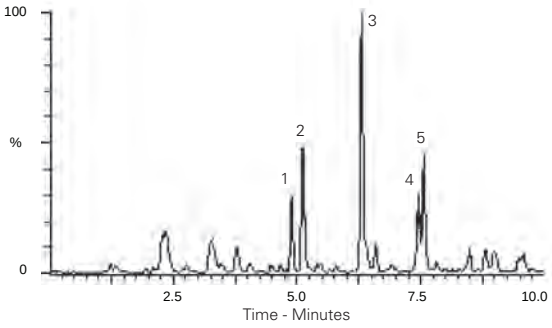
Application #AN3770

Conditions

Column:	ACE Excel 3 SuperC18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-1111-1002U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

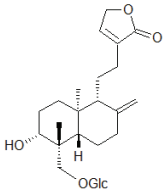
Gradient:	**Time (mins)**	**%B**
	0.0	30
	2.0	40
	8.0	75
	9.0	100
	9.5	30
	15.5	30

Flow Rate:	0.2 mL/min
Injection:	2 µL
Temperature:	35 °C
Detection:	Waters Premier Q-TOF-MS
	ESI in positive ion mode
	Scan Range *m/z* 100-1000 Da

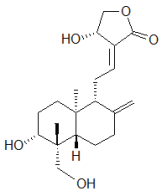


Analytes

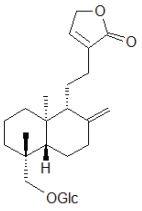
1. 14-Deoxyandrographiside
2. Andrographolide
3. Neoandrographolide
4. 14-Deoxyandrographolide
5. Dehydroandrographolide



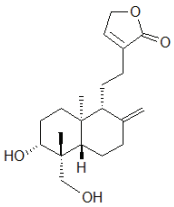
14-Deoxyandrographiside
(*Tentative assignment)



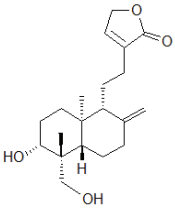
Andrographolide



Neoandrographolide



14-Deoxyandrographolide
(*Tentative assignment)



Dehydroandrographolide

Andrographis Paniculata - used in Chinese medicine.



Song Y-X, Liu S-P, Jin Z, Qin J-F, Jiang Z-Y (2013) Qualitative and quantitative analysis of *Andrographis Paniculata* by rapid resolution liquid chromatography/time-of-flight mass spectrometry. Molecules 189, 12192-12207 doi:10.3390/molecules181012192

Angiotensin II Receptor Antagonists by LC-UV

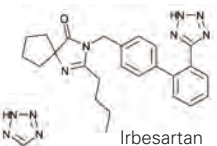
Application #AN3460

Conditions

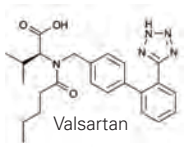
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	0.025 M KH_2PO_4 pH 6.0/MeCN (65:35 v/v)
Flow Rate:	1.5 mL/min
Temperature:	40 °C
Detection:	UV, 220 nm

Analytes

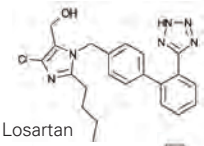
1. Valsartan
2. Losartan
3. Irbesartan
4. Telmisartan



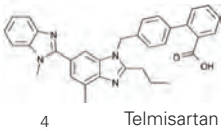
Irbesartan



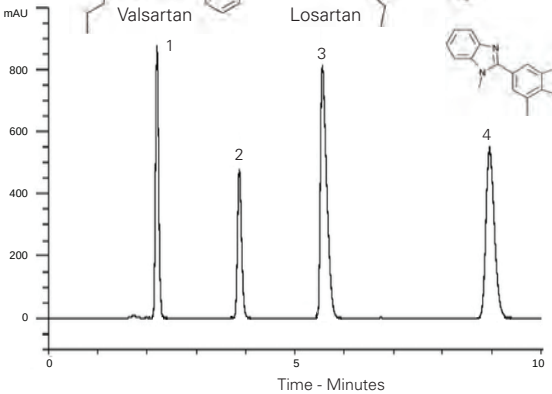
Valsartan



Losartan



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

For further applications

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

Angiotensin Peptides

Application #AN2150

Conditions

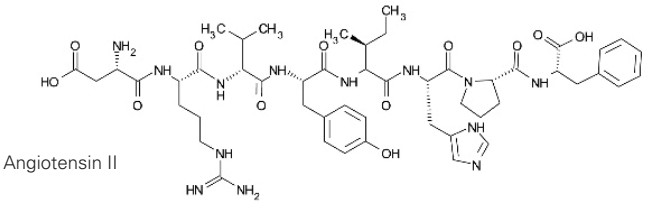
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H_2O
B: 0.1% TFA in H_2O/MeCN (80:20 v/v)
Gradient:

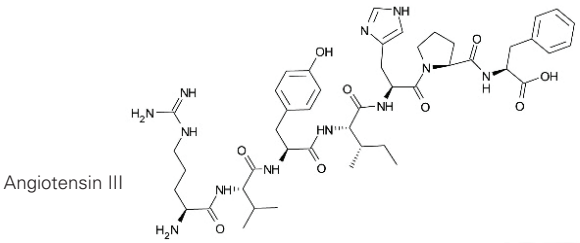
Time (mins)	%B
0	25
15	40

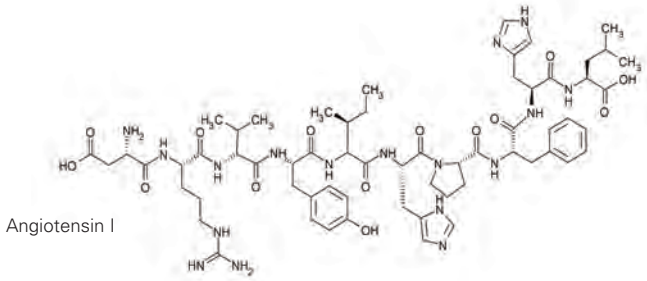
Flow Rate: 1.0 mL/min
Temperature: Ambient
Detection: UV, 215 nm

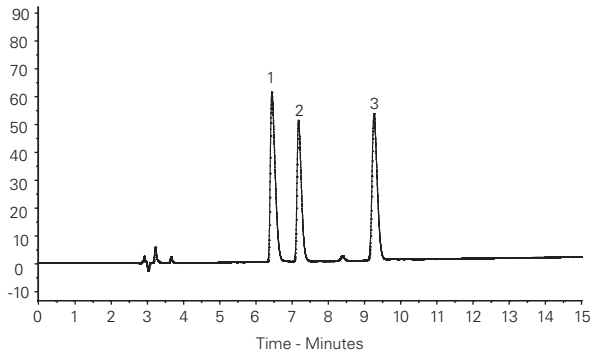
Analytes

1. Angiotensin II (MW 1046.2)
2. Angiotensin III (MW 931.1)
3. Angiotensin I (MW 1296.5)









Annatto

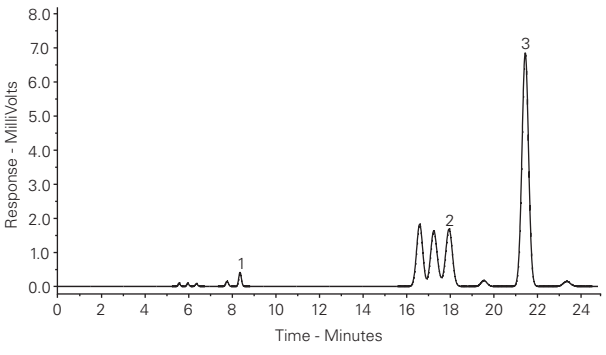
Application #AN2840

Conditions

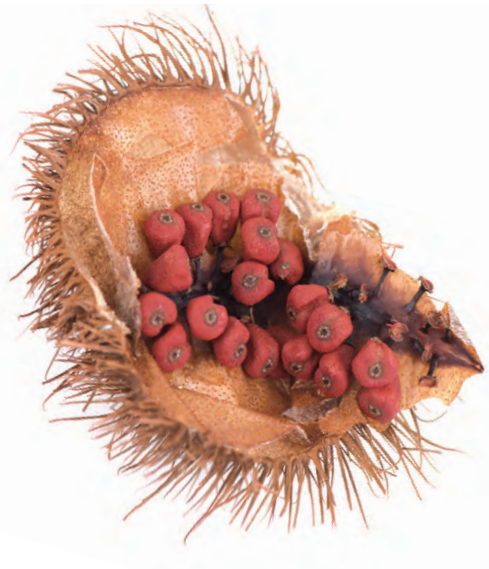
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/0.16% acetic acid in H_20 (70:30 v/v)
Flow Rate: 1.2 mL/min
Temperature: Ambient
Detection: UV-VIS, 478 nm

Analytes

1. Norbixin
2. 9'-trans-Bixin
3. 9'-cis-Bixin



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Annatto - An orange-red condiment and food colouring derived from the seeds of the achiote tree.

Anthocyanins from *Sambucus Nigra* (Elderberry)

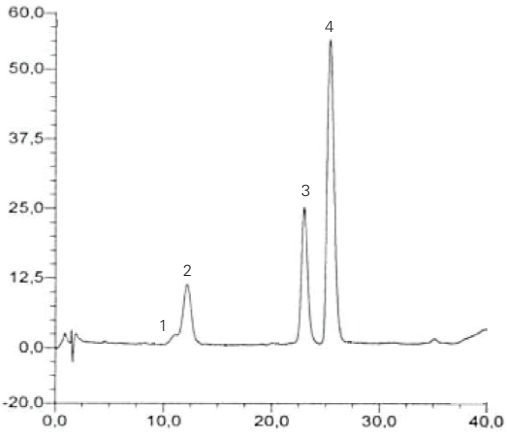
Application #AN2750

Conditions

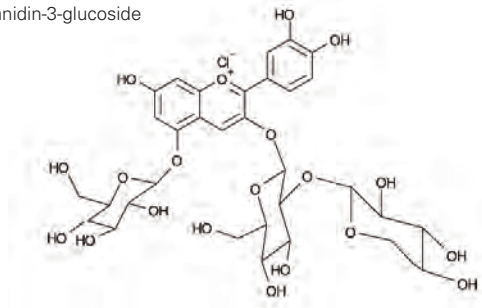
Column:	ACE UltraCore 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	CORE-5A-1546U
Mobile Phase:	A: 5% formic acid in H_2O
	B: MeOH
Gradient:	**Time (mins) %B**
	0 5
	35 10
	55 65
	65 65
Flow Rate:	1 mL/min
Temperature:	40 °C
Detection:	UV-Vis, 525 nm

Analytes

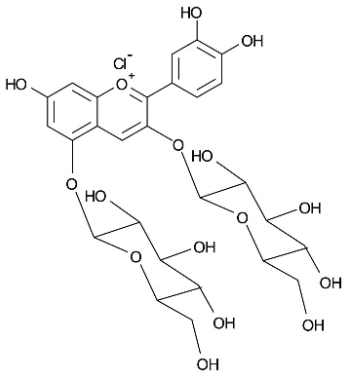
1. Cyanidin-3-sambubioside-5-glucoside
2. Cyanidin-3,5-diglucoside
3. Cyanidin-3-sambubioside
4. Cyanidin-3-glucoside



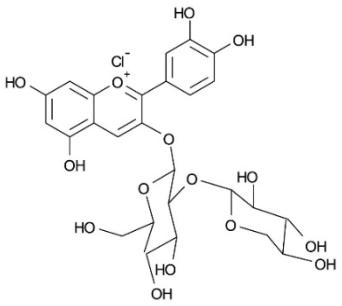
Reproduced with permission of University of Vila Real, Portugal



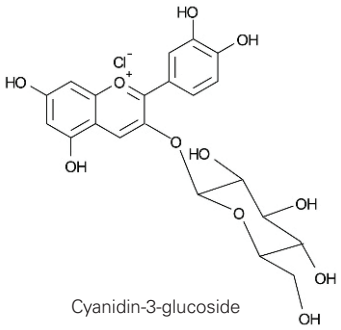
Cyanidin-3-sambubioside-5-glucoside



Cyanidin-3,5-diglucoside



Cyanidin-3-sambubioside



Cyanidin-3-glucoside

Antihistamines

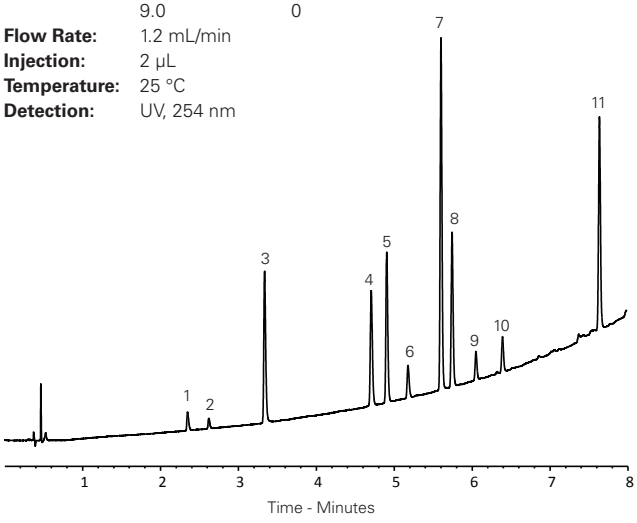
Application #AN1400

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)
Gradient:	**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

Analytes

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



Antihistamines and Expectorants

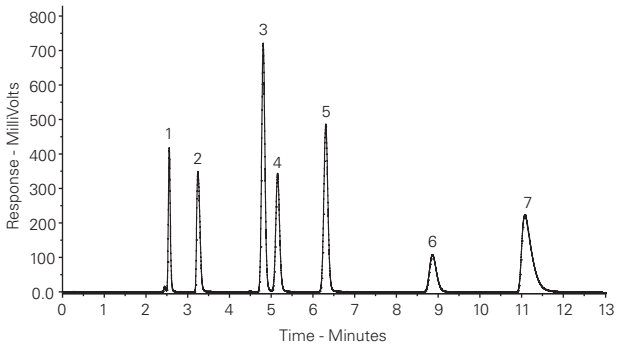
Application #AN3190

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	MeOH/50 mM KH_2PO_4 (pH 3.0) (50:50 v/v)
Flow Rate:	1.0 mL/min
Temperature:	22 °C
Detection:	UV, 220 nm

Analytes

1. Maleic acid
2. Norephedrine
3. Salicylamide
4. Guaifenesin
5. Guaiacol
6. Chlorpheniramine maleate
7. Dextromethorphan



Antihistamines and Expectorants – Mobile Phase Effects

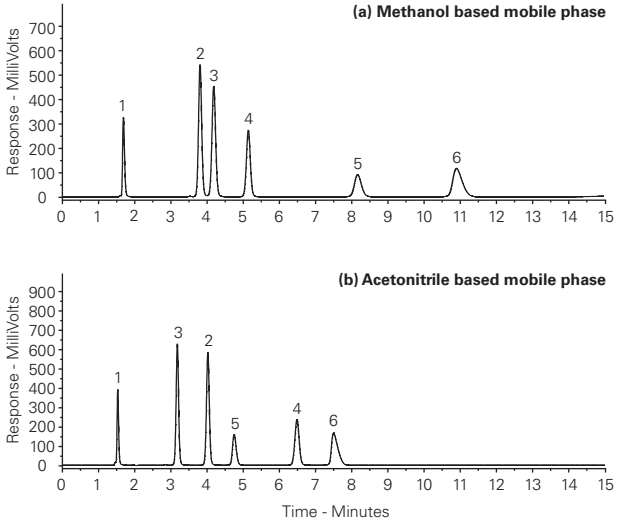
Application #AN3960

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: (a) MeOH/50 mM KH_2PO_4 (pH 3.0) (45:55 v/v)
(b) MeCN/50 mM KH_2PO_4 (pH 3.0) (28:72 v/v)
Flow Rate: 1.0 mL/min
Temperature: Ambient
Detection: UV, 220 nm

Analytes

1. Maleic acid
2. Salicylamide
3. Guaifenesin
4. Guaiacol
5. Chlorpheniramine maleate
6. Dextromethorphan



Antihistamines – Fast Analysis

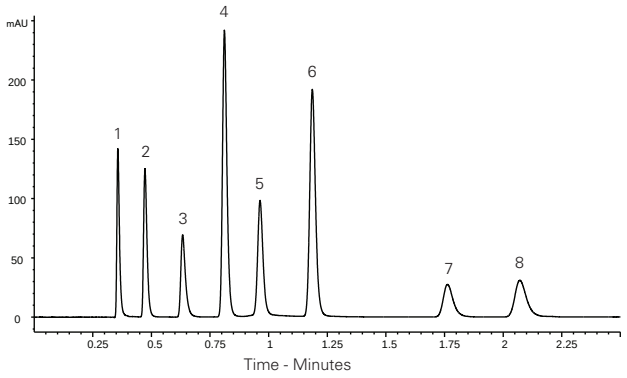
Application #AN4290

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: 30 mM KH_2PO_4 pH 2.7 in H_2O/MeOH (60:40 v/v)
Flow Rate: 0.85 mL/min
Injection: 0.9 µL
Temperature: 30 °C
Detection: UV, 214 nm

Analytes

1. Maleic acid
2. Norephedrine
3. Doxylamine
4. Salicylamide
5. Guaifenesin
6. Guaiacol
7. Chlorpheniramine
8. Triprolidine



Anti-Ulcer Drugs in Basic Mobile Phase Conditions

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)

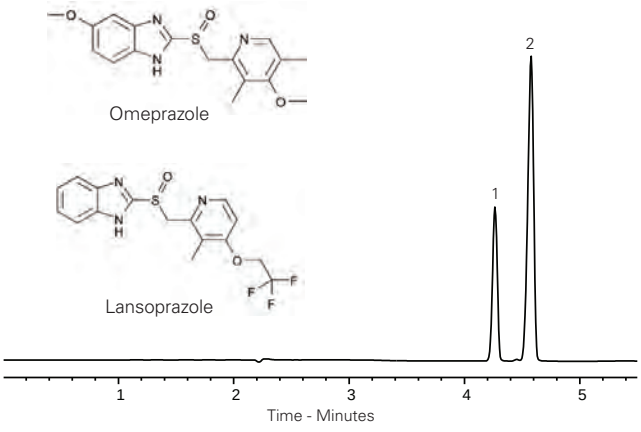
Gradient:

Time (mins)	%B
0	10
5	90

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

Analytes

1. Omeprazole
2. Lansoprazole



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Antimycins from Marine Sponge *Streptomyces* sp. by LC-HRMS

Application #AN4380

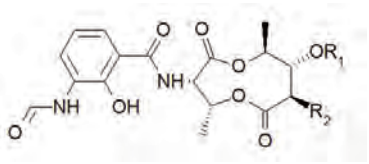
Conditions

Column: ACE 5 C18
Dimensions: 75 x 3.0 mm
Part Number: ACE-121-7503
Mobile Phase: A: 0.1% (v/v) formic acid in H_2O
B: 0.1% (v/v) formic acid in MeCN

Gradient:

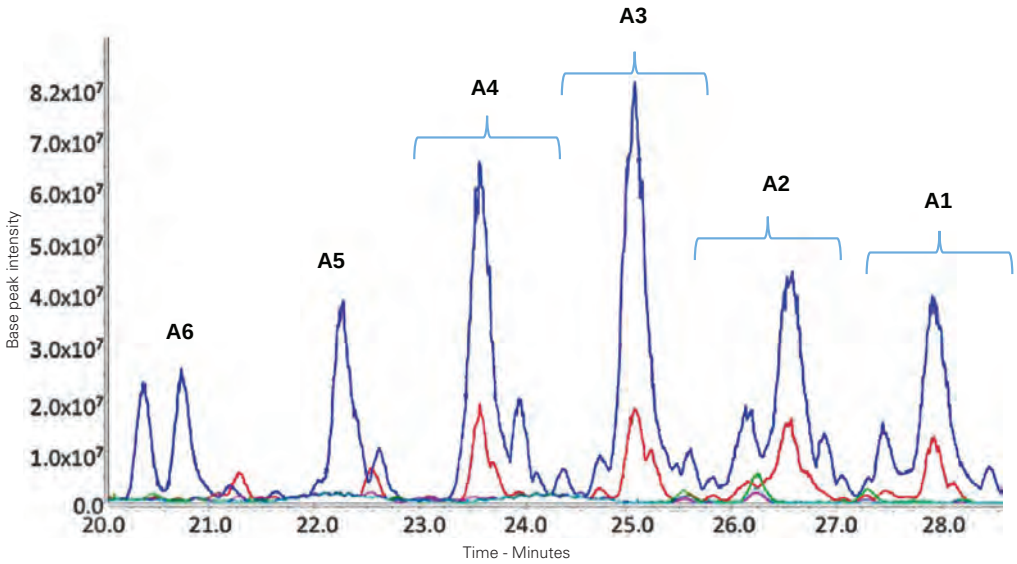
Time (mins)	%B
0	10
30	100
35	100

Flow Rate: 0.3 mL/min
Injection: 10 µL
Detection: Thermo Exactive Orbitrap
High resolution (15,000)
ESI in positive ion mode
Spray Voltage: 4.5 kV
Capillary Temperature: 268 °C
Capillary Voltage: 30 V
Sample: Antifungal fraction from *Streptomycin* sp.
SM8 extract from *Haliclona simulans* marine sponge



Antimycin A

Antimycin	R_1	R_2
A1a	$C{=}OCH(CH_3)CH_2CH_3$	$(CH_2)_5CH_3$
A1b	$C{=}OCH_2CH(CH_3)_2$	$(CH_2)_5CH_3$
A2a	$C{=}OCH(CH_3)_2$	$(CH_2)_5CH_3$
A2b	$C{=}OCH_2CH_2CH_3$	$(CH_2)_5CH_3$
A3a	$C{=}OCH(CH_3)CH_2CH_3$	$(CH_2)_3CH_3$
A3b	$C{=}OCH_2CH(CH_3)_2$	$(CH_2)_3CH_3$
A4a	$C{=}OCH(CH_3)_2$	$(CH_2)_3CH_3$
A4b	$C{=}OCH_2CH_2CH_3$	$(CH_2)_3CH_3$
A5	$C{=}OCH_2CH(CH_3)_2$	CH_2CH_3
A6	$C{=}OCH_2CH_2CH_3$	CH_2CH_3



Viegelmann C, Margassery LM, Kennedy J, Zhang T, O'Brien C, O'Gara F, Morrissey JP, Dobson ADW, Edrada-Ebel R. Metabolomic profiling and genomic study of a marine sponge-associated *Streptomyces* sp. Marine Drugs 12, 3323-3351 (2014). doi:10.3390/md12063323

Appetite Suppressants by LC-MS

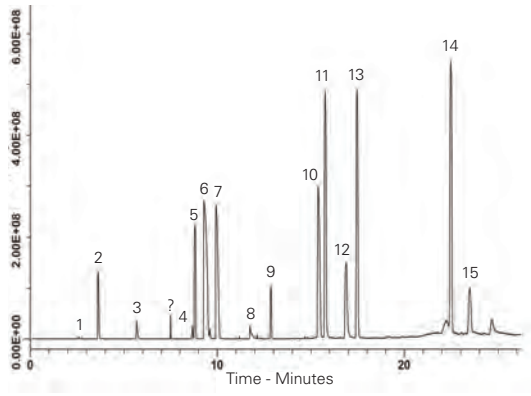
Application #AN1960

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)
Gradient:	**Time (mins) %B** 0.0 11.11 1.0 11.11 21.0 100.00 23.0 100.00
Flow Rate:	0.5 mL/min
Injection:	2 µL
Temperature:	25 °C
Detection:	MS

Analytes

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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Aromatic Nitrobenzenes

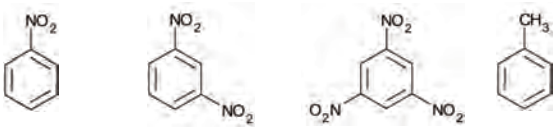
Application #AN2480

Conditions

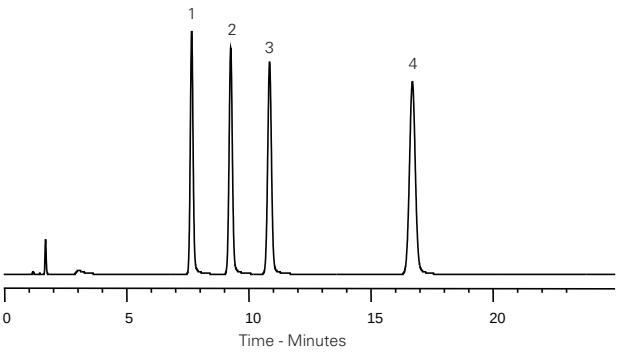
Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	H_2O/MeOH (50:50 v/v)
Flow Rate:	1 mL/min
Temperature:	40 °C
Detection:	UV, 210 nm

Analytes

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



Nitrobenzene 1,3-Dinitrobenzene 1,3,5-Trinitrobenzene Toluene



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

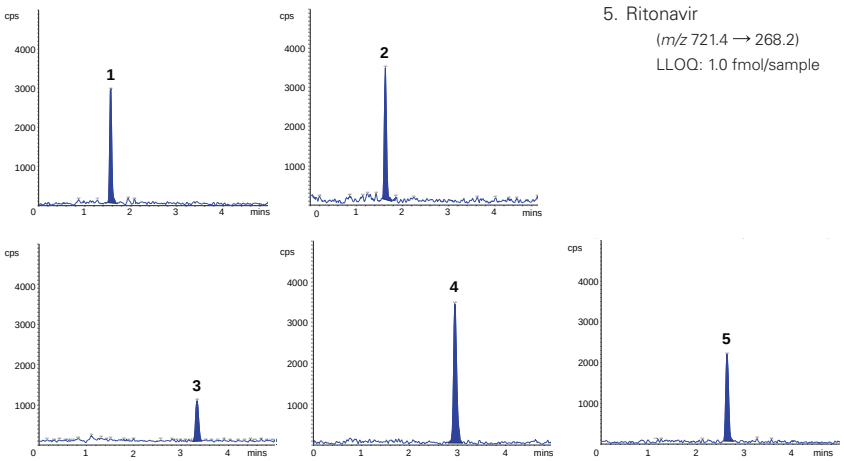
Application #AN3470

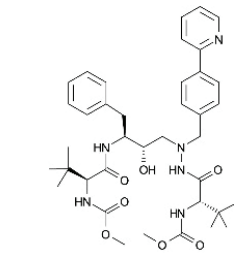
Conditions

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)

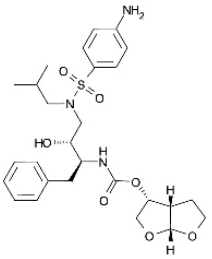
Analytes

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

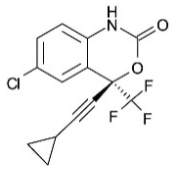




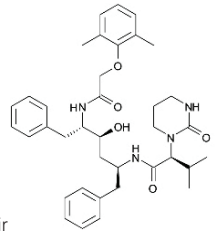
Atazanavir



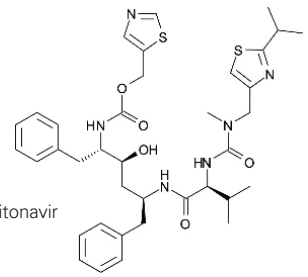
Darunavir



Efavirenz



Lopinavir



Ritonavir

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Arsenolipids from Edible Seaweed *(Alaria Esculenta)* by LC-ICP-MS and LC-ESI-MS

Application #AN1970

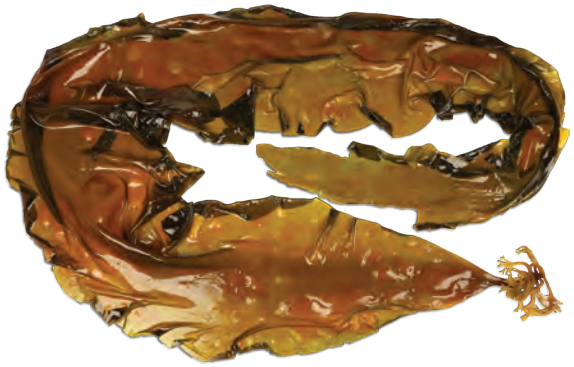
Conditions

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: 0.1% formic acid in MeOH

Gradient:

Time (mins)	%B
0	0
20	100
45	100

Flow Rate: 1 mL/min
Injection: 100 µL
Temperature: 45 °C
Detection: Split ratio: 75% ESI-MS: 25% ICP-MS
Thermo Scientific Element 2 ICP-MS
Mode: Organic mode
Medium resolution
Thermo Scientific Orbitrap Discovery
Positive ESI mode
Spray voltage: 4.5 kV
Capillary temperature: 320 °C
Capillary voltage: 42 V



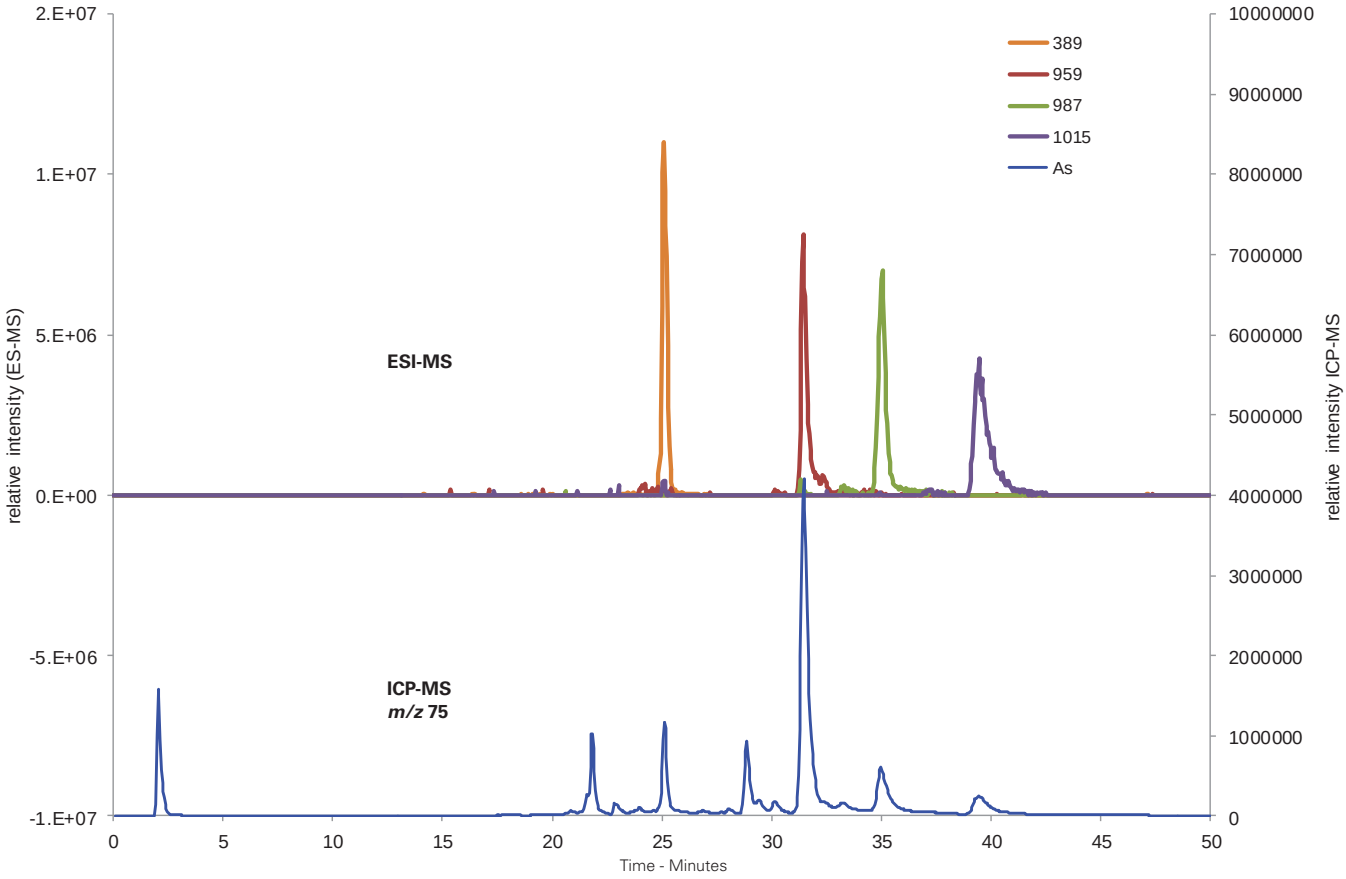
Alaria esculenta is an edible seaweed. It is a traditional food found along the coasts of the far north Atlantic Ocean.

Arsenic-containing hydrocarbon:

***m/z* 389** $[M + H]^+$ for $C_{21}H_{46}AsO$

Arsenic-containing phospholipids:

***m/z* 959** $[M + H]^+$ for $C_{45}H_{89}AsO_{14}P$ (C16:0/C16:0)
***m/z* 987** $[M + H]^+$ for $C_{47}H_{93}AsO_{14}P$ (C18:0/C16:0)
***m/z* 1015** $[M + H]^+$ for $C_{49}H_{97}AsO_{14}P$ (C20:0/C16:0)



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Artemisinin

Application #AN3140

Conditions

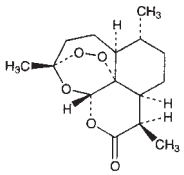
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: H_2O
	B: MeOH

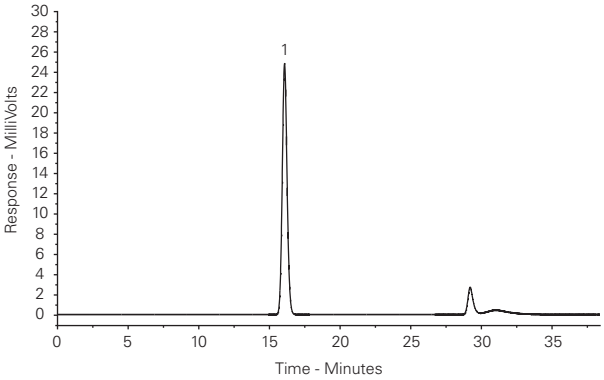
Gradient:	**Time (mins)**	**%B**
	0	50
	25	100
	35	100

Flow Rate:	1.0 mL/min
Injection:	20 µL
Temperature:	20 °C
Detection:	ELSD

Analyte

1. Artemisinin





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Artificial Food Colours

Application #AN2960

Conditions

Column:	ACE 3 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-111-1046
Mobile Phase:	A: 3.1 mM TBAB[1] and 5 mM KH_2PO_4 in H_2O
	B: 5 mM KH_2PO_4 in MeOH

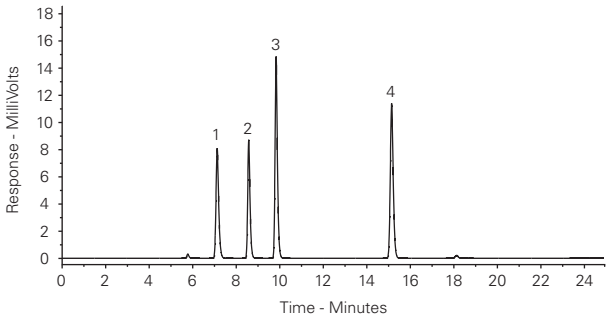
Gradient:	**Time (mins)**	**%B**
	0	45
	12	60
	25	45

Flow Rate:	0.8 mL/min
Injection:	10 µL
Temperature:	Ambient
Detection:	UV-VIS, 480 nm

[1] Tetrabutylammonium bromide

Analytes

1. Tartrazine
2. Amaranth
3. Sunset Yellow
4. Ponceau 4R



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Artificial Sweeteners Global Method

Application #AN1980

Conditions

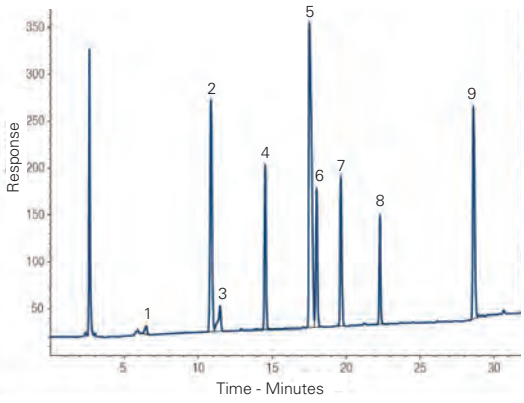
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: H_2O
	B: MeCN
	C: 0.1% TFA

Gradient:	**Time (mins)**	**%A**	**%B**	**%C**
	0	88	2	10
	25	50	40	10
	30	30	60	10
	35	88	2	10

Flow Rate:	1 mL/min
Injection:	50 µL
Temperature:	30 °C
Detection:	Corona CAD

Analytes

1. Acesulfame K
2. Cyclamate
3. Saccharin
4. Sucralose
5. Aspartame
6. Neotame
7. Alitame
8. Neohesperidin dihydrochalcone
9. Dulcin



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Artificial Sweeteners (Stevia Glycosides)

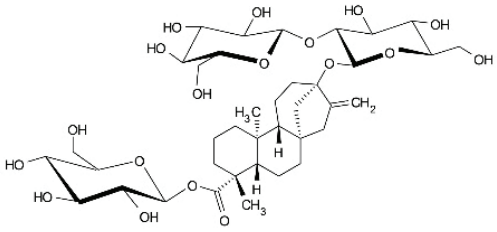
Application #AN1020

Conditions

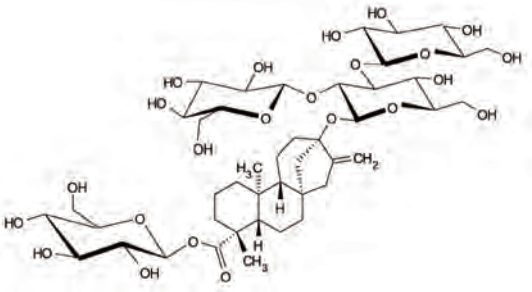
Column:	ACE Excel 2 SuperC18
Dimensions:	150 x 2.1 mm
Part Number:	EXL-1011-1502U
Mobile Phase:	A: 10 mM sodium dihydrogen phosphate pH 2.8 in H_2O
	B: 10 mM sodium dihydrogen phosphate pH 2.8 in H_2O/MeCN (20:80 v/v)
Gradient:	**Time (mins) %B**
	0 39.5
	4 48.0
Flow Rate:	0.6 mL/min
Injection:	1 µL
Temperature:	50 °C
Detection:	UV, 200 nm

Analytes

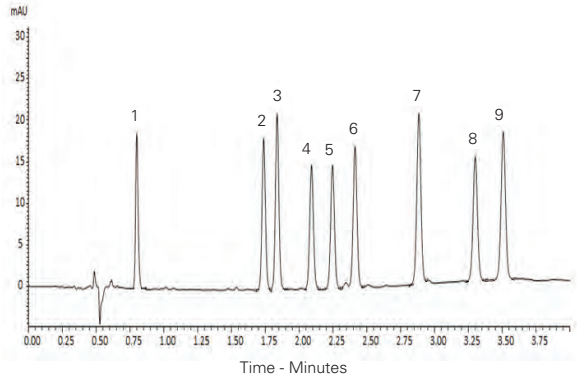
1. Rebaudioside D
2. Rebaudioside A
3. Stevioside
4. Rebaudioside F
5. Rebaudioside C
6. Dulcoside A
7. Rubusoside
8. Rebaudioside B
9. Steviolbioside



Stevioside
MW 804.87



Rebaudioside A
MW 967.01



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Aspirin and Related Substances (I)

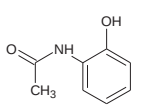
Application #AN1050

Conditions

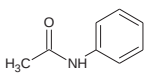
Column:	ACE Excel 3 CN-ES
	ACE Excel 3 C18
	ACE Excel 3 CN
Dimensions:	50 x 2.1 mm
Part Numbers:	EXL-1113-0502U,
	EXL-111-0502U,
	EXL-114-0502U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH
Gradient:	**Time (mins) %B**
	0.00 5
	3.75 38
	5.00 38
Flow Rate:	0.6 mL/min
Temperature:	40 °C
Detection:	UV, 240 nm

Analytes

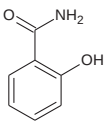
1. 2-Acetamidophenol
2. Acetanilide
3. Salicylamide
4. Aspirin
5. Phenacetin
6. Salicylic acid



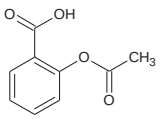
2-Acetamidophenol



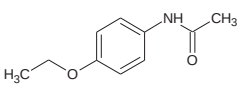
Acetanilide



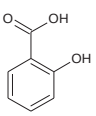
Salicylamide



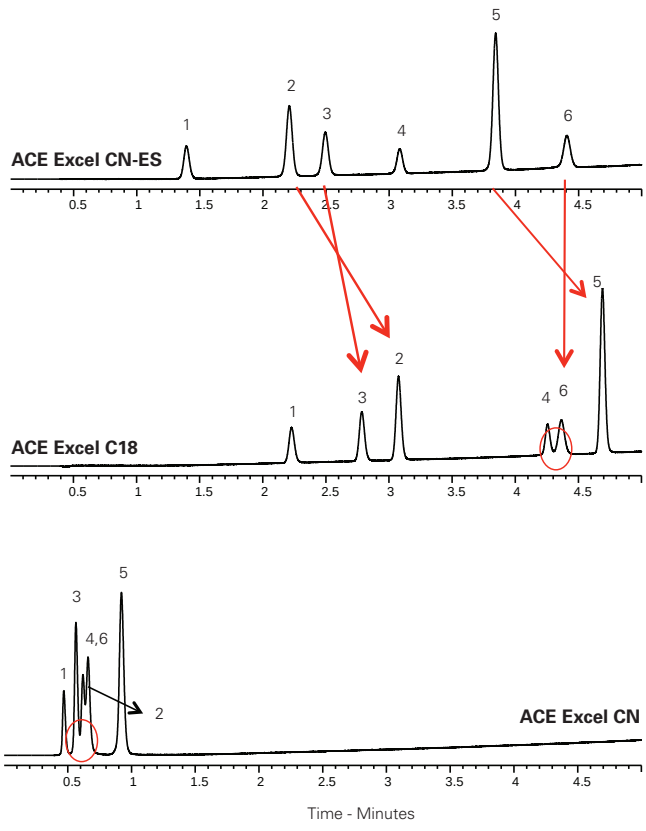
Aspirin



Phenacetin



Salicylic acid



Aspirin and Related Substances (II)

Application #AN2280

Conditions

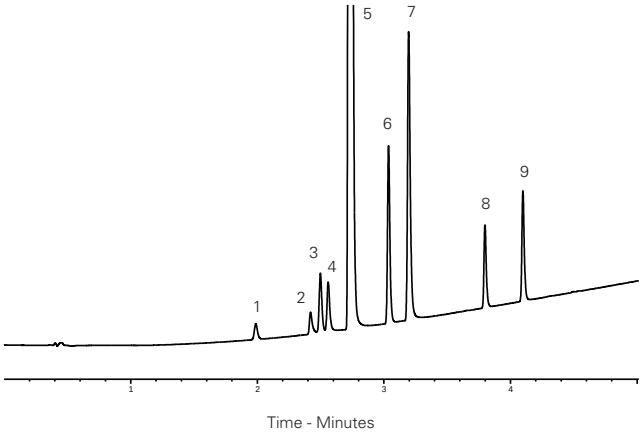
Column:	ACE Excel 1.7 CN-ES
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1713-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0,0	5
	5.0	90
	6.0	90
	6.5	5

Flow Rate:	0.7 mL/min
Injection:	0.5 µL
Temperature:	30 °C
Detection:	UV, 240 nm

Analytes

1. 2-Acetamidophenol
2. 4-Hydroxyisophthalic acid
3. Acetanilide
4. Salicylamide
5. Aspirin
6. Phenacetin
7. Salicylic acid
8. Acetylsalicylsalicylic acid
9. Salsalate



Avenacins

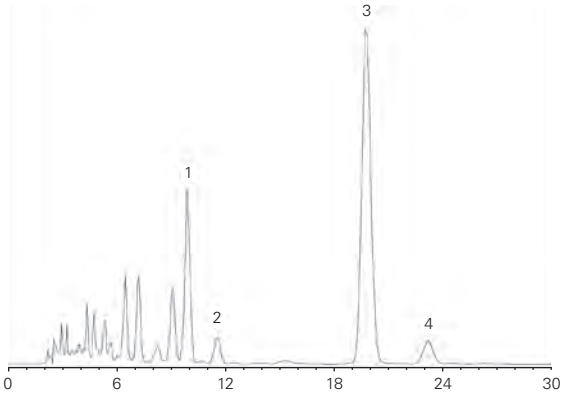
Application #AN2740

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	H_2O/MeOH (30:70 v/v)
Flow Rate:	1.0 mL/min
Temperature:	Ambient
Detection:	UV, 225 nm
Sample:	Partially purified extract from oat root

Analytes

1. Avenacin A-2
2. Avenacin B-2
3. Avenacin A-1
4. Avenacin B-1



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β-Antagonists and Diuretics

Application #AN1410

Conditions

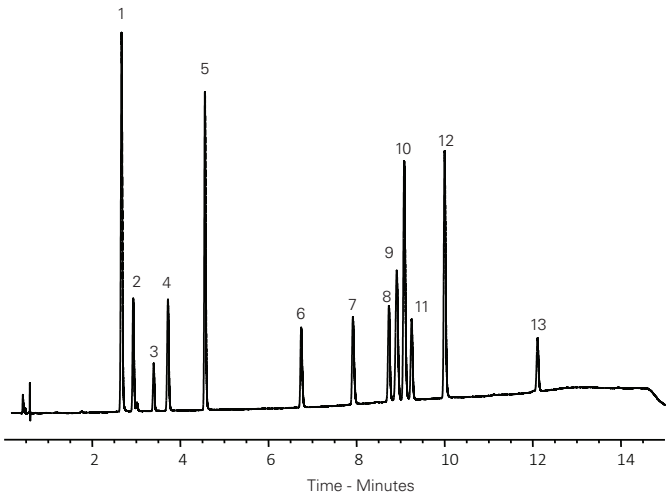
Column:	ACE 3 C18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-111-1002
Mobile Phase:	A: 20 mM KH_2PO_4, pH 2.7
	B: 20 mM KH_2PO_4, pH 2.7
	in MeCN/H_2O (65:35 v/v)

Gradient:	**Time (mins)**	**%B**
	0	5
	1	5
	12	95
	13	95
	14	5
	17	5

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

Analytes

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



β-Blockers at High pH

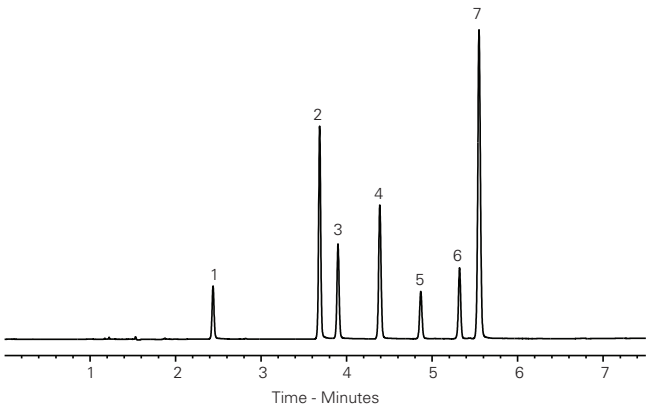
Application #AN1420

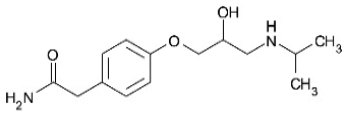
Conditions

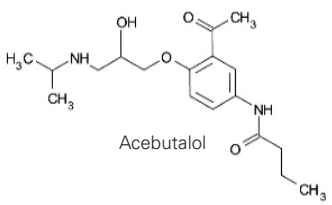
Column:	ACE Excel 5 SuperC18	
Dimensions:	150 x 4.6 mm	
Part Number:	EXL-1211-1546U	
Mobile Phase:	A: 0.1% ammonia in H_2O	
	B: 0.1% ammonia in MeCN	
Gradient:	**Time (mins)**	**%B**
	0.0	30
	5.0	90
	7.0	90
	7.5	30
	22.5	30
Flow Rate:	1 mL/min	
Injection:	5 µL	
Temperature:	35 °C	
Detection:	UV, 230 and 254 nm	

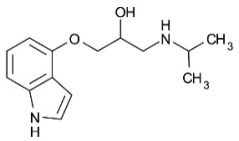
Analytes

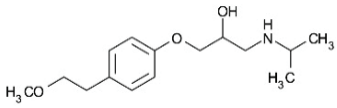
1. Atenolol
2. Acebutalol
3. Pindolol
4. Metoprolol
5. Oxprenolol
6. Carvedilol
7. Propranolol

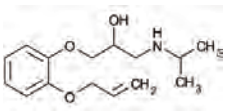


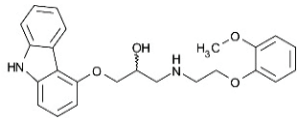

Atenolol

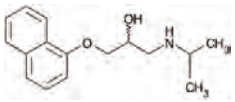

Acebutalol


Pindolol


Metoprolol


Oxprenolol


Carvedilol


Propranolol

β-Blockers at High pH – Fast Analysis

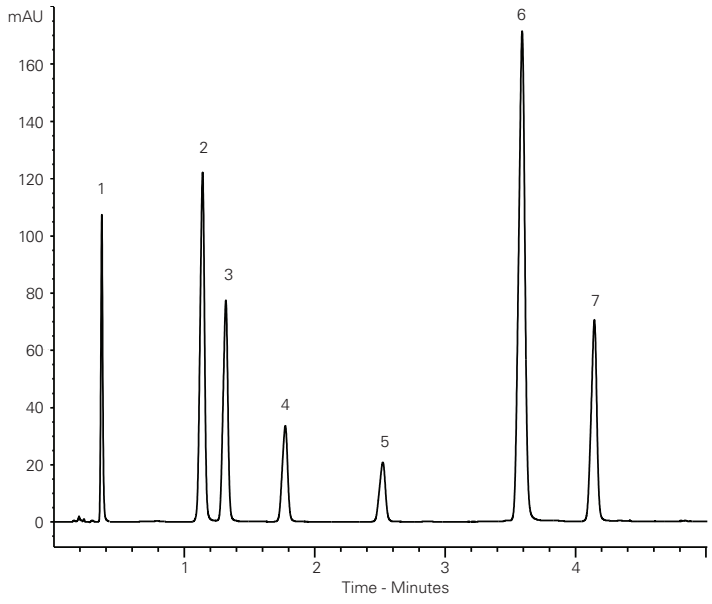
Application #AN2160

Conditions

Column:	ACE Excel 1.7 SuperC18	
Dimensions:	50 x 3.0 mm	
Part Number:	EXL-1711-0503U	
Mobile Phase:	A: 0.1% ammonia in H_2O	
	B: 0.1% ammonia in MeCN	
Gradient:	**Time (mins)**	**%B**
	0.0	30
	4.3	55
	5.0	55
	6.0	30
	9.0	30
Flow Rate:	1 mL/min	
Injection:	0.7 µL	
Temperature:	20 °C	
Detection:	UV, 230 nm	

Analytes

1. Atenolol
2. Acebutalol
3. Pindolol
4. Metoprolol
5. Oxprenolol
6. Carvedilol
7. Propranolol



β-Blockers by LC-MS/MS

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

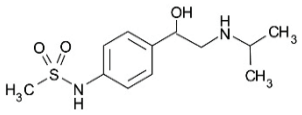
Gradient:

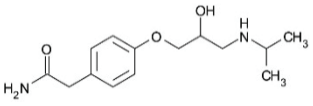
Time (mins)	%B
0.0	10
3.0	50
3.1	10

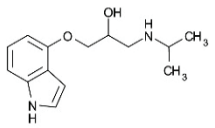
Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: MS/MS ESI in positive ion mode
Sample: 2.5 pg/µL

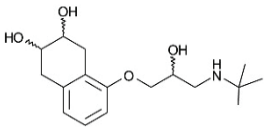
Analytes

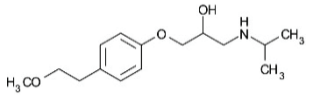
1. Sotalol (*m/z* 272.9 → 212.8)
2. Atenolol (*m/z* 267.0 → 189.8)
3. Pindolol (*m/z* 248.9 → 115.8)
4. Nadolol diastereomers (*m/z* 310.0 → 253.9)
5. Metoprolol (*m/z* 268.0 → 115.8)
6. Labetalol (*m/z* 329.1 → 161.8)
7. Propranolol (*m/z* 260.0 → 115.7)
8. Alprenolol (*m/z* 250.0 → 115.8)

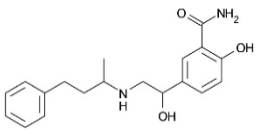

Sotalol

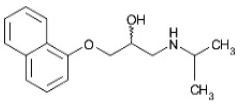

Atenolol

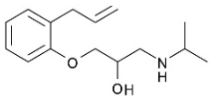

Pindolol

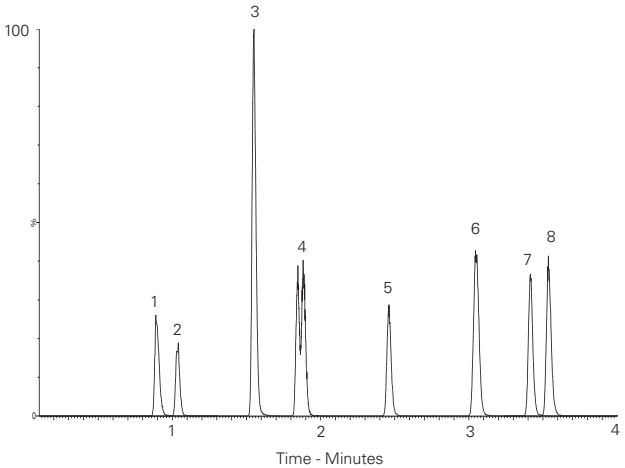

Nadolol diastereomers


Metoprolol


Labetalol


Propranolol


Alprenolol



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β-Blockers

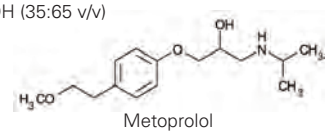
Application #AN3160

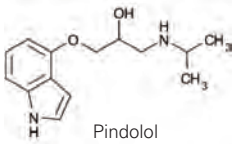
Conditions

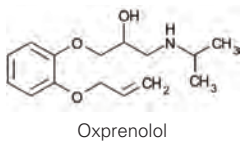
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM 1-methylpiperidine pH 11/MeOH (35:65 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 215 nm

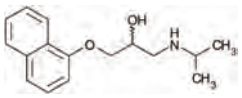
Analytes

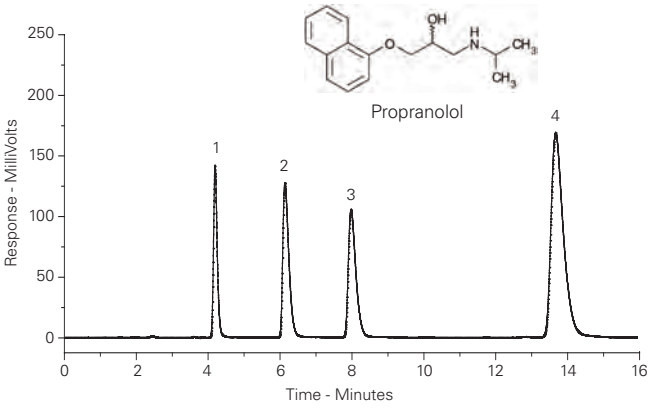
1. Pindolol
2. Metoprolol
3. Oxprenolol
4. Propranolol


Metoprolol


Pindolol


Oxprenolol


Propranolol



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

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

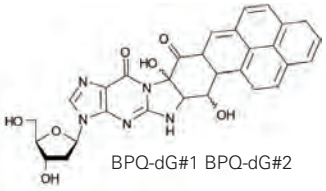
Gradient:

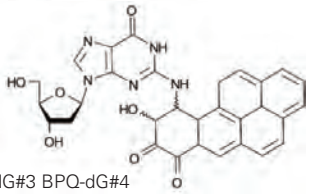
Time (mins)	%B
0	25
8	55

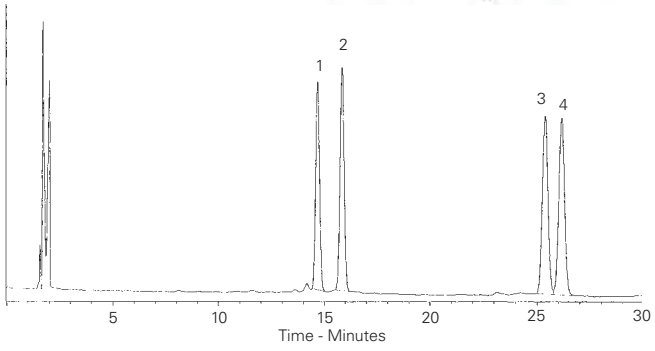
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 35 °C
Detection: UV, 285 nm

Analytes

1. BPQ-dG#1
2. BPQ-dG#2
3. BPQ-dG#3
4. BPQ-dG#4


BPQ-dG#1 BPQ-dG#2


BPQ-dG#3 BPQ-dG#4



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Benzodiazepines from Drugs of Abuse Screen (#AN2190)

Application #AN2370

Conditions

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

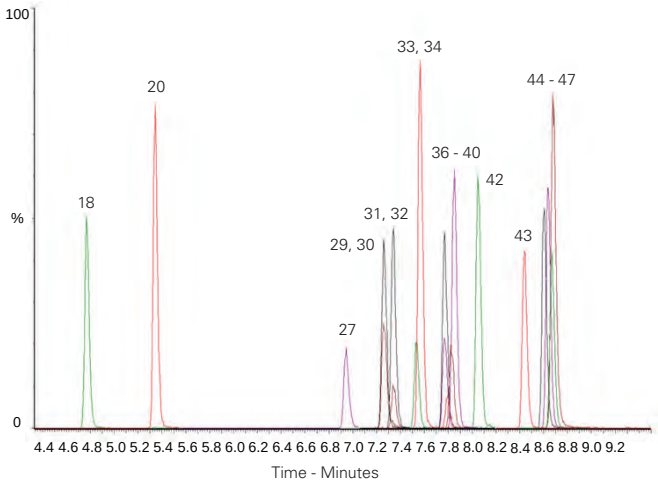
Gradient:

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

Flow Rate: 0.3 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: MS Quattro Premier XE triple quad
MRM, positive and negative ESI mode
Desolvation temperature: 450 °C
IonSource temperature: 150 °C
Collision gas pressure: 3.5 x10^{-3} mbar

Analytes

18. 7-Amino-clonazepam (*m/z* 286.2 → 121.0)
20. 7-Amino-flunitrazepam (*m/z* 284.2 → 135.0)
27. Bromazepam (*m/z* 316.1 → 182.1)
29. Clonazepam (*m/z* 316.1 → 270.1)
30. Nitrazepam (*m/z* 282.2 → 236.1)
31. α-Hydroxytriazolam (*m/z* 359.1 → 331.1)
32. Flunitrazepam (*m/z* 314.2 → 268.2)
33. α-Hydroxyalprazolam (*m/z* 325.2 → 297.1)
34. Estazolam (*m/z* 295.2 → 267.2)
36. Triazolam (*m/z* 343.0 → 308.1)
37. 2-Hydroxyethylflurazapam (*m/z* 333.2 → 109.0)
38. Lorazepam (*m/z* 321.1 → 275.1)
39. Oxazepam (*m/z* 287.2 → 241.0)
40. Alprazolam (*m/z* 309.2 → 281.2)
42. Temazepam (*m/z* 301.1 → 255.1)
43. Nordiazepam (*m/z* 271.1 → 139.9)
44. Midazolam (*m/z* 326.2 → 291.2)
45. Diazepam-d5 (*m/z* 290.2 → 154.0)
46. Diazepam (*m/z* 285.2 → 154.0)
47. Flurazepam (*m/z* 388.2 → 315.1)



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Biomarker Analysis for Gaucher Disease by LC-MS/MS

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)

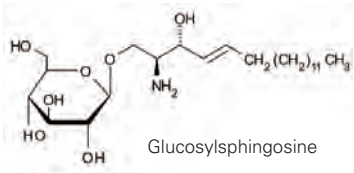
Gradient:

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

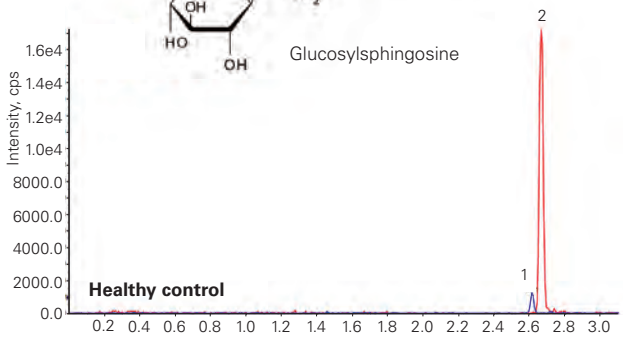
Flow Rate: 0.9 mL/min
Injection: 5 µL
Temperature: 60 °C
Detection: API 4000 triple quad MS
ESI in positive ion mode
Temperature: 500 °C

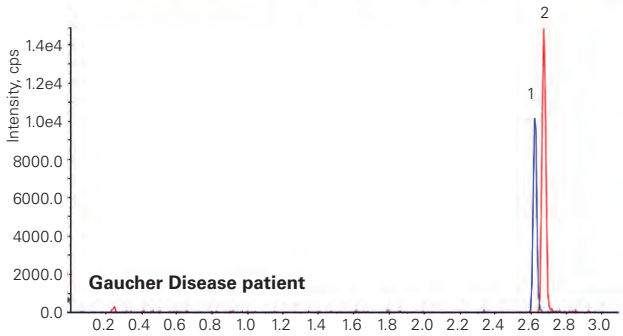
Analytes

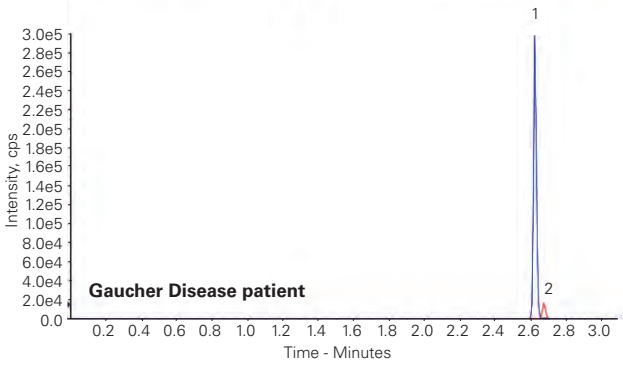
1. Glucosylsphingosine (*m/z* 462 → 282)
2. Lyso-Gb2 (IS) (*m/z* 624 → 282)



Glucosylsphingosine







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

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

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)

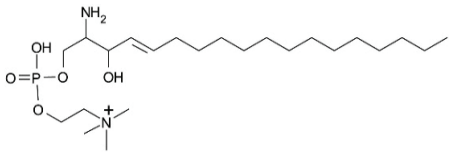
Gradient:

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

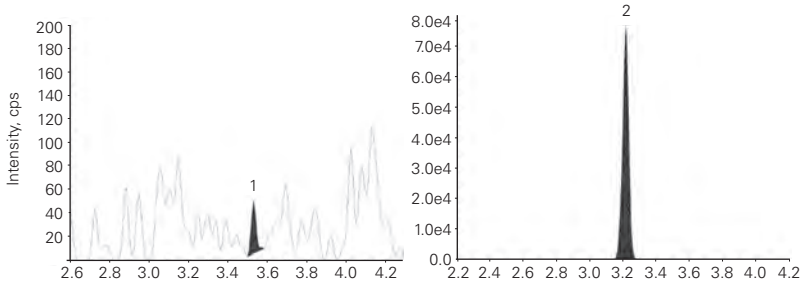
Analytes

1. Lyso-SM-509
   (*m/z* 509 → 184)
2. Lyso-Gb2 (IS)
   (*m/z* 624 → 282)

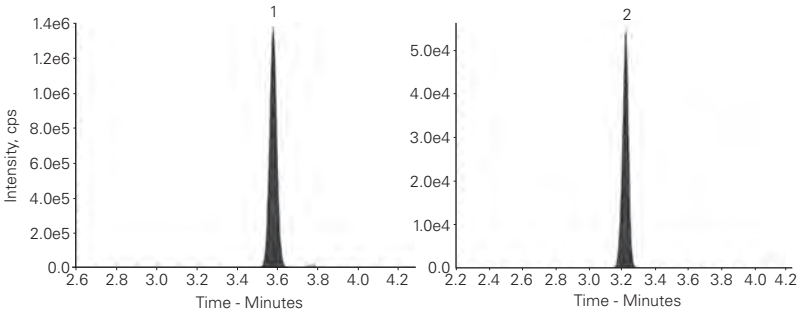


Lyso-SM (lyso-sphingomyelin)

Human Control Plasma



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

Biomarker Profiling

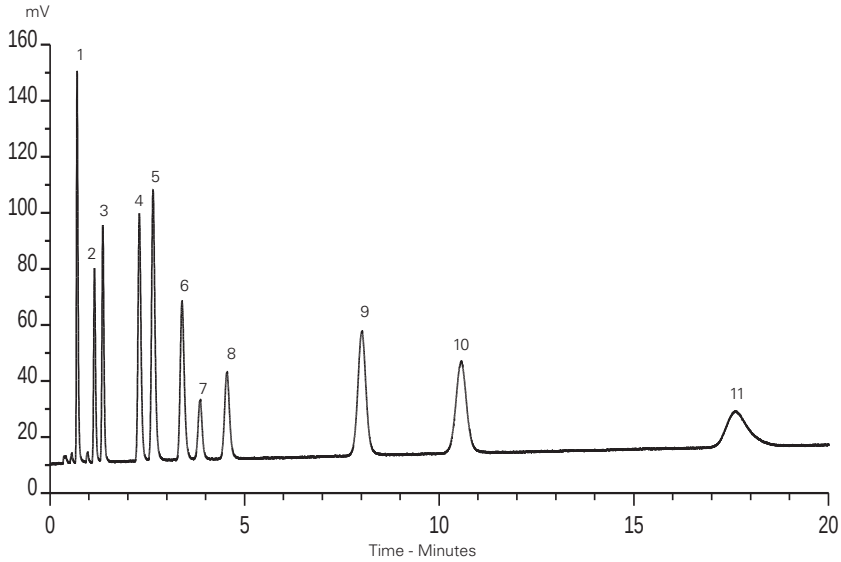
Application #AN1990

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
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

Analytes

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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Brazilian Red Propolis Biomarkers by LC-FTMS

Application #AN3370

Conditions

Column: ACE 5 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-121-1046
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

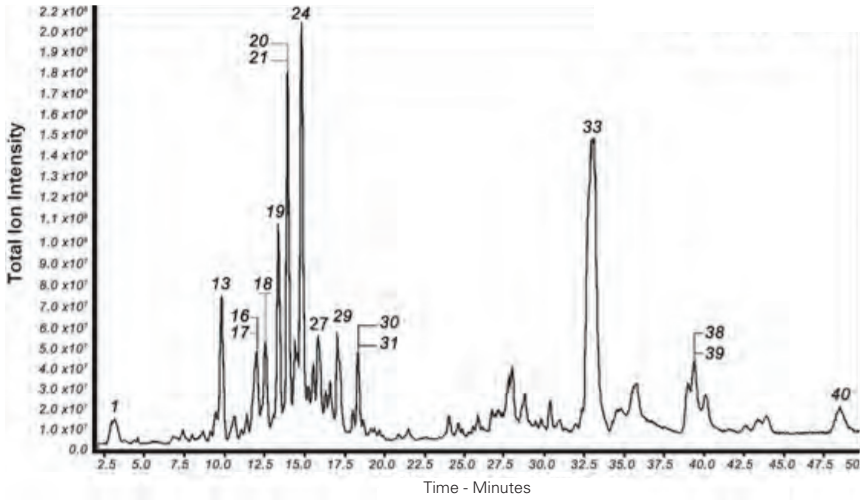
Gradient:

Time (mins)	%B
0	30
6	45
10	60
14	75
18	90
22	100
47	100
52	30
58	30

Flow Rate: 0.3 mL/min
Injection: 10 µL
Detection: Thermo Scientific LC-Orbitrap FTMS
Negative ion mode
Scan range 50-1200 amu
Sample: Ethanolic extract of red propolis

Analytes

1. Caffeic acid
13. Liquiritigenin
16/17. Naringenin/Pinobanksin
19. Isoliquiritigenin
20/21. Formononetin/isoformonetin
24. Vestitol
27. 2′,6′-dihydroxy-4′-methoxydihydrochalcone
29. 3′,4′-di-O-benzyl-7O-(2-hydroxyethyl)-3-O-methylquercetin
30/31. (3S)-7-O-methylvestitol/Calycosin/7,3′-dihydroxy-4′-methoxy-8-methylflavane
33. Cycloartenol/α-amyrin/β-amyrin
38/39. Guttiferone C/Guttiferone D
40. 19-nor-10-keto-25-hydroxyvitamin D3



Reference: de Mendonca et al, BMC Complement Altern Med. 2015; 15: 357. Published online 2015 Oct 14, doi:10.1186/s12906-015-0888-9

Brompheniramine Maleate

Application #AN3150

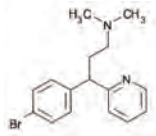
Conditions

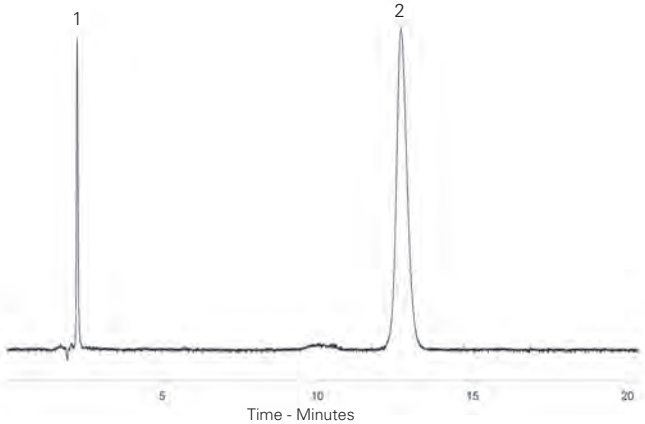
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: 20 mM ammonium formate pH 3.0 in H_2O/MeOH (95:5 v/v)
Flow Rate: 1.0 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV, 265 nm

Analytes

1. Maleic acid
2. Brompheniramine


Maleic acid


Brompheniramine



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BSA Tryptic Digest Profiling

Application #AN2000

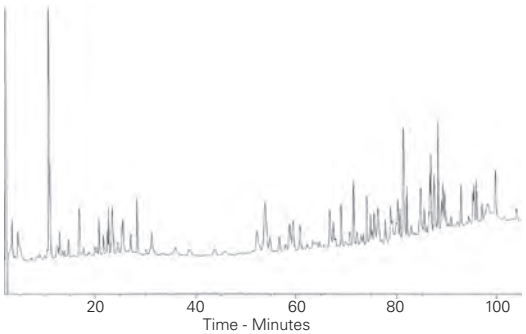
Conditions

Column: ACE 5 C18-300
Dimensions: 150 x 4.6 mm
Part Number: ACE-221-1546
Mobile Phase: A: 1% TFA in H_2O
B: 1% TFA in MeCN/H_2O (1:1 v/v)

Gradient:

Time (mins)	%B
0	4
5	4
25	20
45	20
75	40
95	65
115	70
120	4

Flow Rate: 1.0 mL/min
Temperature: Ambient
Detection: UV, 214 nm



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Bufotenine Extract from *Rhinella Jimi* Toad Skin Secretions

Application #AN3800

Conditions

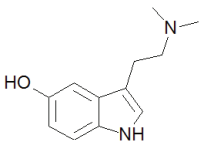
Column: ACE 5 C18
Dimensions: 250 x 7.75 mm (semi-preparative separation) and 250 x 4.6 mm (analytical)
Part Number: ACE-121-2508 and ACE-121-2546
Mobile Phase: A: 0.1% TFA in H_2O
B: 0.1% TFA in H_2O/MeCN (10:90 v/v)

Gradient:	**Semi-Preparative**		**Analytical**	
	Time (mins)	**%B**	**Time (mins)**	**%B**
	0	10	0	13
	35	70	15	15

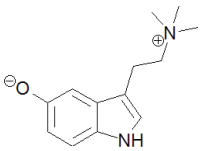
Flow Rate: 1.7 mL/min (semi-preparative) and 1.1 mL/min (analytical)
Temperature: 4 °C
Detection: UV, 214 nm
MS positive ESI mode for peak identification
Sample: Aqueous extract from liquid-liquid partition of toad skin secretion Fraction* from semi-preparative separation injected into analytical system.

Analytes

1. Bufotenine ([M+H]$^+$ *m/z* 205)
2. Bufotenidine (5-HTQ) ([M+H]$^+$ *m/z* 219)

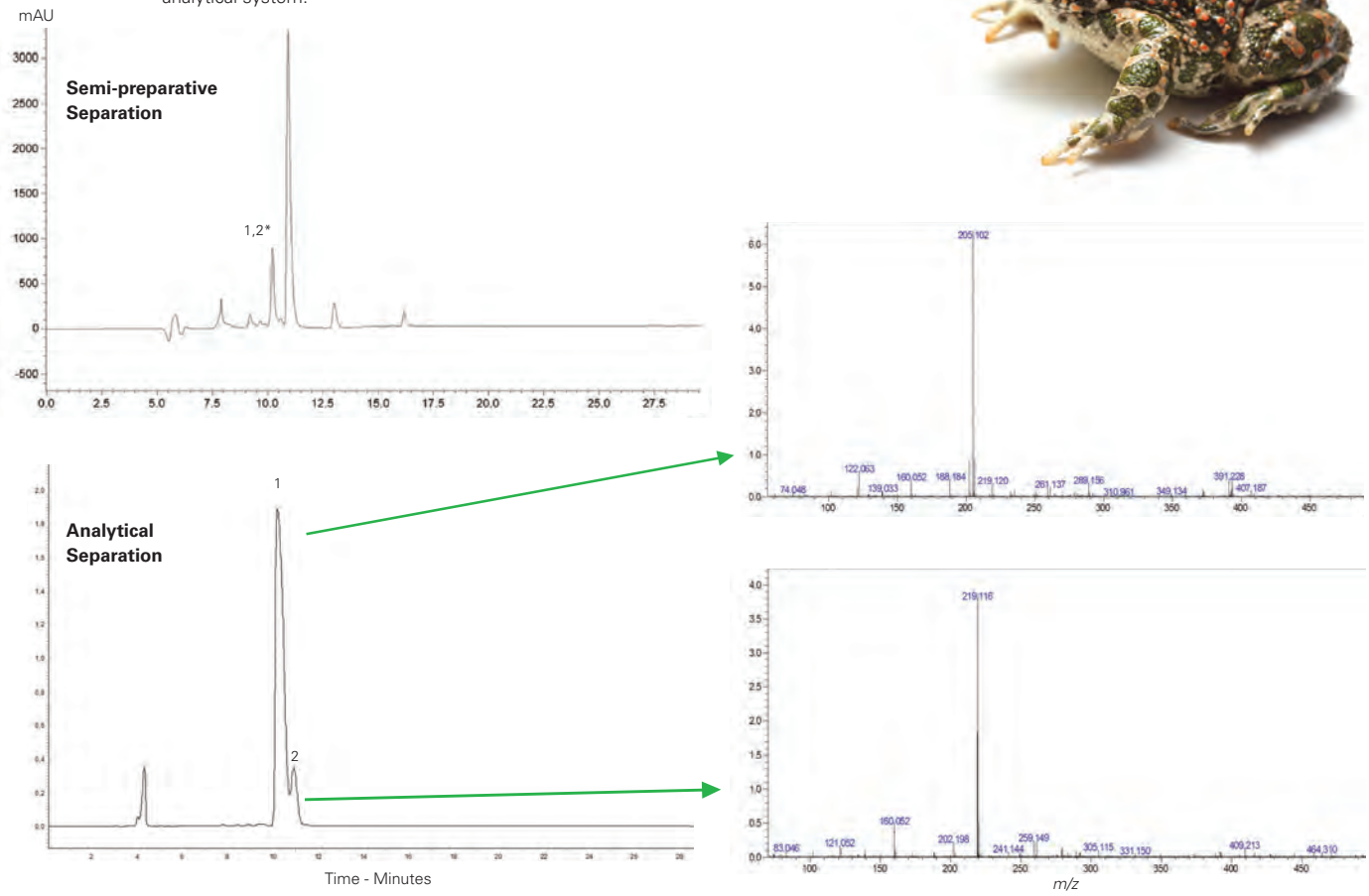


Bufotenine



Bufotenidine (5-HTQ)





Vigerelli H, Sciani JM, Jared C, Antoniazzi MM, Caporale GMM, Rodrigues da Silva A, Pimenta DC. Bufotenine is able to block rabies virus infection in BHK-21 cells. Journal of Venomous Animals and Toxins including Tropical Diseases 2014, 20:45. doi:10.1186/1678-9199-20-45

Caffeine and Metabolites

Application #AN2010

Conditions

Column: ACE Excel 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)

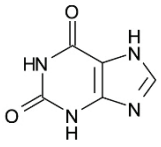
Gradient:

Time (mins)	%B
0	2
45	15
48	15
49	2
59	2

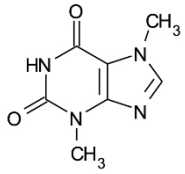
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: 60 °C
Detection: UV, 273 nm

Analytes

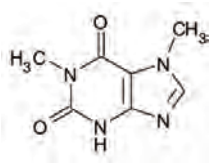
1. Xanthine
2. Theobromine
3. Paraxanthine
4. Theophylline
5. Caffeine



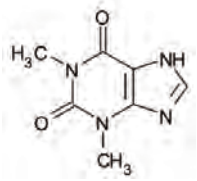
Xanthine



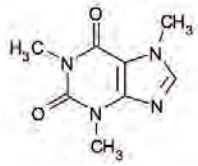
Theobromine



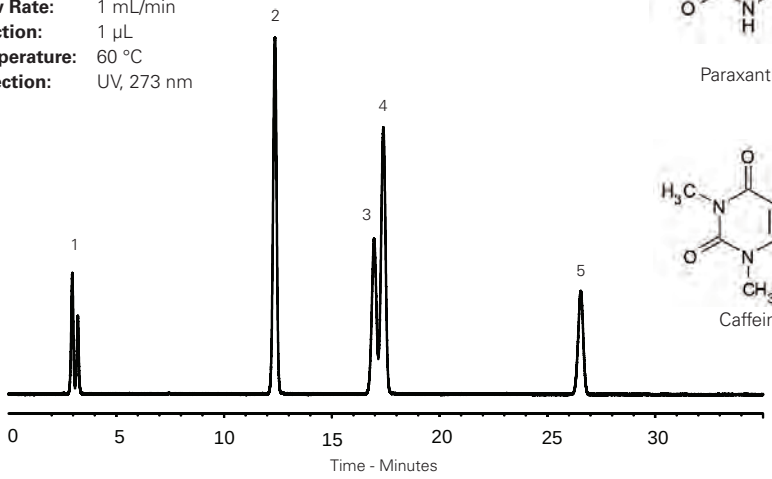
Paraxanthine



Theophylline



Caffeine



Caffeoylquinic and Dicaffeoylquinic Acids

Application #AN3520

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 4.6 mm
Part Number: CORE-25A-1046U
Mobile Phase: A: 0.2% phosphoric acid in H_2O
B: MeCN

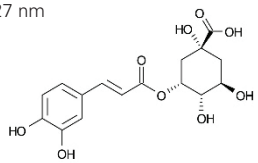
Gradient:

Time (mins)	%B
0	5
1	5
9	18
14	28
15	70

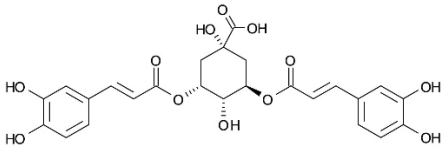
Flow Rate: 0.8 mL/min
Temperature: 35 °C
Detection: UV-Vis, 327 nm

Analytes

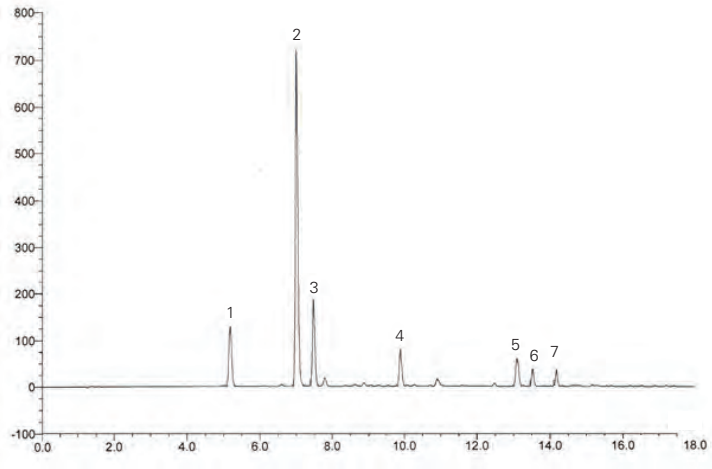
1. 3-Caffeoylquinic acid (chlorogenic acid)
2. 5-Caffeoylquinic acid (neochlorogenic acid)
3. 4-Caffeoylquinic acid (cryptochlorogenic acid)
4. Feruloylquinic acid
5. 3,4-Dicaffeoylquinic acid (isochlorogenic acid B)
6. 3,5-Dicaffeoylquinic acid (isochlorogenic acid A)
7. 4,5-Dicaffeoylquinic acid (isochlorogenic acid C)



5-Caffeoylquinic acid (neochlorogenic acid)



3,5-Dicaffeoylquinic acid (isochlorogenic acid A)



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Cannabinoids (Synthetic) by LC-MS/MS

Application #AN2540

Conditions

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

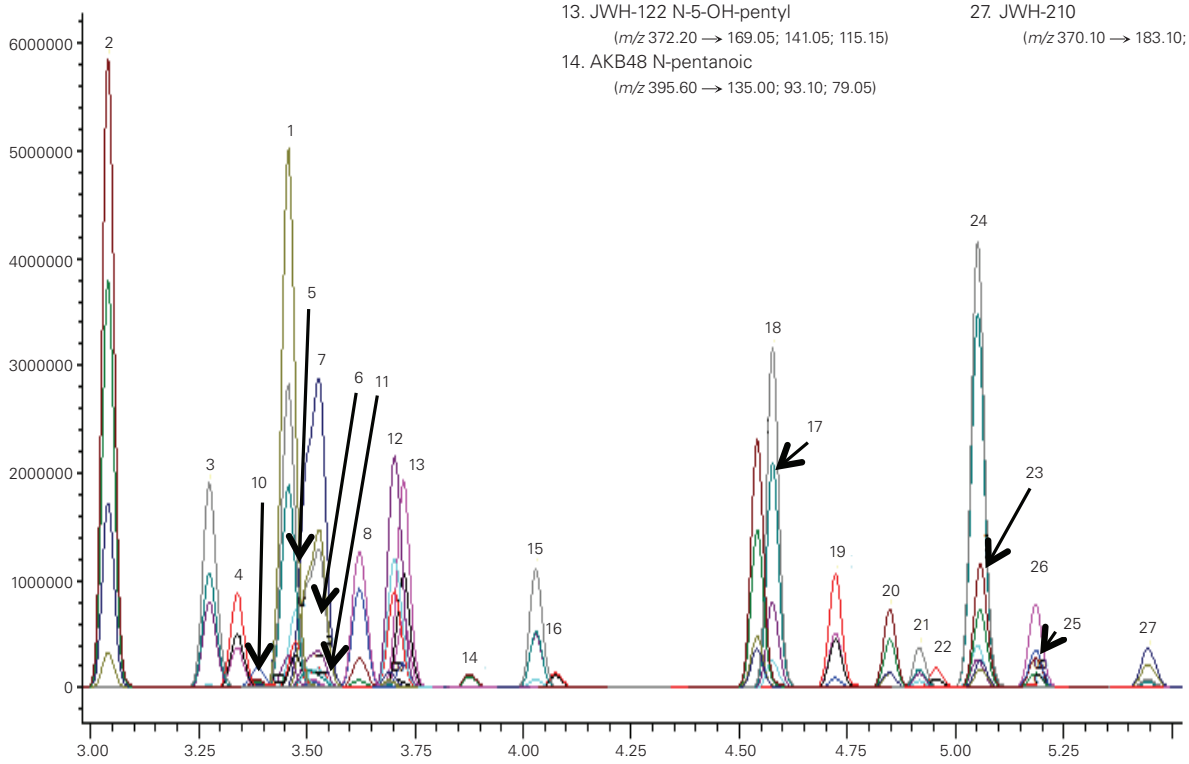
Gradient:

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

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

Analytes

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



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Cannabinoids in Rat Plasma

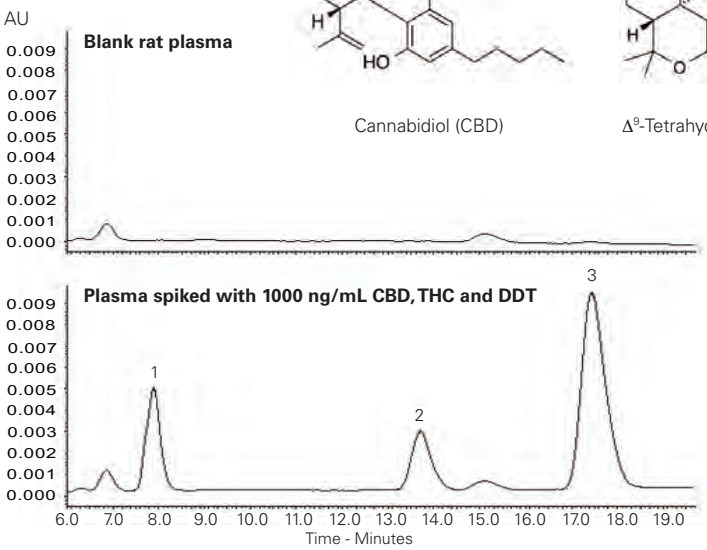
Application #AN2310

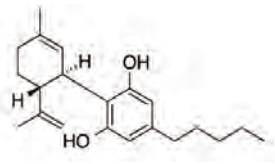
Conditions

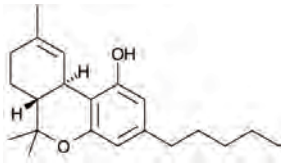
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: H_2O/MeCN (38:62 v/v)
Flow Rate: 1 mL/min
Injection: 30 µL
Temperature: 55 °C
Detection: UV, 220 nm

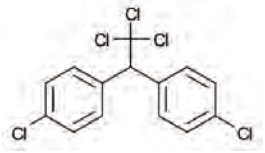
Analytes

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




Cannabidiol (CBD)


Δ^9-Tetrahydrocannabinol (THC)


4,4-Dichlorodiphenyltrichloroethane (DDT) (IS)



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

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Carglumic Acid in Human Plasma by LC-MS/MS

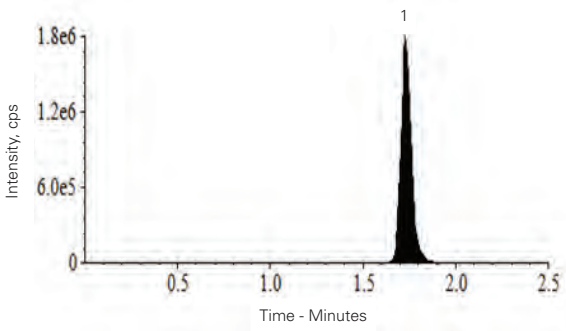
Application #AN3750

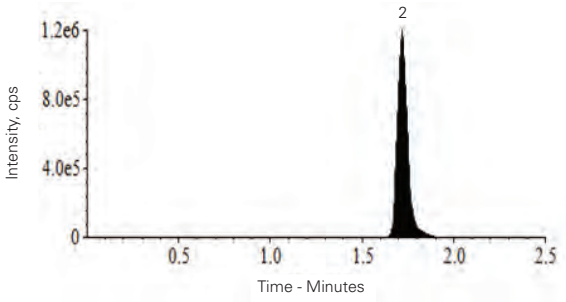
Conditions

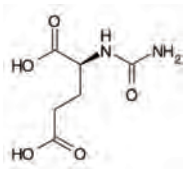
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: MeCN/MeOH/0.1% acetic acid pH 3.2 (40:40:20 v/v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: MDS Sciex API-4000 triple quad MS
Negative ion mode ESI
Ion source temperature: 500 °C
Ion spray voltage: -4500 V
20%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

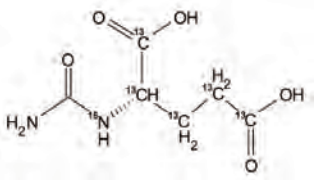
Analytes

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






Carglumic acid


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

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Catechins

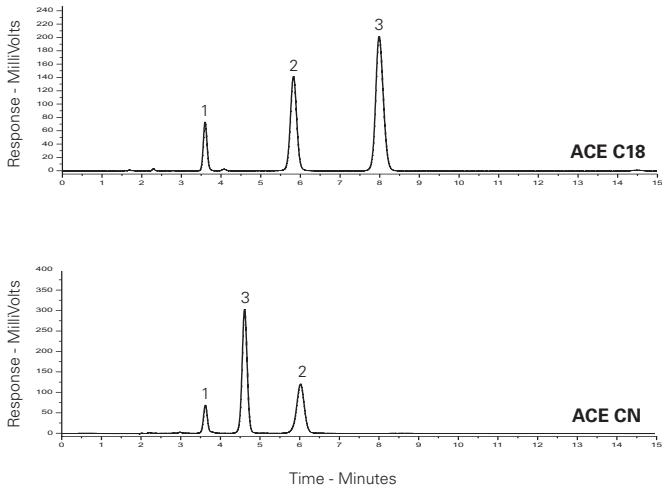
Application #AN3950

Conditions

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

Analytes

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



Catecholamine Analysis (I)

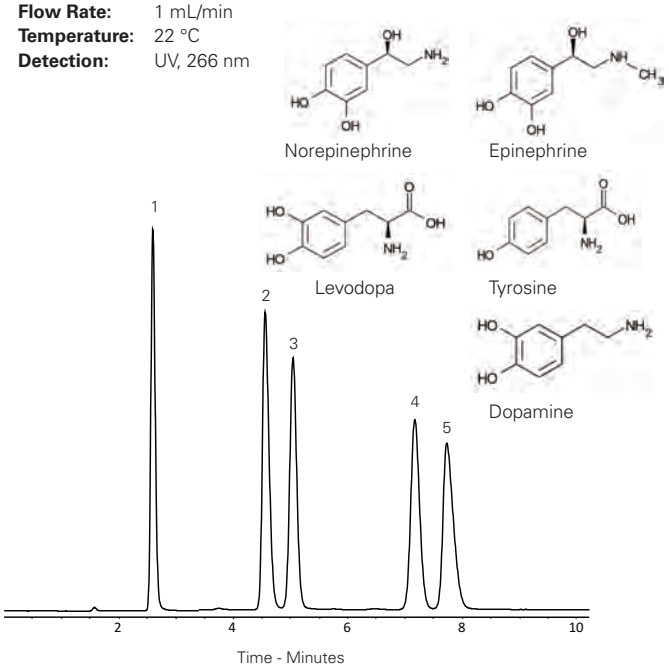
Application #AN2020

Conditions

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

Analytes

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



Catecholamine Analysis (II)

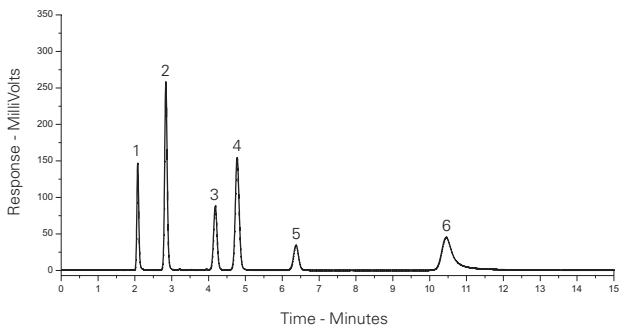
Application #AN3910

Conditions

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

Analytes

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



Catecholamines by LC-MS/MS

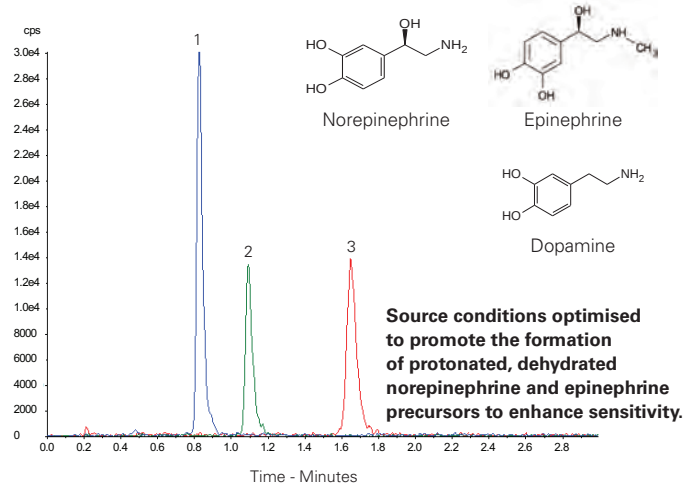
Application #AN2320

Conditions

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

Analytes

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



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

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

Application #AN4040

Conditions

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

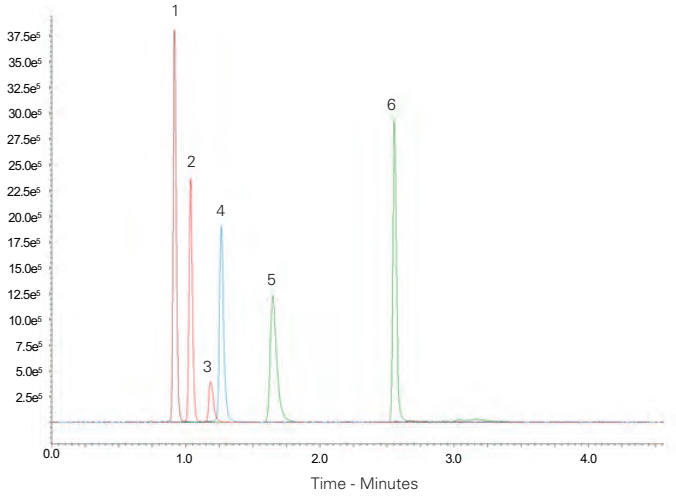
Gradient:

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

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

Analytes

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



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Catecholamines and Metanephrines Separation (Gradient)

Application #AN1480

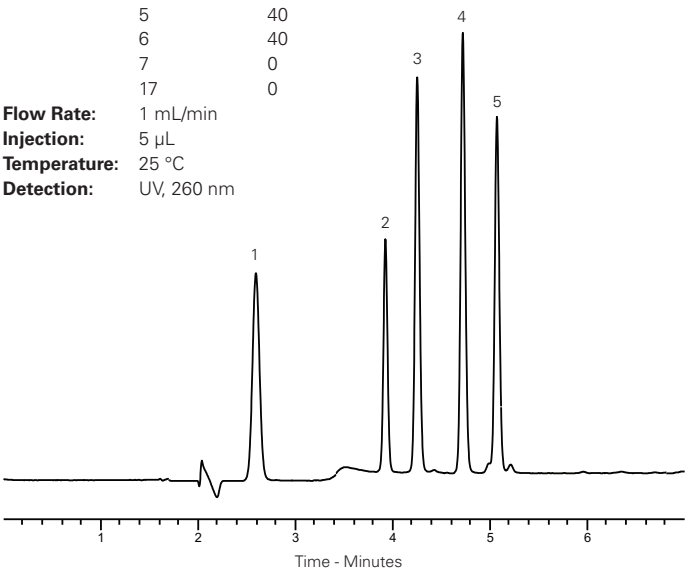
Conditions

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

Gradient:

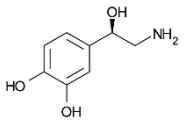
Time (mins)	%B
0	0
5	40
6	40
7	0
17	0

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

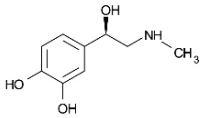


Analytes

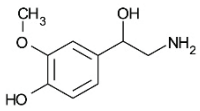
1. Norepinephrine
2. Epinephrine
3. Normetanephrine
4. Dopamine
5. Metanephrine



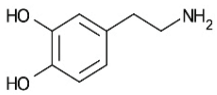
Norepinephrine



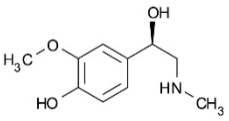
Epinephrine



Normetanephrine



Dopamine



Metanephrine

Catecholamines and Metanephrines Separation (Isocratic)

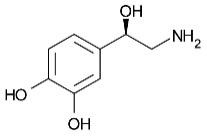
Application #AN1490

Conditions

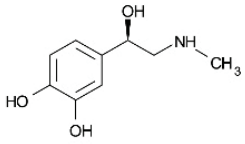
Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: 20 mM ammonium formate pH 3.0 in H_2O
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 260 nm

Analytes

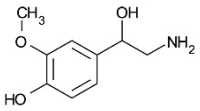
1. Norepinephrine
2. Epinephrine
3. Normetanephrine
4. Dopamine
5. Metanephrine



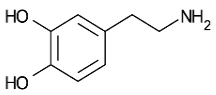
Norepinephrine



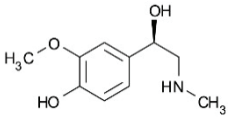
Epinephrine



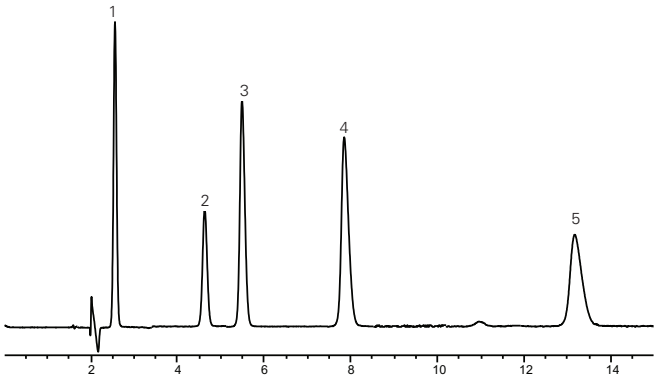
Normetanephrine



Dopamine



Metanephrine



Catecholamines from Plasma

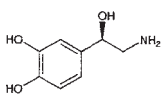
Application #AN3210

Conditions

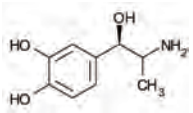
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 50 mM sodium acetate pH 7.0/MeCN/MeOH (50:35:15 v/v/v)
Flow Rate: 0.9 mL/min
Temperature: Ambient
Detection: Fluorescence – λ_{Ex} 350 nm, λ_{Em} 480 nm
Sample: Ion pair extraction using diphenyl-borate-ethanolamine. Derivatisation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

Analytes

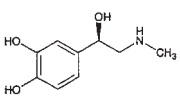
1. Noradrenaline (Norepinephrine)
2. 3,4-Dihydroxynorephedrine (I.S.)
3. Adrenaline (Epinephrine)



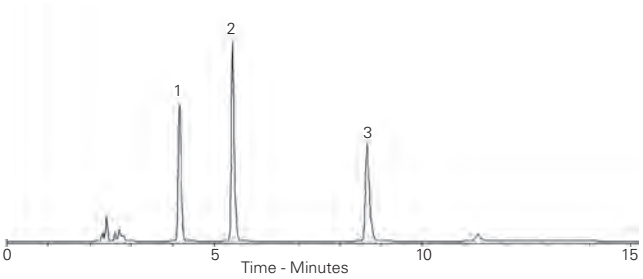
Noradrenaline



3,4-Dihydroxynorephedrine (I.S.)



Adrenaline



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Catecholamines from Urine

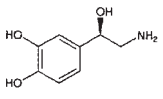
Application #AN3200

Conditions

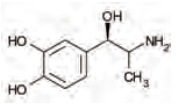
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 50 mM sodium acetate pH 7.0/MeCN/MeOH (50:35:15 v/v/v)
Flow Rate: 0.9 mL/min
Temperature: Ambient
Detection: Fluorescence – λ_{Ex} 350 nm, λ_{Em} 480 nm
Sample: Ion pair extraction using diphenyl-borate-ethanolamine. Derivatisation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

Analytes

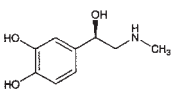
1. Noradrenaline (Norepinephrine)
2. 3,4-Dihydroxynorephedrine (I.S.)
3. Adrenaline (Epinephrine)
4. Dopamine



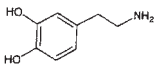
Noradrenaline



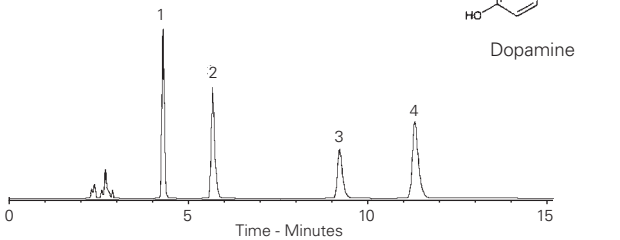
3,4-Dihydroxynorephedrine (I.S.)



Adrenaline



Dopamine



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Catechols Mixture Separations (I) and (II)

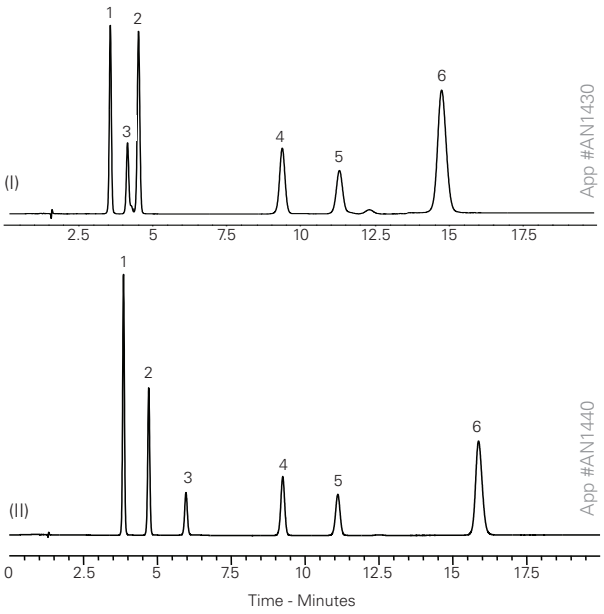
Application #AN1430 and #AN1440

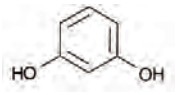
Conditions

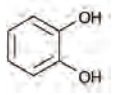
Column: (I) ACE Excel 3 CN-ES (II) ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: (I) EXL-1113-1546U (II) EXL-1112-1546U
Mobile Phase: (I) 20 mM H_3PO_4 in MeCN/H_2O (25:75 v/v)
(II) 20 mM H_3PO_4 in MeCN/H_2O (10:90 v/v)
Flow Rate: 1.5 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: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

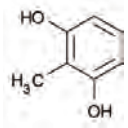
Analytes

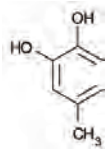
1. Resorcinol
2. Catechol
3. 2-Methylresorcinol
4. 4-Methylcatechol
5. 3-Methylcatechol
6. 4-Nitrocatechol

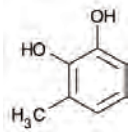


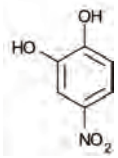

Resorcinol


Catechol


2-Methylresorcinol


4-Methylcatechol


3-Methylcatechol


4-Nitrocatechol

Cathinone Psychoactive Substances by LC-UV and LC-Amperometry

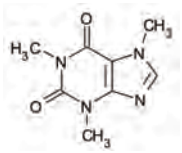
Application #AN3500

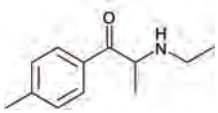
Conditions

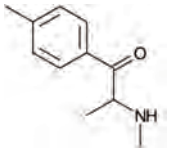
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: 10 mM ammonium acetate-100 mM KCl pH 4.3/MeOH (70:30 v/v)
Flow Rate: 0.8 mL/min
Injection: 10 µL
Temperature: 22 °C
Detection: UV, 264 nm
Amperometric Potential +1.4 V

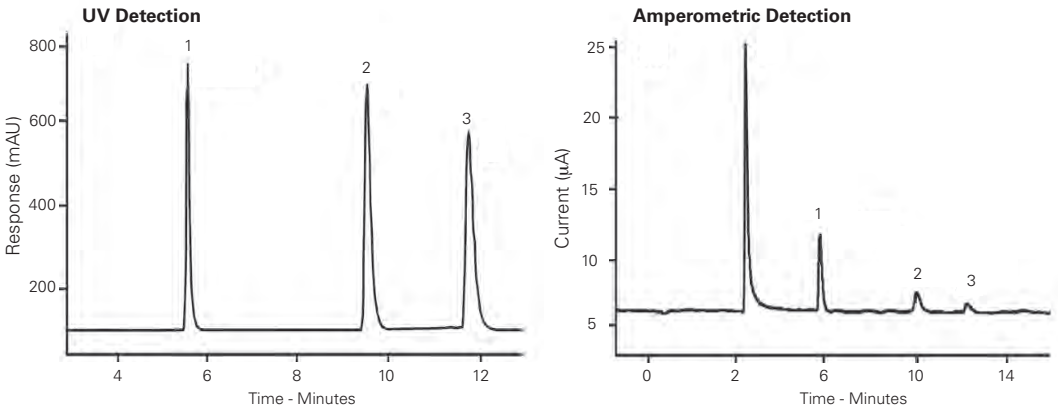
Analytes

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


Caffeine


4-Methylethcathinone (4-MEC)


4-Methylmethcathinone (4-MMC, mephedrone)



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

Cefquinome by LC-MS

Application #AN3130

Conditions

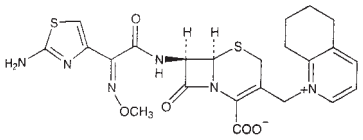
Column: ACE 5 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-121-1502
Mobile Phase: A: 2 mM formic acid in H_2O
B: 2 mM formic acid in MeCN
Gradient:

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

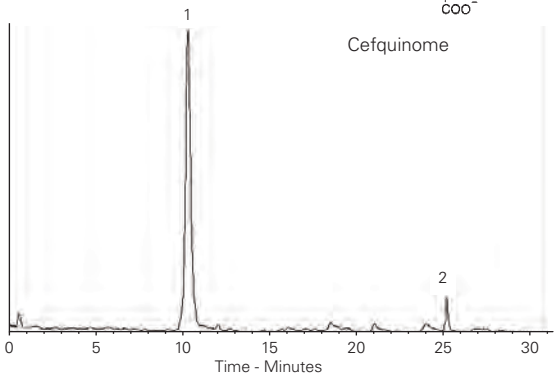
Flow Rate: 0.2 mL/min
Temperature: 25 °C
Detection: ESI-MS (+)

Analytes

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



Cefquinome



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Ciprofibrate from Human Plasma by LC-MS/MS

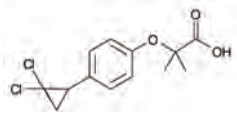
Application #AN2670

Conditions

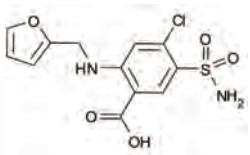
Column: ACE 5 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-121-0546
Mobile Phase: 0.001% ammonia in MeOH/MeCN/H_2O (70:20:10 v/v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: API 3200 triple quad MS
ESI in negative ion mode
Ion source temperature: 550 °C
Ion spray voltage: 4500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

Analytes

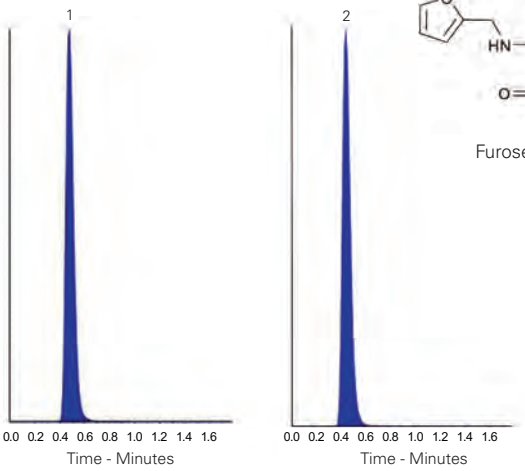
1. Ciprofibrate
(*m/z* 287.0 → 85.0)
2. Furosemide (IS)
(*m/z* 328.9 → 204.9)



Ciprofibrate



Furosemide (IS)



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Chloramphenicol in Milk by LC-MS/MS

Application #AN2030

Conditions

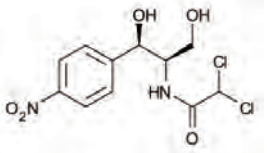
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: H_2O
B: MeOH
Gradient:

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

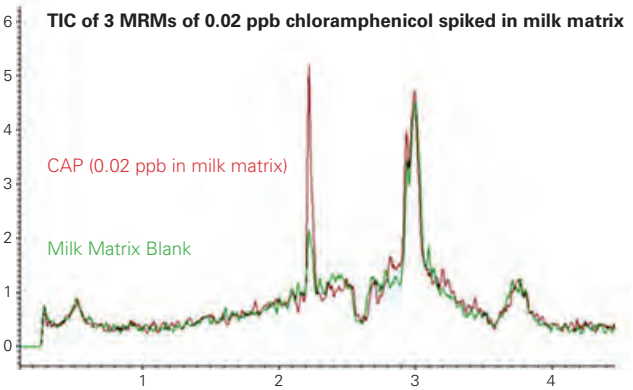
Flow Rate: 0.5 mL/min
Injection: 10 µL
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 400 °C
Cone gas temperature: 350 °C
Spray voltage: -4500 V

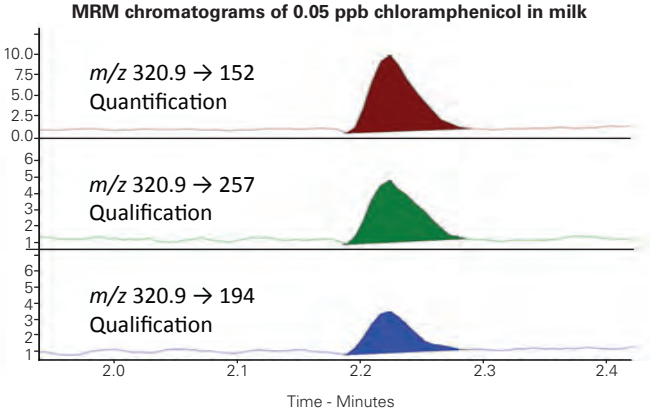
Analyte

1. Chloramphenicol









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Chocolate Analysis

Application #AN2040

Conditions

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

Gradient:

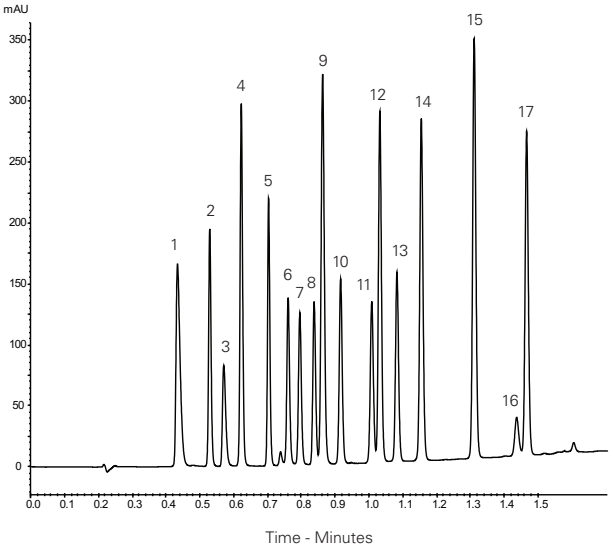
Time (mins)	%B
0.0	5
1.5	85

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

Analytes

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





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Clenbuterol in Equine Plasma by LC-MS/MS

Application #AN2050

Conditions

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

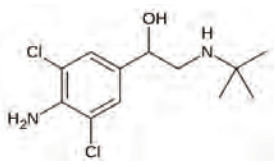
Gradient:

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

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

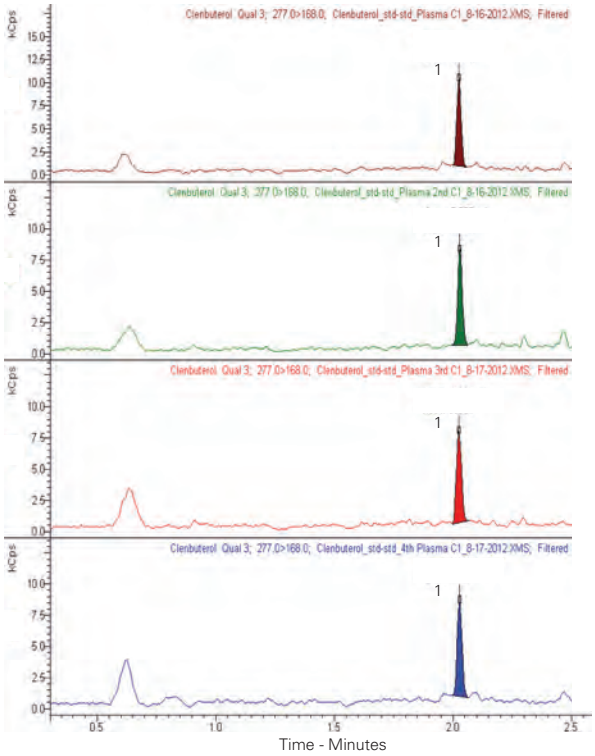
Analyte

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



Clenbuterol

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



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Clonidine Hydrochloride Oral Solution Containing Preservatives

Application #AN2060

Conditions

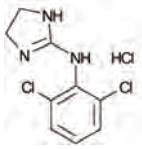
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 4.6 mm
Part Number:	CORE-25A-0546U
Mobile Phase:	A: 0.2% w/v phosphate buffer/ MeOH/MeCN (80:10:10 v/v/v) B: MeCN

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

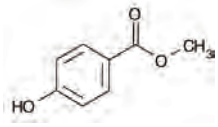
Flow Rate:	2 mL/min
Injection:	100 µL
Temperature:	20 °C
Detection:	UV, 220 nm

Analytes

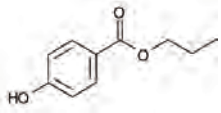
1. Clonidine HCl (10 µg/mL)
2. Methyl paraben (1.5 g/mL)
3. Propyl paraben (1.5 g/mL)



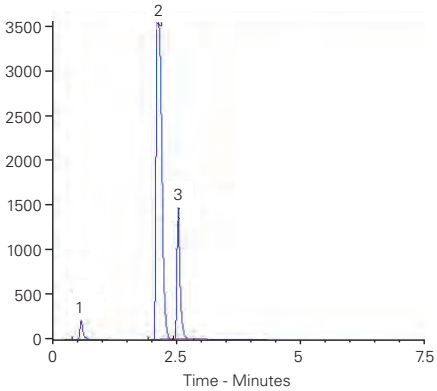
Clonidine HCl



Methyl paraben



Propyl paraben



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Clopidogrel and Photodegradation Products

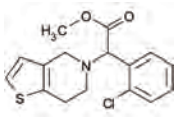
Application #AN3110

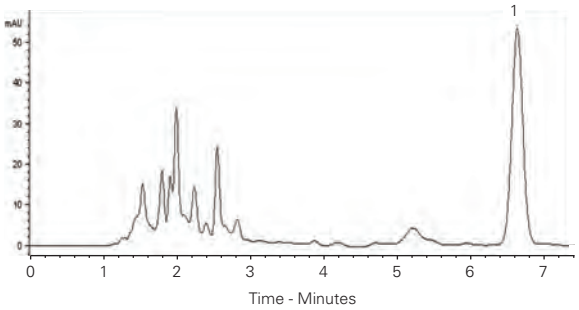
Conditions

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

Analyte

1. Clopidogrel





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

email: info@ace-hplc.com

Coffee Metabolite Profiling by LC-MS

Application #AN2590

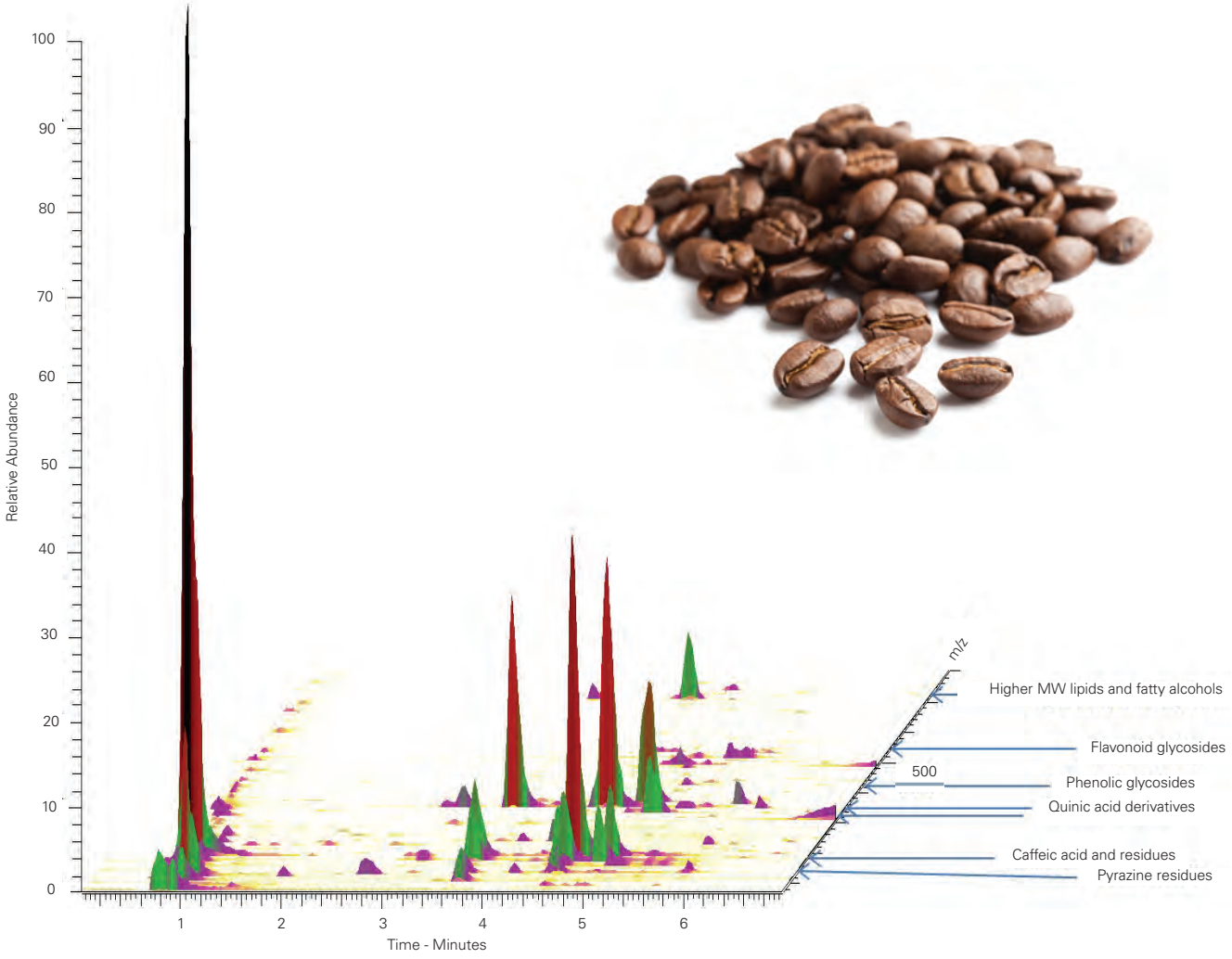
Conditions

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

Gradient:

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

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



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Cold Medicine Analytes (I) and (II)

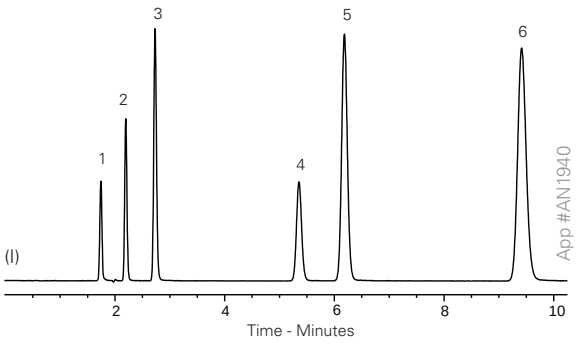
Application #AN1940 and #AN2410

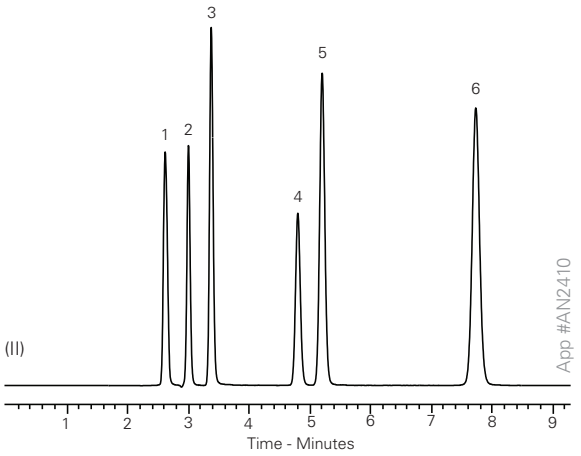
Conditions

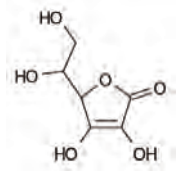
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: (I) 20 mM phosphoric acid in MeOH/H_2O (25:75 v/v)
(II) 0.1% formic acid in MeOH/H_2O (55:45 v/v)
Flow Rate: (I) 1.5 mL/min (II) 1.0 mL/min
Injection: 5 µL
Temperature: (I) 40 °C (II) 25 °C
Detection: (I) UV, 280 nm (II)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

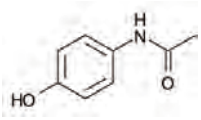
Analytes

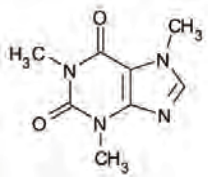
1. Ascorbic acid
2. Paracetamol
3. Caffeine
4. Aspirin
5. Ethenzamide
6. Salicylic acid

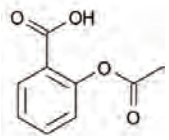


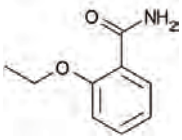


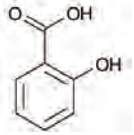

Ascorbic acid


Paracetamol


Caffeine


Aspirin


Ethenzamide


Salicylic acid

Corticosteroids by LC-MS/MS

Application #AN1030

Conditions

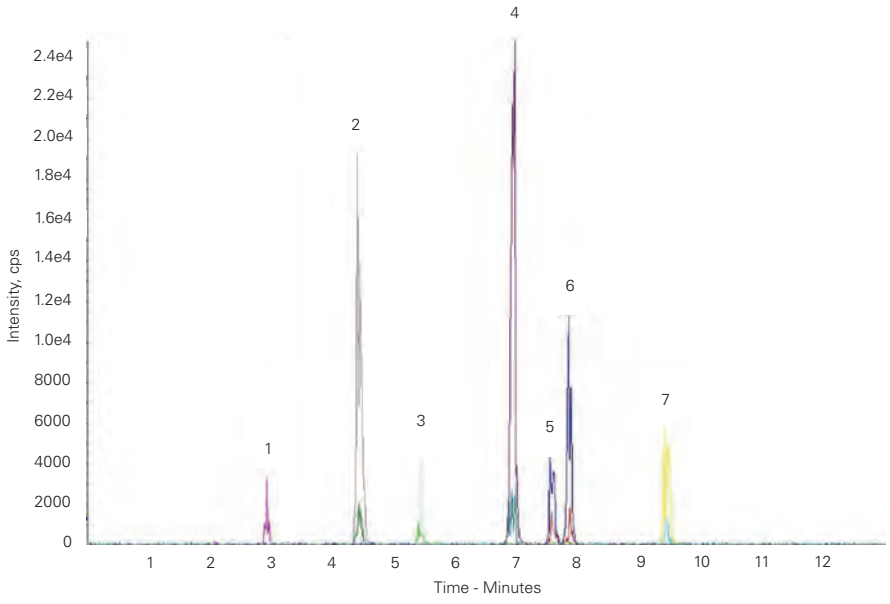
Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeCN/0.1% formic acid in H_2O (90:10 v/v)
Gradient:

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

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

Analytes

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



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Cortisol in Urine by LC-MS/MS

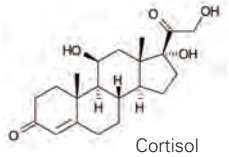
Application #AN2680

Conditions

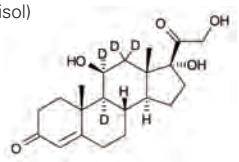
Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: 4 mM ammonium acetate in H_2O/0.2% (v/v) formic acid in MeOH (71.5:28.5 v/v)
Flow Rate: 0.7 mL/min
Injection: 50 µL
Temperature: 50 °C
Detection: Applied Biosystems 5000 MS/MS APCI in positive ion mode
Sample: BioRad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

Analytes

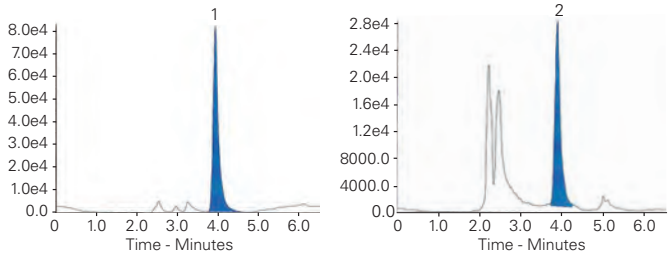
1. Cortisol
   (*m/z* 363.5 → 121.3)
2. Cortisol-d4 (IS)
   (*m/z* 367.3 → 331.3)



Cortisol



Cortisol-d4 (IS)



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Cyclosporin Mixture

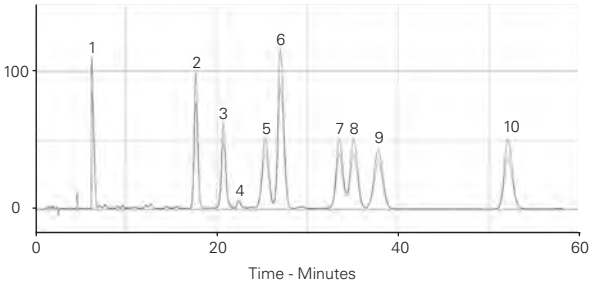
Application #AN3270

Conditions

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

Analytes

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



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Cyclodextrin-Encapsulated Flavour Compounds in Beer

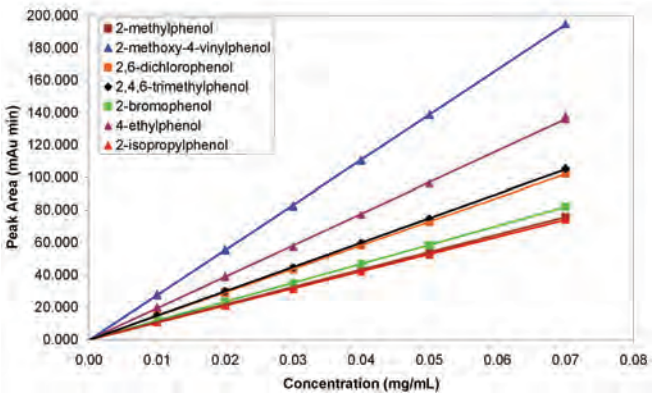
Application #AN2300

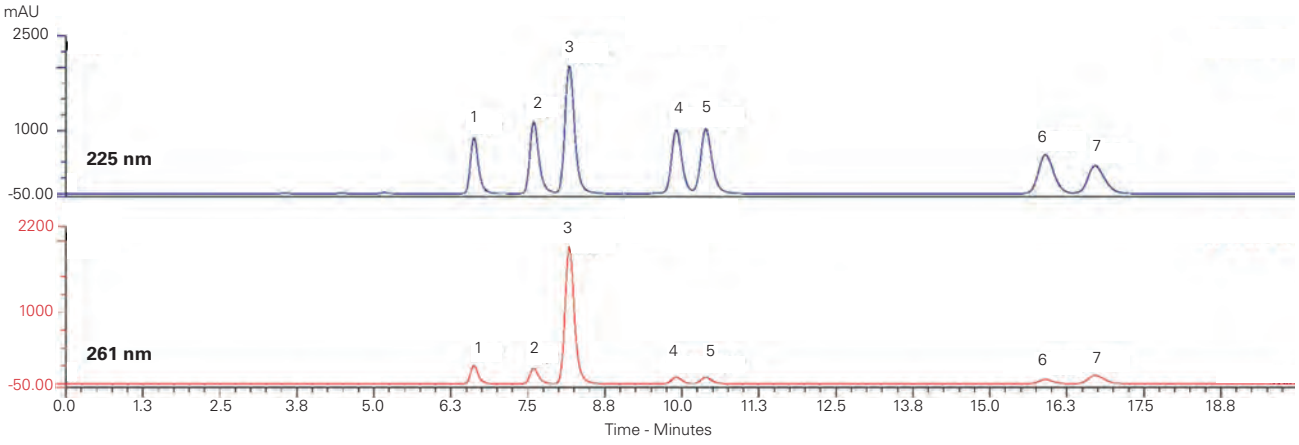
Conditions

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

Analytes

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





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Cytarabine Analogues by Ion-Pairing LC-MS/MS

Application #AN2070

Conditions

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

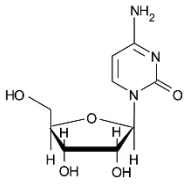
Gradient:

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

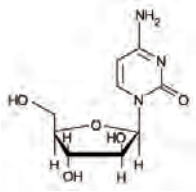
Flow Rate: 0.7 mL/min
Detection: API 4000 MS
TurbolonSpray, positive mode
Source Temperature 550 °C

Analytes

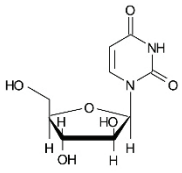
1. Uracil arabinofuranoside
   (*m/z* 245 → 113)
2. 5-Fluorocytidine (IS)
   (*m/z* 262 → 130)
3. Cytidine
   (*m/z* 244 → 112)
4. Cytarabine
   (*m/z* 244 → 112)



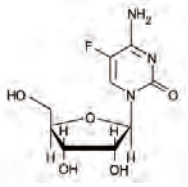
Cytidine



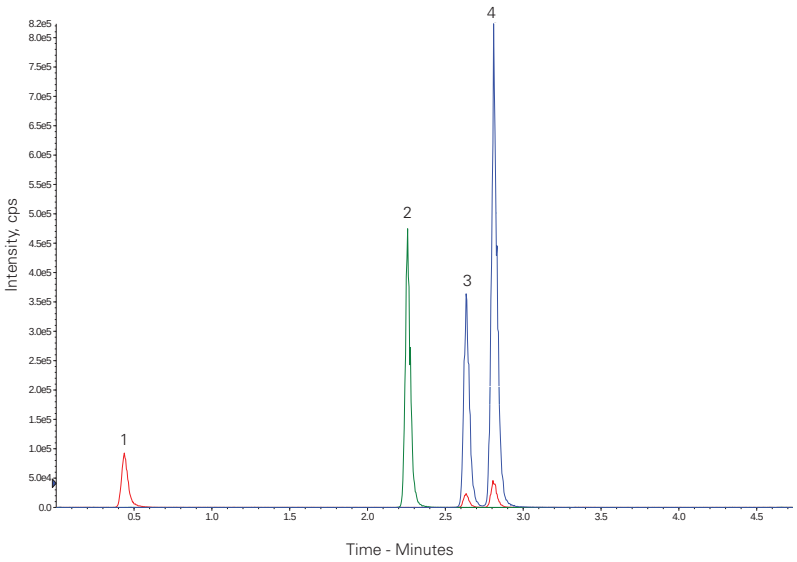
Cytarabine



Uracil arabinofuranoside



5-Fluorocytidine (IS)



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Cytotoxic Agents by UHPLC-MS/MS

Application #AN1070

Conditions

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

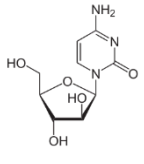
Gradient:

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

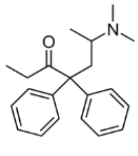
Flow Rate: 0.25 mL/min
Detection: Thermo Vantage triple quadrupole MS
MRM +ve ESI mode
Spray voltage: 3500 V
Nitrogen sheath and auxiliary gas
CID with argon: 1.5 mTorr

Analytes

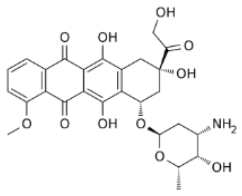
1. AraC
   (*m/z* 244.1 → 112.2)
2. Methadone
   (*m/z* 310.2 → 265.3)
3. Doxorubicin
   (*m/z* 544.2 → 361.2)
4. Etoposide
   (*m/z* 589.2 → 185.1)



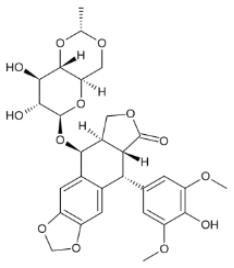
AraC



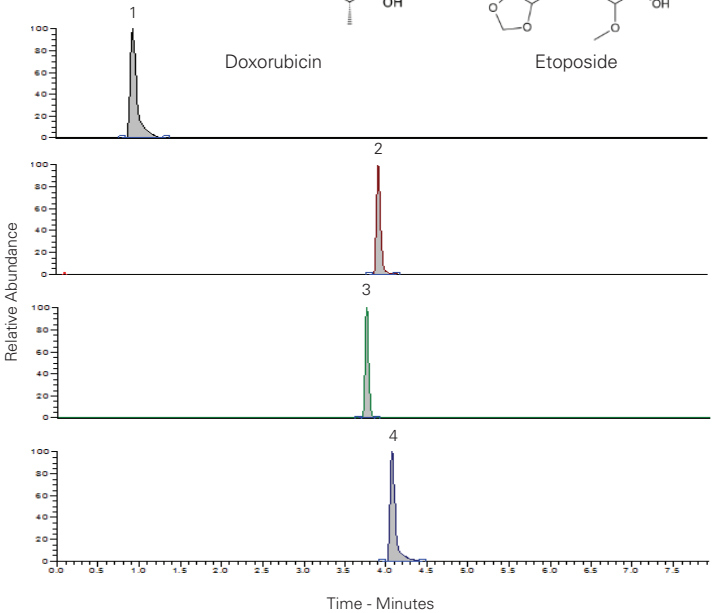
Methadone



Doxorubicin



Etoposide



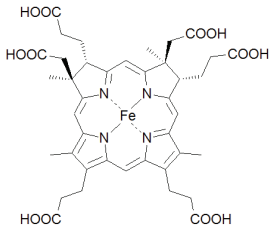
Reproduced with permission of Barts Cancer Institute, Queen Mary University of London

Decarboxylation of Sirohaem by Sirohaem Decarboxylase

Application #AN3830

Conditions

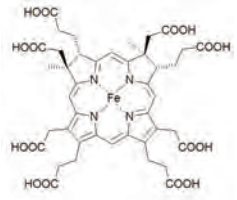
Column:	ACE 5 AQ	
Dimensions:	150 x 2.1 mm	
Part Number:	ACE-126-1502	
Mobile Phase:	A: 0.1% TFA in H_2O	
	B: MeCN	
Gradient:	**Time (mins)**	**%B**
	0	5
	6	20
	25	30
	35	100
	40	100
Flow Rate:	0.2 mL/min	
Detection:	DAD, 380 nm	



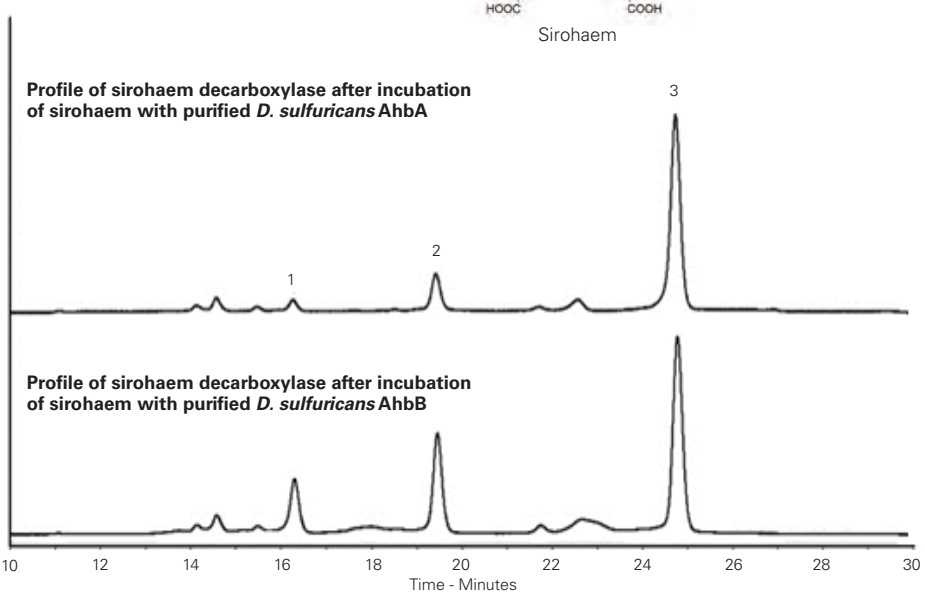
12,18-Didecarboxysirohaem

Analytes

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



Sirohaem



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

Defensins (Human) in Saliva Matrix

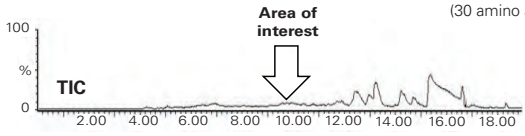
Application #AN1270

Conditions

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

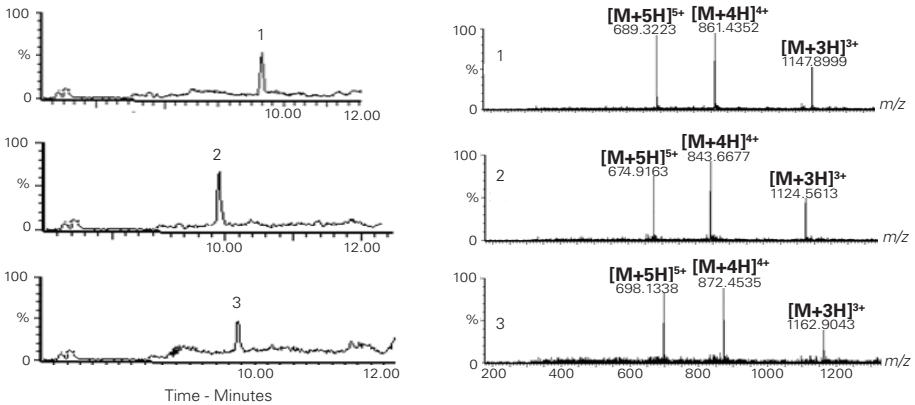
Defensin Human Neutrophil Peptides

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



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

Mass spectra



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Dermorphin in Equine Urine by LC-MS/MS

Application #AN1040

Conditions

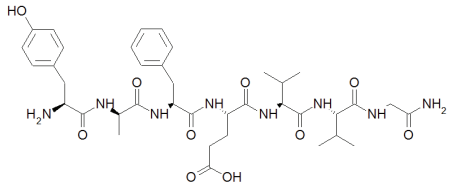
Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.2% formic acid in H_2O
B: 0.2% formic acid in MeCN

Gradient:

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

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

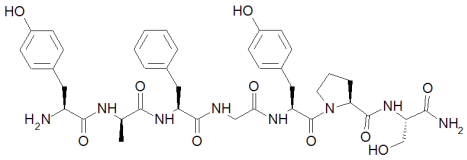
Accurate quantification of dermorphin in equine urine in range 0.05 – 100 ng/mL
LLOQ = 0.05 ng/mL



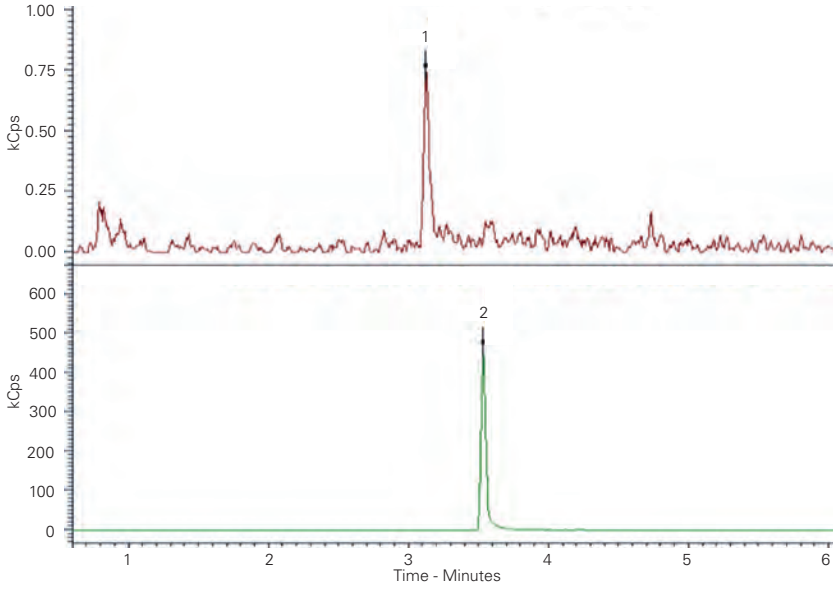
Deltorphin-II (IS)

Analytes

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



Dermorphin



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Didanosine

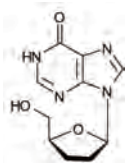
Application #AN3590

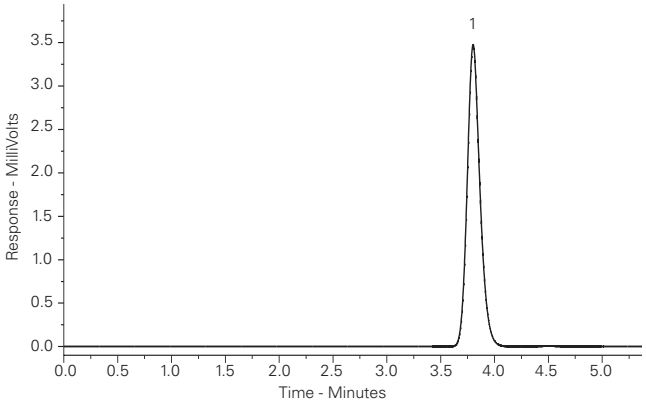
Conditions

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

Analyte

1. Didanosine





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Diuretics (Isocratic)

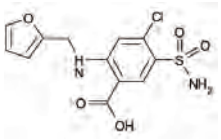
Application #AN2140

Conditions

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

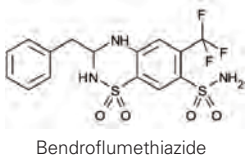
Analytes

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

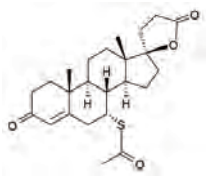


Furosemide

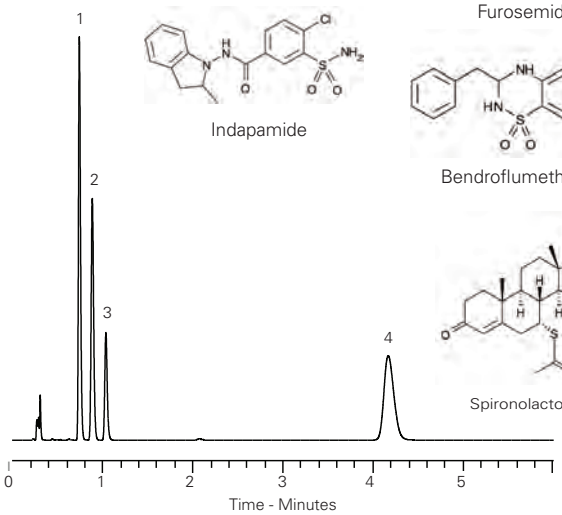
Indapamide



Bendroflumethiazide



Spironolactone



Diuretics

Application #AN1450

Conditions

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

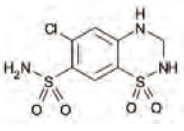
Gradient:

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

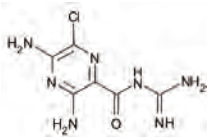
Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: UV, 254 nm

Analytes

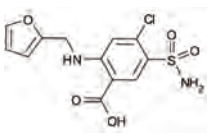
1. Hydrochlorothiazide
2. Amiloride
3. Furosemide
4. Indapamide
5. Bendroflumethiazide
6. Spironolactone



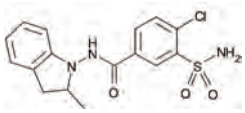
Hydrochlorothiazide



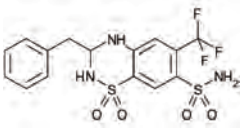
Amiloride



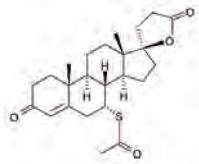
Furosemide



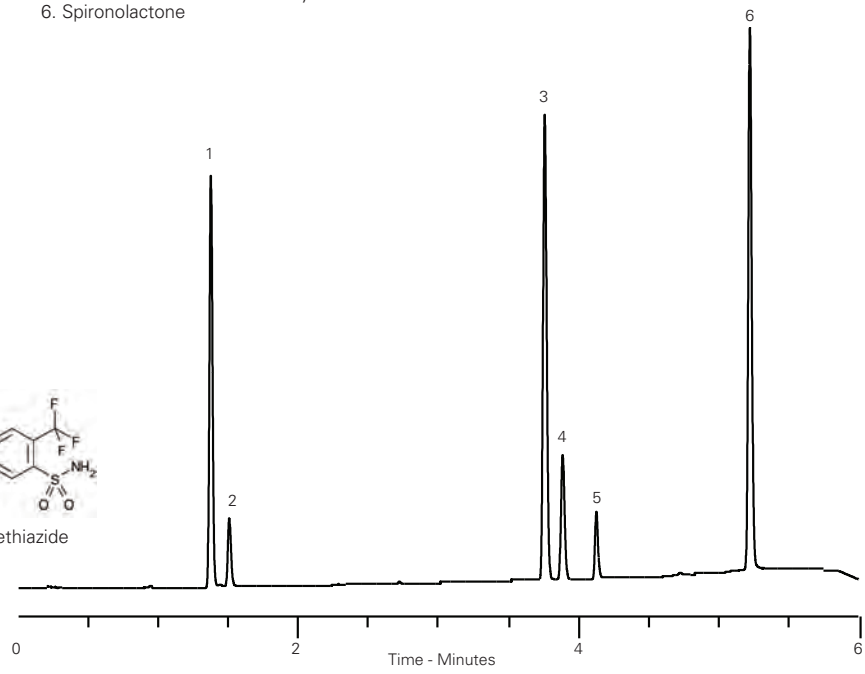
Indapamide



Bendroflumethiazide



Spironolactone



DOTATATE and Octreotide

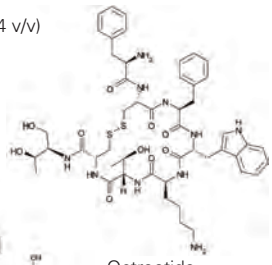
Application #AN2730

Conditions

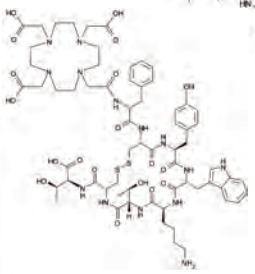
Column: ACE 3 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-111-1503
Mobile Phase: 0.1% TFA in H_2O/MeCN (76:24 v/v)
Flow Rate: 0.6 mL/min
Injection: 20 µL
Detection: UV, 220 nm

Analytes

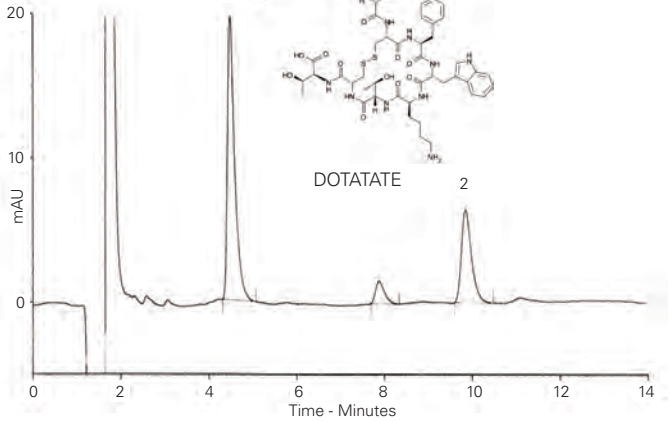
1. DOTATATE
2. Octreotide



Octreotide



DOTATATE



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

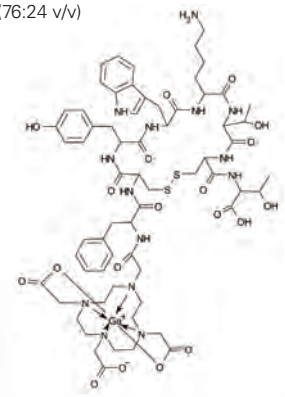
Application #AN2720

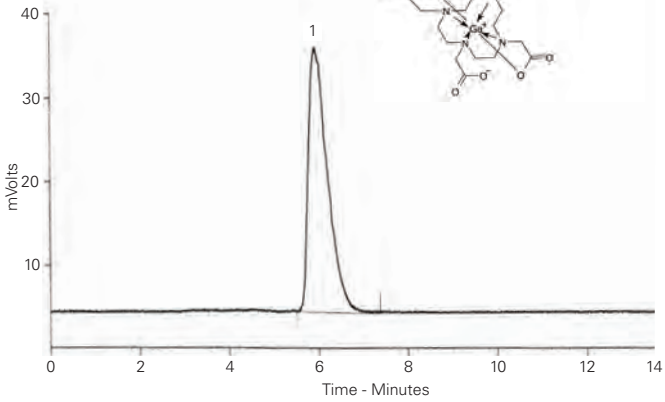
Conditions

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

Analyte

1. ^{68}Ga-DOTATATE





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

Application #AN2710

Conditions

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

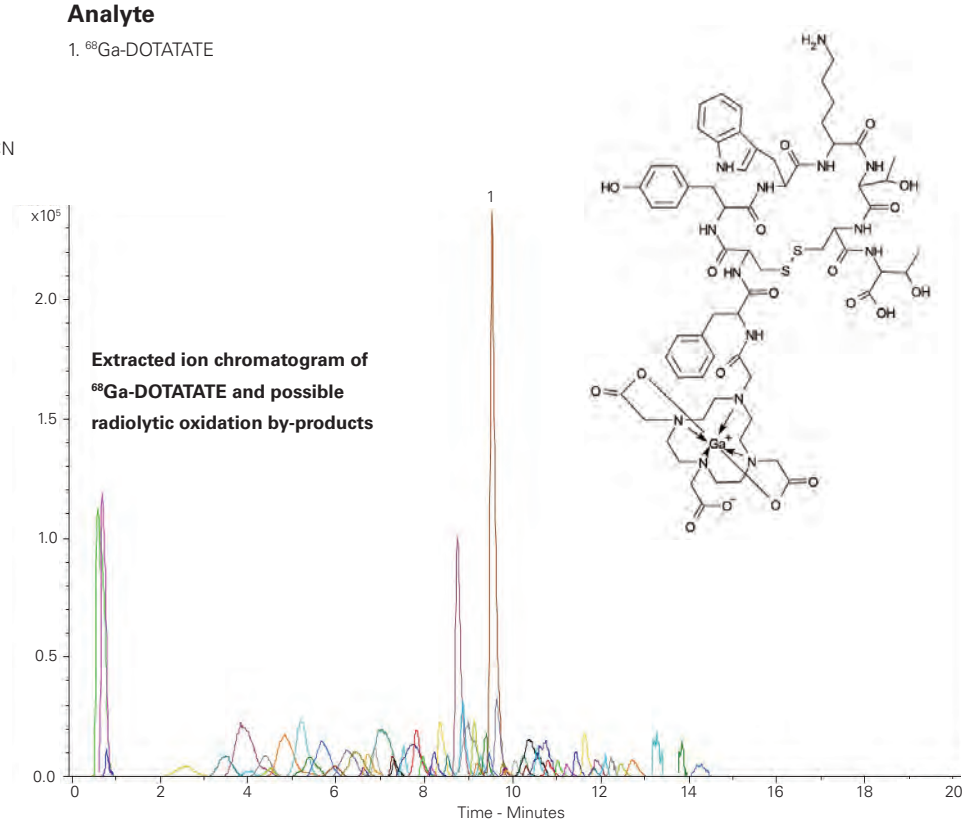
Gradient:

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

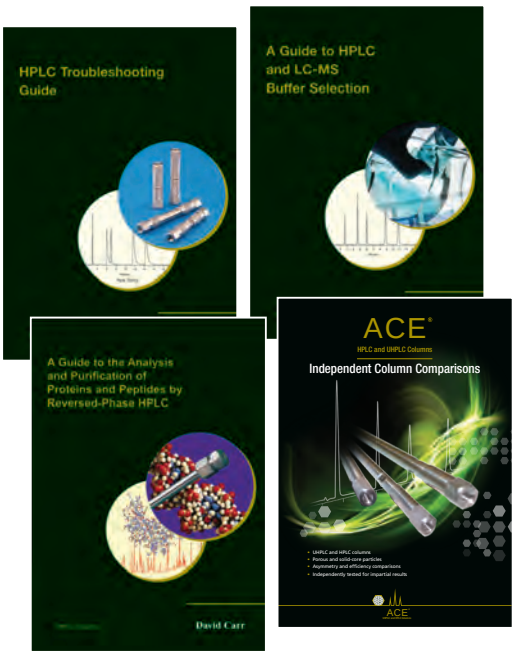
Flow Rate: 1 mL/min
Injection: 10 µL
Detection: Bruker ESI-Q-TOF
ESI positive ion mode

Analyte

1. ^{68}Ga-DOTATATE



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Drugs of Abuse Screen by UHPLC-MS/MS

Application #AN2190

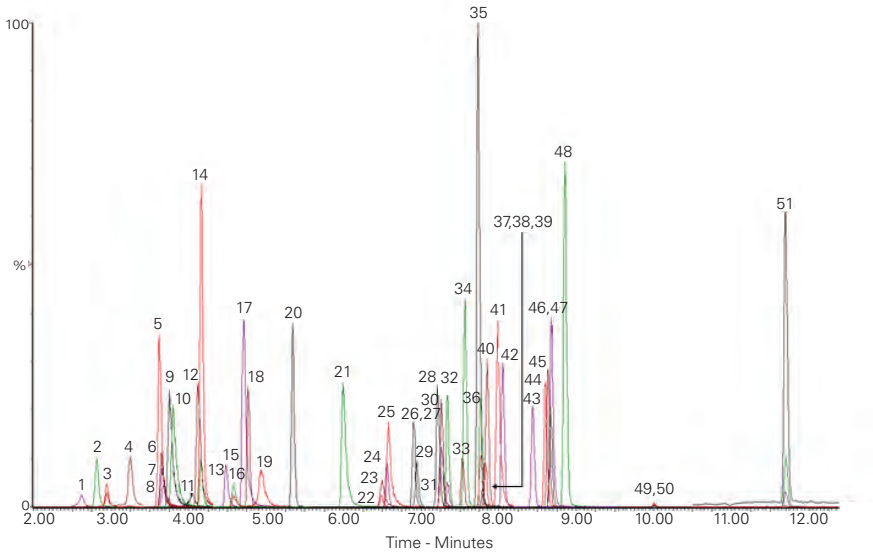
Conditions

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

Gradient:

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

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



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

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

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

Conditions

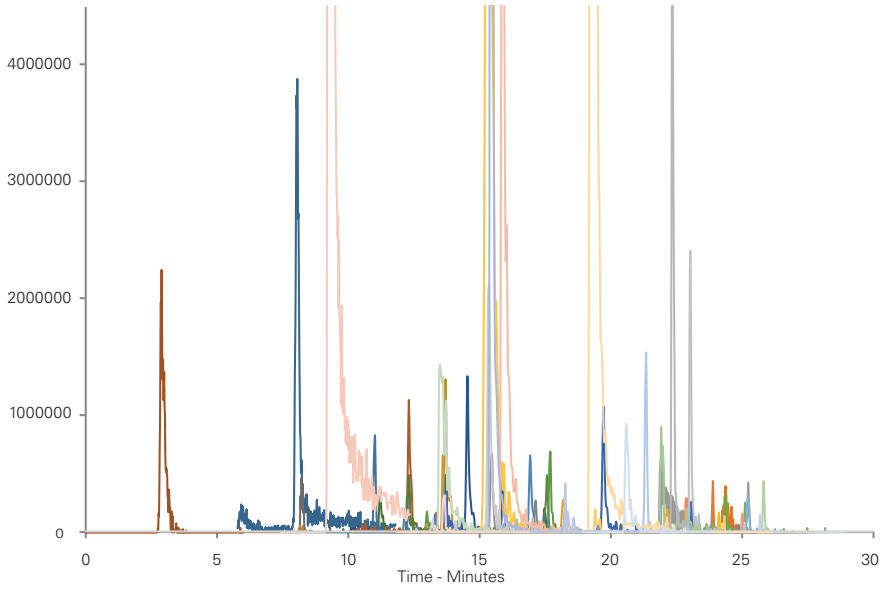
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 2 mM ammonium acetate + 0.1% formic acid in H_2O
B: 2 mM ammonium acetate + 0.1% formic acid in MeOH

Gradient:

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

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

Analytes in blue are included in Extracted Ion Chromatogram



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

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

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

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

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

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

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

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

Echinacea

Application #AN4270

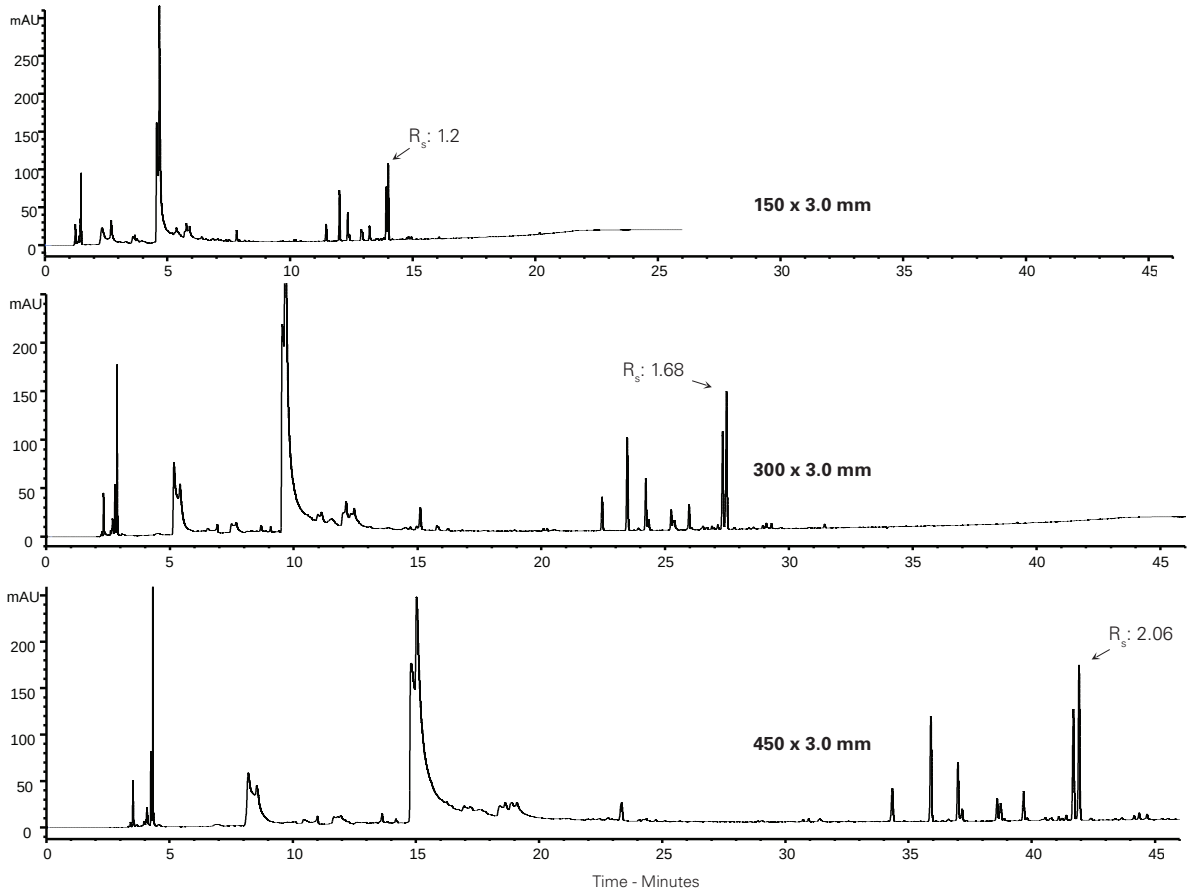
Conditions

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

Gradient:

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

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



Entacapone

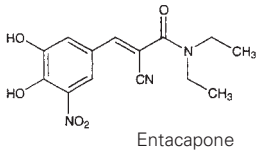
Application #AN3600

Conditions

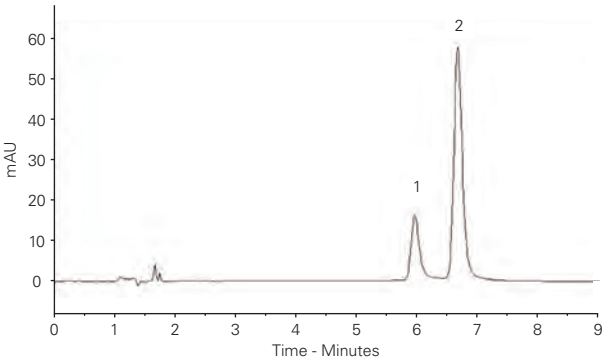
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: Phosphoric acid pH 3.0/MeCN (65:35 v/v)
Flow Rate: 2.0 mL/min
Injection: 20 µL
Temperature: 25 °C
Detection: UV, 305 nm
Sample: Entacapone standard in MeOH solution exposed to direct UV radiation (254 nm)

Analytes

1. Degradation Product
2. Entacapone



Entacapone



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Epanolol

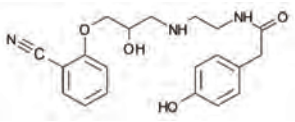
Application #AN3610

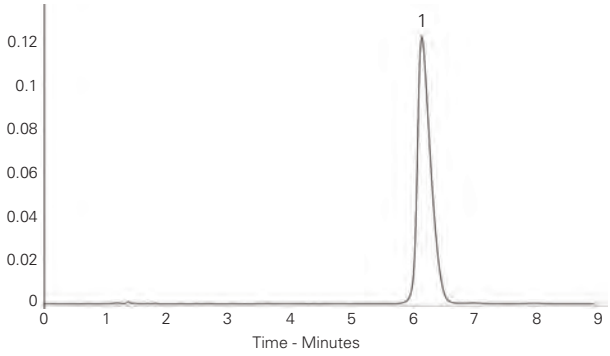
Conditions

Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: 20 mM ammonium formate pH 3.0/MeOH (85:15 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Epanolol





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Epinastine

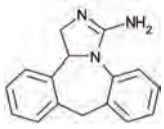
Application #AN3620

Conditions

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

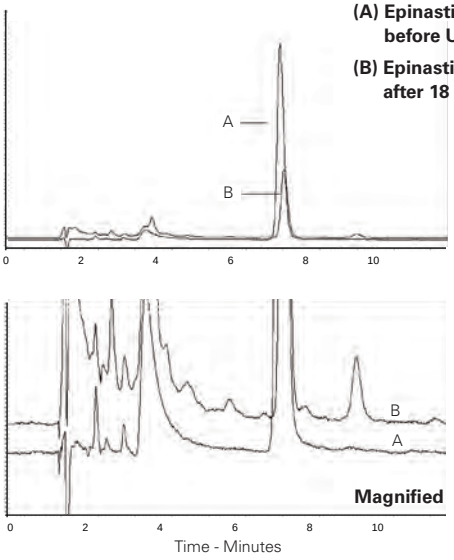
Analyte

1. Epinastine



(A) Epinastine Hydrochloride before UV radiation

(B) Epinastine Hydrochloride after 18 hours UV radiation



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Ethanol Extract from Seed Cover (*Acacia Farnesiana*)

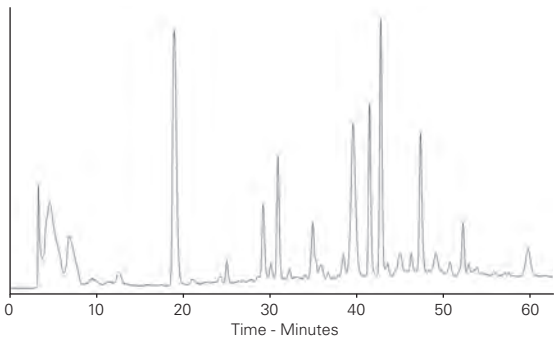
Application #AN2900

Conditions

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

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

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



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Ethyl Glucuronide in Water by LC-MS/MS

Application #AN1100

Conditions

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

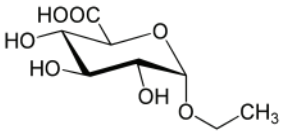
Gradient:

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

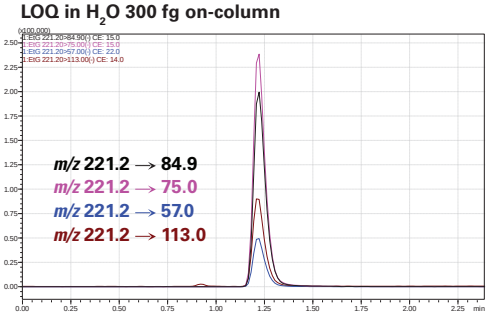
Flow Rate: 0.4 mL/min
Injection: 3 µL
Temperature: 40 °C
Detection: Shimadzu LCMS-8050
ESI voltage: -3 kV
Desolvation line: 250 °C
Interface heater: 380 °C
Nebulizing gas: 3 L/min
Heat block: 400 °C

Analyte

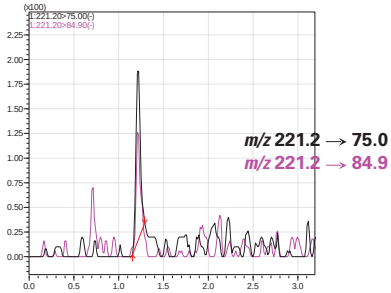
1. Ethyl glucuronide



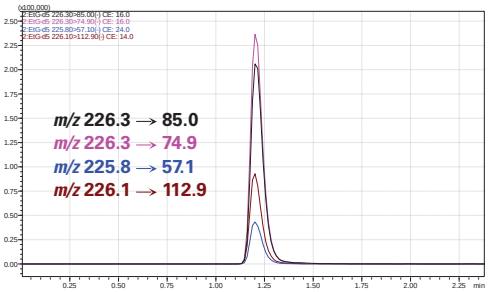
Ethyl glucuronide (EtG)
LOQ in H_2O 300 fg on-column



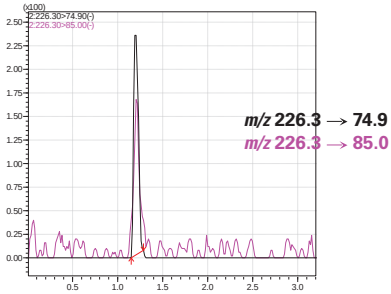
EtG 100 pg/mL



Ethyl glucuronide-d5 (EtG-d5)



EtG-d5 100 pg/mL



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Exploiting Selectivity by Adjusting pH

Application #AN2440

Conditions

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

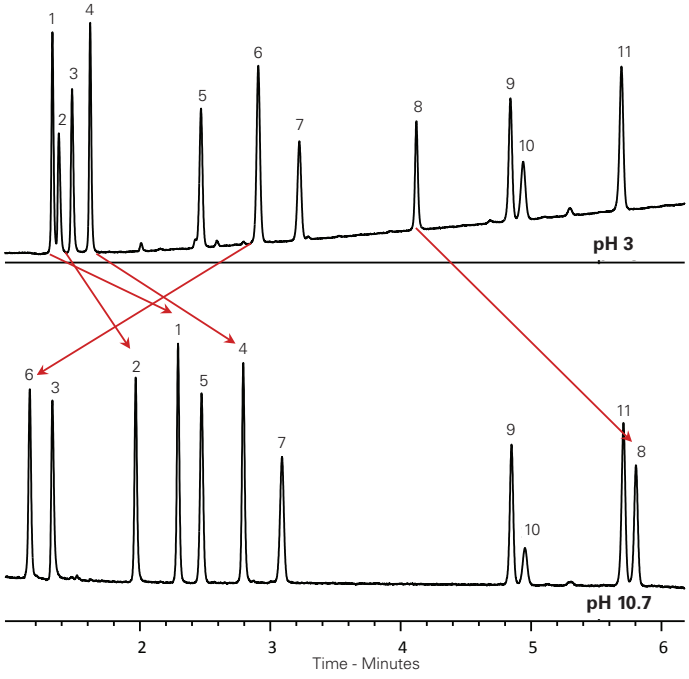
Gradient:

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

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

Analytes

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



Explosive Analytes (I)

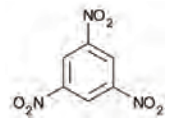
Application #AN1460

Conditions

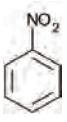
Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	MeOH/H_2O (50:50 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	20 °C
Detection:	UV, 254 nm

Analytes

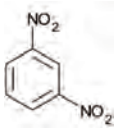
1. 1,3,5-Trinitrobenzene
2. Nitrobenzene
3. 1,3-Dinitrobenzene
4. 2,4-Dinitrotoluene



1,3,5-Trinitrobenzene

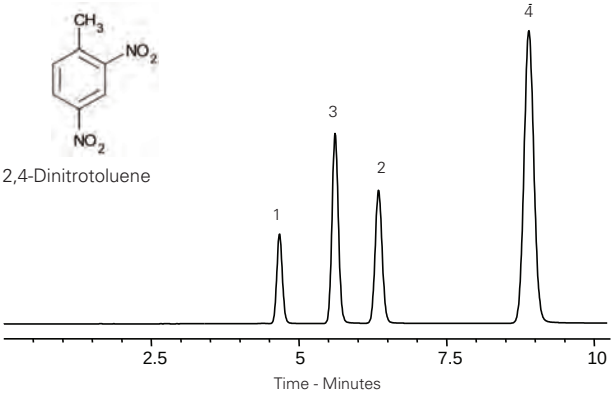


Nitrobenzene



1,3-Dinitrobenzene

2,4-Dinitrotoluene



Explosive Analytes (II)

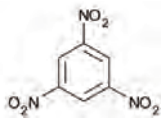
Application #AN1470

Conditions

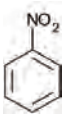
Column:	ACE 5 CN-ES
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1213-1546U
Mobile Phase:	MeOH/H_2O (50:50 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	20 °C
Detection:	UV, 254 nm

Analytes

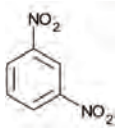
1. 1,3,5-Trinitrobenzene
2. Nitrobenzene
3. 1,3-Dinitrobenzene
4. 2,4-Dinitrotoluene



1,3,5-Trinitrobenzene

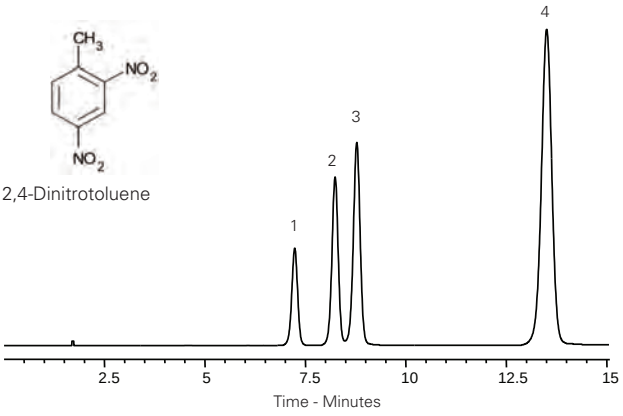


Nitrobenzene



1,3-Dinitrobenzene

2,4-Dinitrotoluene



Fingerprinting of *Cuscuta Chinensis* Flavonoids

Application #AN4250

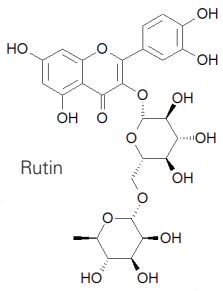
Conditions

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

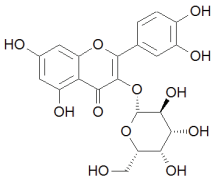
***Cuscuta chinensis* is used in traditional medicines in eastern and southern Asia**

Analytes

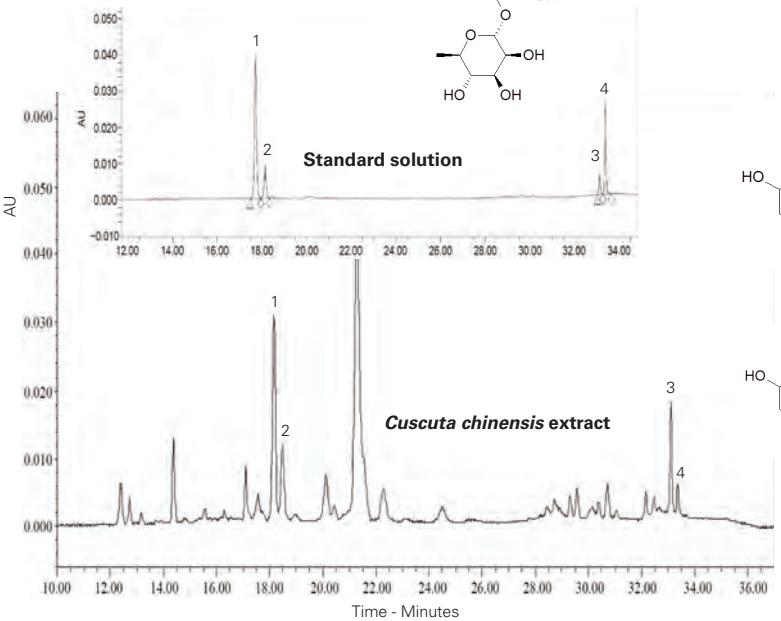
1. Rutin
2. Hyperoside
3. Isorhamnetin
4. Kaempferol

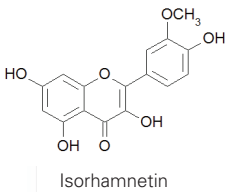


Rutin

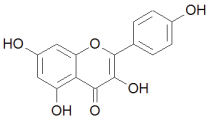


Hyperoside





Isorhamnetin



Kaempferol

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

Flavone and Dibucaine

Application #AN2850

Conditions

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

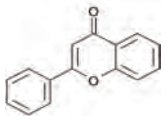
Gradient:

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

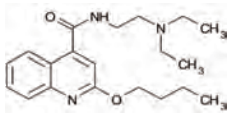
Flow Rate: 2 mL/min
Temperature: 60 °C
Detection: UV, 200-450 nm

Analytes

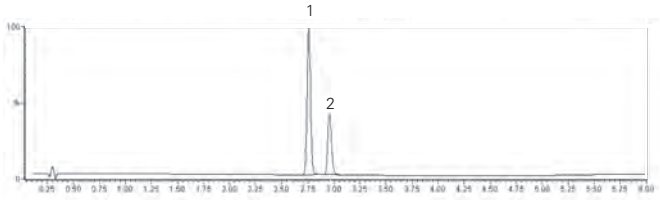
1. Flavone
2. Dibucaine



Flavone



Dibucaine



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Flavonoids

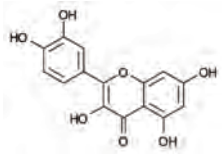
Application #AN2810

Conditions

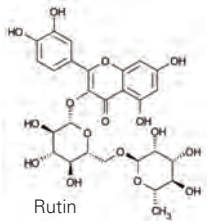
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/0.1% formic acid in H_2O (40:60 v/v)
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: Ambient
Detection: UV, 254 nm

Analytes

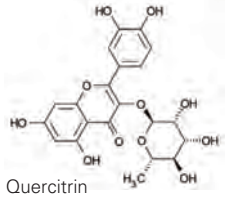
1. Rutin
2. Quercetin
3. Quercitrin
4. Kaempferol



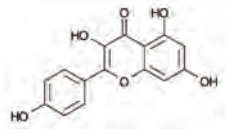
Quercetin



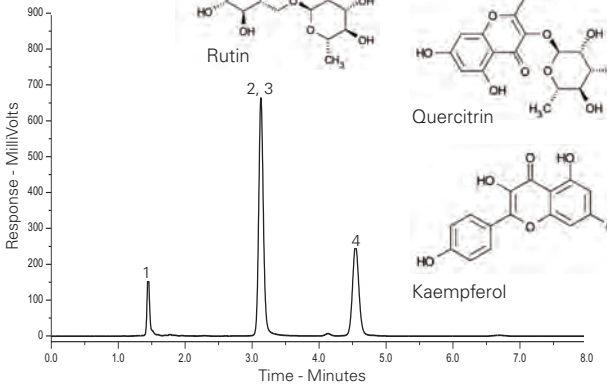
Rutin



Quercitrin



Kaempferol



Flurbiprofen and Related Substances

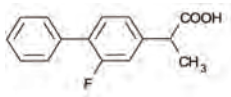
Application #AN3630

Conditions

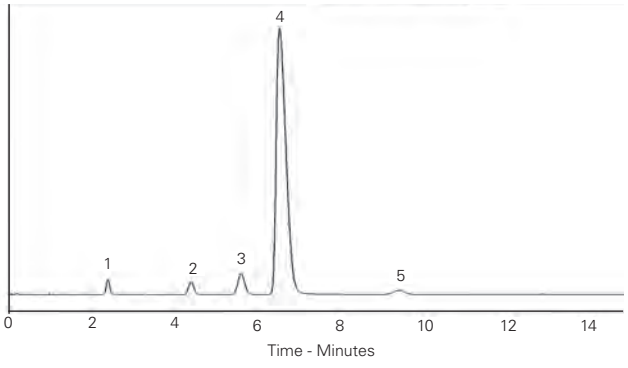
Column: ACE 3 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-111-0546
Mobile Phase: H_2O/MeCN/TFA (64:34:0.5 v/v/v)
Flow Rate: 2 mL/min
Injection: 20 µL
Temperature: 28 °C
Detection: UV, 254 nm

Analytes

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



Flurbiprofen



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Formoterol from Human Plasma by LC-MS/MS

Application #AN3100

Conditions

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

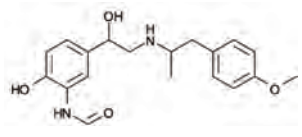
Gradient:

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

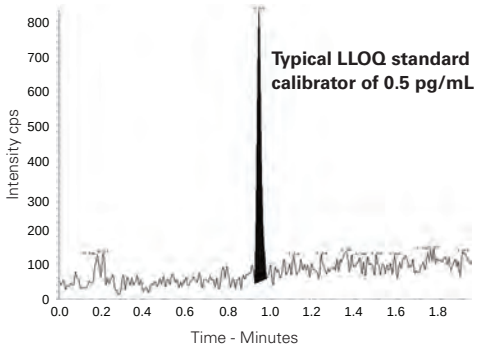
Flow Rate: 0.75 mL/min
Temperature: 60 °C
Detection: AB SCIEX QTRAP 5500 LC-MS/MS system
Sample: Extracted by mixed mode cation exchange SPE

Analyte

1. Formoterol (*m/z* 345 → 149)



Formoterol



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Galanthamine

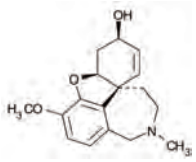
Application #AN3640

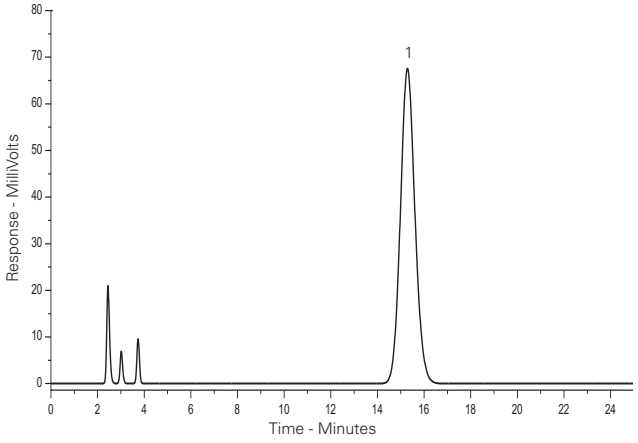
Conditions

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

Analyte

1. Galanthamine





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

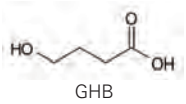
Application #AN1500

Conditions

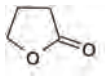
Column: ACE Excel 2 C18-AR
Dimensions: 100 x 3.0 mm
Part Number: EXL-109-1003U
Mobile Phase: 20 mM KH_2PO_4 pH 2.5 in H_2O/MeCN (98:2 v/v)
Flow Rate: 0.43 mL/min
Injection: 2 µL
Temperature: 30 °C
Detection: UV, 215 nm

Analytes

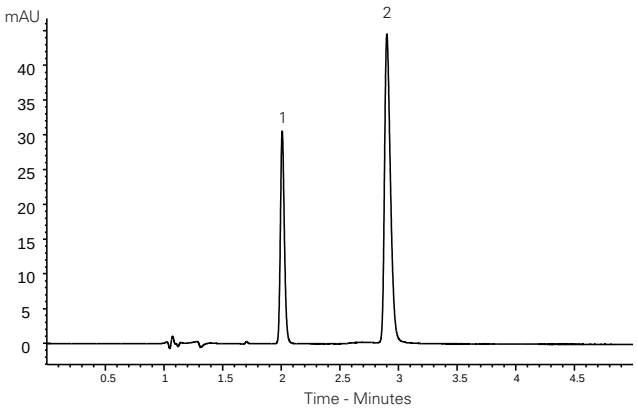
1. GHB
2. GBL



GHB



GBL



Garlic Analysis (I)

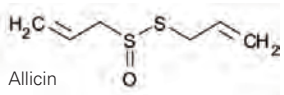
Application #AN2820

Conditions

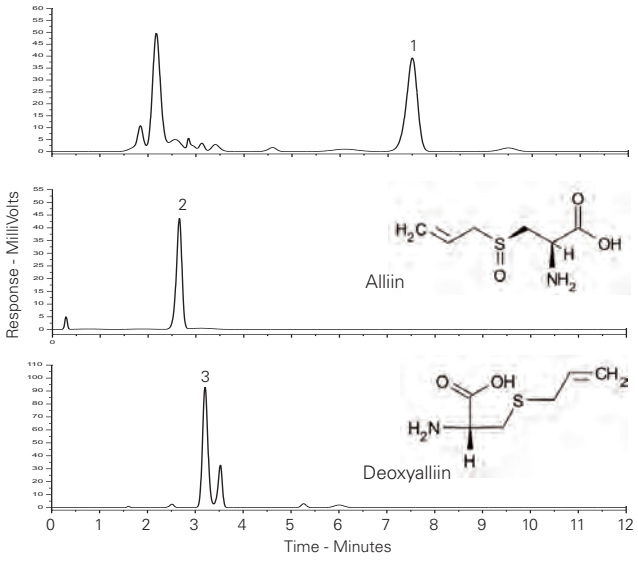
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: H_2O/MeOH (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 210 nm

Analytes

1. Allicin
2. Alliin
3. Deoxyalliin



Allicin



Alliin

Deoxyalliin

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Garlic Analysis (II)

Application #AN2830

Conditions

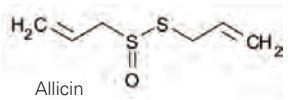
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: H_2O
B: MeCN

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

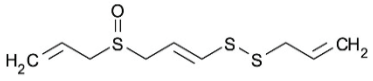
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 254 nm

Analytes

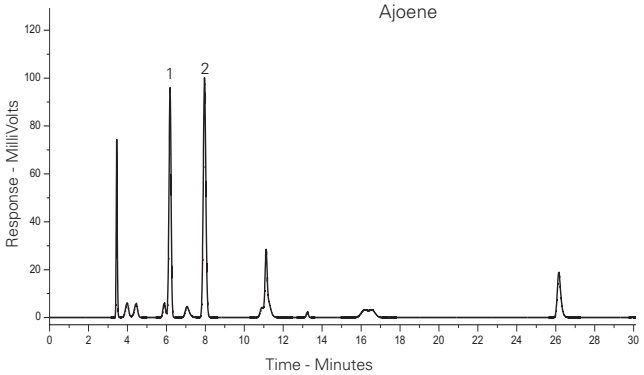
1. Allicin
2. Ajoene



Allicin



Ajoene



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Ginkgo Biloba – Ultra Resolution

Application #AN2270

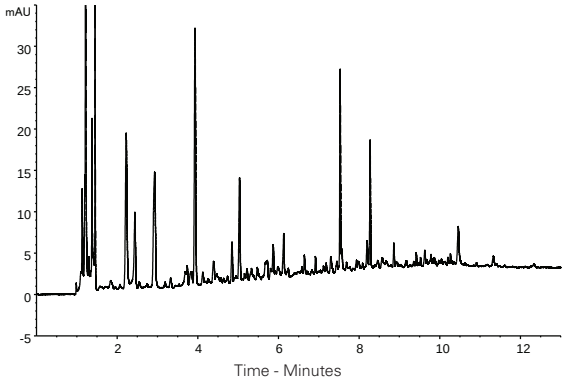
Conditions

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

Gradient:

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

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



Need a custom column for your application?

Please enquire

email: info@ace-hplc.com



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

Ginsenosides from Chinese Medicine by UHPLC-MS/MS

Application #AN3540

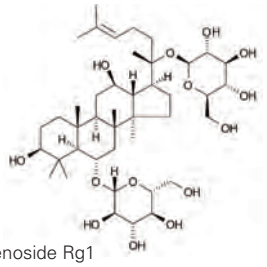
Conditions

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

Gradient:

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

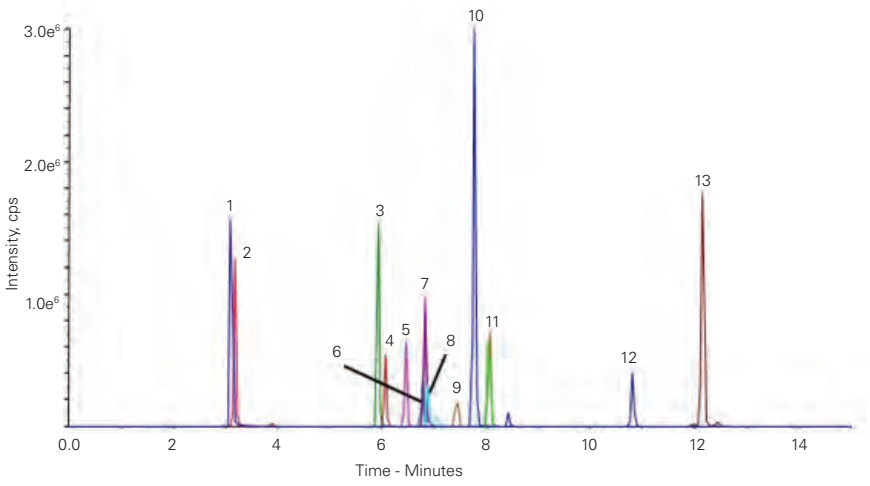
Flow Rate: 0.4 mL/min
Injection: 2 µL
Temperature: 45 °C
Detection: AB SCIEX 5500 Qtrap MS
ESI in negative ion mode
Source temperature: 450 °C
Sprayer voltage: -4500 V
Stepwise MRM mode for
$[M + HCOO]^-$ > $[M - H]^-$ ion transitions
Mass range 501 – 1250 u (step size 2 u)



Ginsenoside Rg1

Analytes

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



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Ginseng Extract

Application #AN4260

Conditions

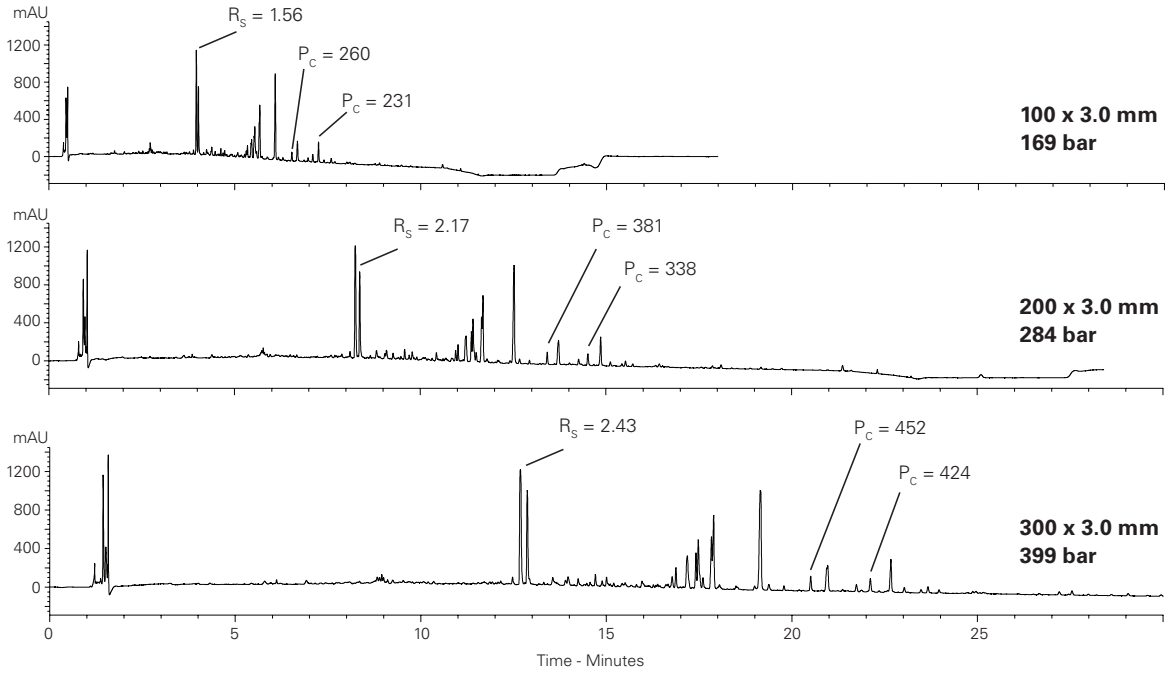
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 3.0 mm; 2 x 100 x 3.0 mm (coupled); 3 x 100 x 3.0 mm (coupled)
Part Number: CORE-25A-1003U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

Gradient:

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

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





Gliotoxin from *Aspergillus Fumigatus* Liquid Culture

Application #AN3780

Conditions

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

Gradient:

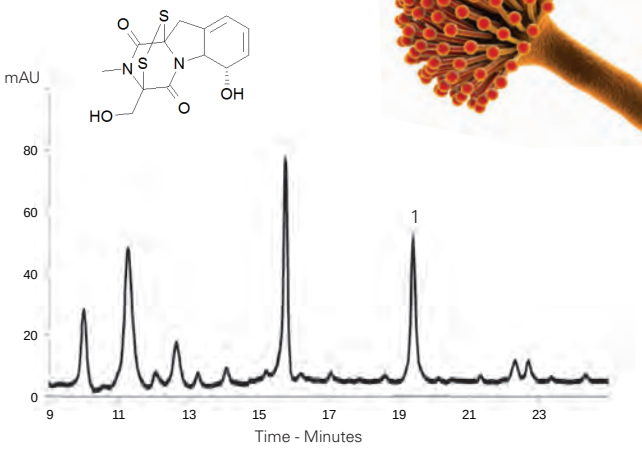
Time (mins)	%B
0	10
21	100

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

Analyte

1. Gliotoxin





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

Glyphosate and Related Compounds as FMOC Derivatives (Gradient)

Application #AN3850

Conditions

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

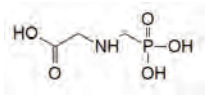
Gradient:

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

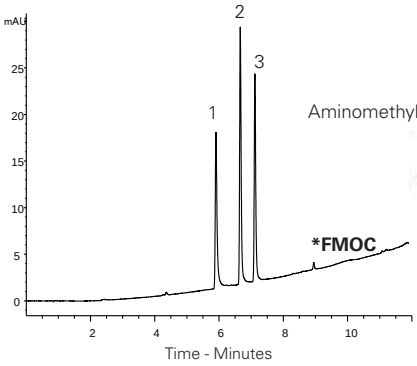
Flow Rate: 0.4 mL/min
Injection: 0.1 µL
Temperature: 60 °C
Detection: UV, 254 nm
Sample: Standards derivatised with FMOC-Cl

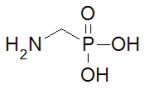
Analytes

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

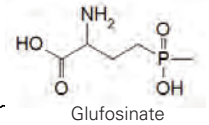


Glyphosate





Aminomethylphosphonic acid (AMPA)



Glufosinate

Glyphosate and Related Compounds as FMOC Derivatives (Isocratic)

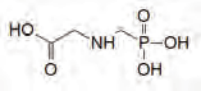
Application #AN3860

Conditions

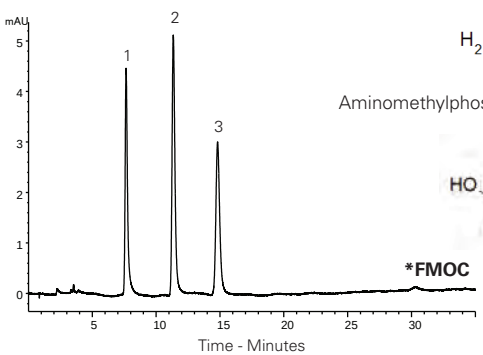
Column: ACE Excel 3 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: EXL-1111-1502U
Mobile Phase: 5 mM ammonium formate pH 3.0 in H_2O/MeOH (55:45 v/v)
Flow Rate: 0.4 mL/min
Injection: 0.1 µL
Temperature: 25 °C
Detection: UV, 254 nm
Sample: Standards derivatised with FMOC-Cl

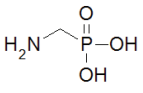
Analytes

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

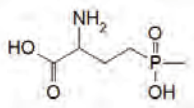


Glyphosate





Aminomethylphosphonic acid (AMPA)



Glufosinate

Green Tea Extract

Application #AN4280

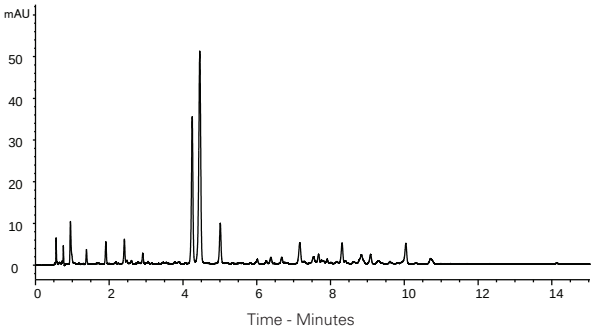
Conditions

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

Gradient:

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

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



Green Tea Metabolite Profiling by LC-MS

Application #AN2580

Conditions

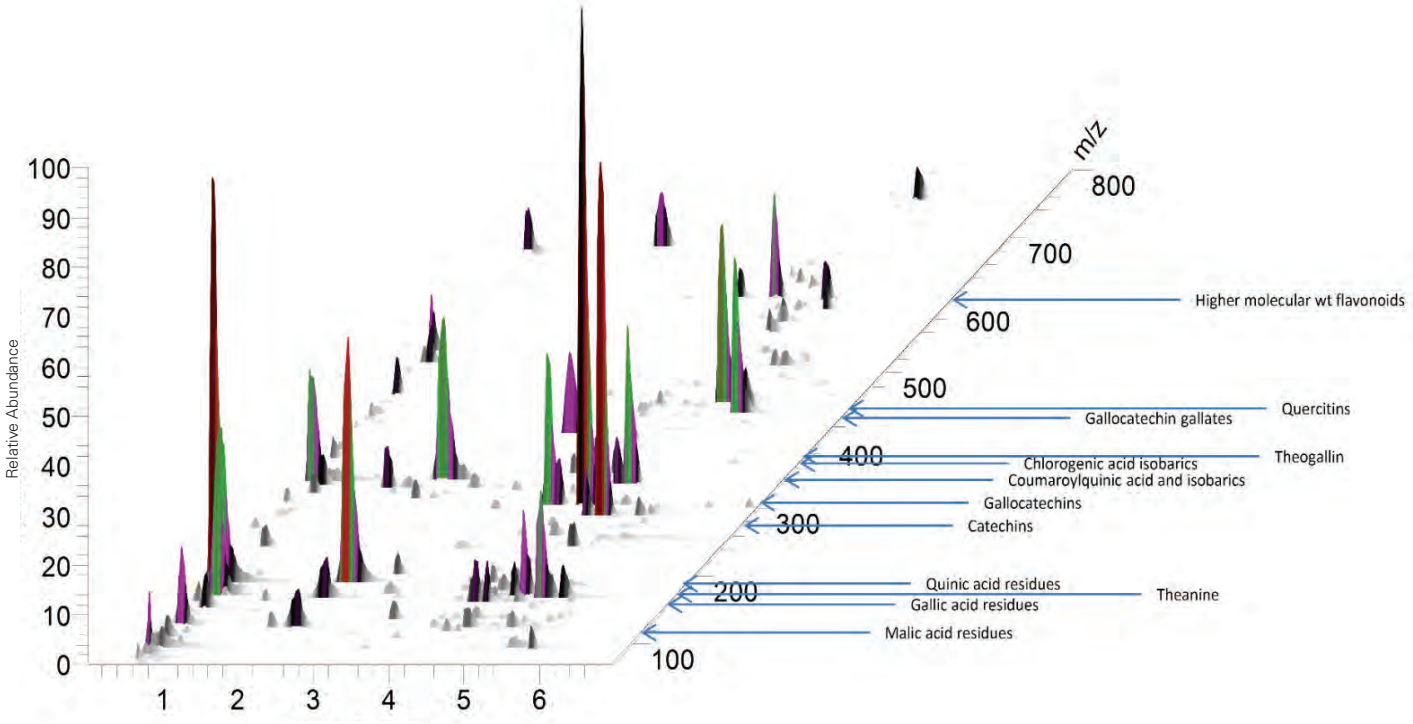
Column: ACE Excel 1.7 C18-Amide
Dimensions: 100 x 2.1 mm
Part Number: EXL-1712-1002U
Mobile Phase: A: 0.01% formic acid in H_2O
B: 0.01% formic acid in MeCN

Gradient:

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

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





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Hair Dye Restricted Components (I)

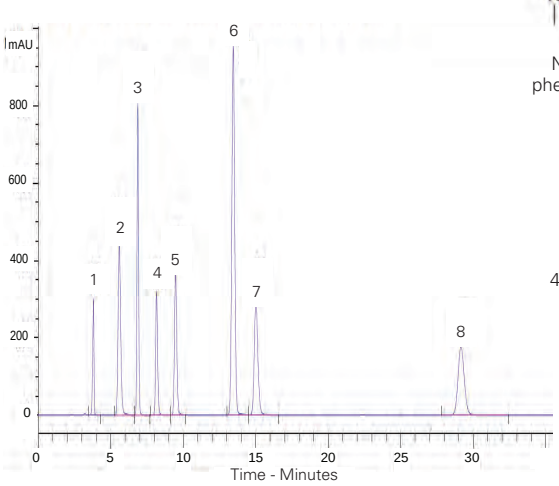
Application #AN2100

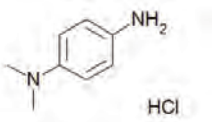
Conditions

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

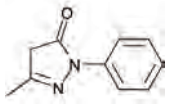
Analytes

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

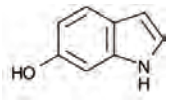




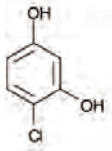
N,N-Dimethyl-1,4-phenylenediamine HCl



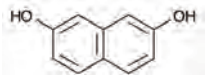
5-Methyl-2-phenyl-1,2-dihydropyrazol-3-one



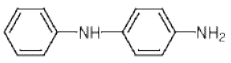
6-Hydroxyindole



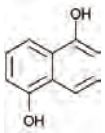
4-Chlororesorcinol



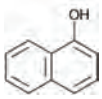
2,7-Dihydroxynaphthalene



4-Aminodiphenylamine



1,5-Dihydroxynaphthalene



1-Naphthol

Hair Dye Restricted Components (II)

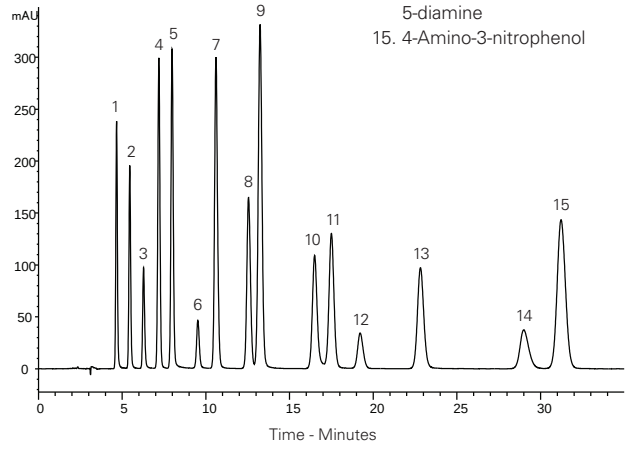
Application #AN2110

Conditions

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

Analytes

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



Halogenated Positional Isomer Separations

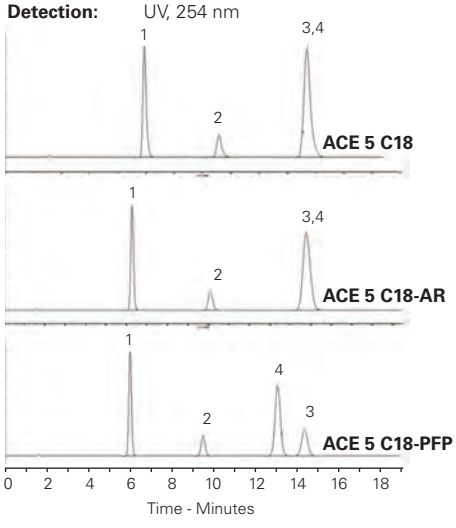
Application #AN1510

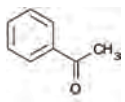
Conditions

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

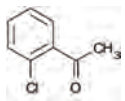
Analytes

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

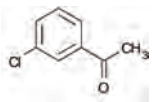




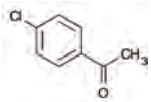
Acetophenone



o-Chloroacetophenone



m-Chloroacetophenone



p-Chloroacetophenone

Hepcidin-25 and Truncated Isoforms by LC-HRMS

Application #AN3090

Conditions

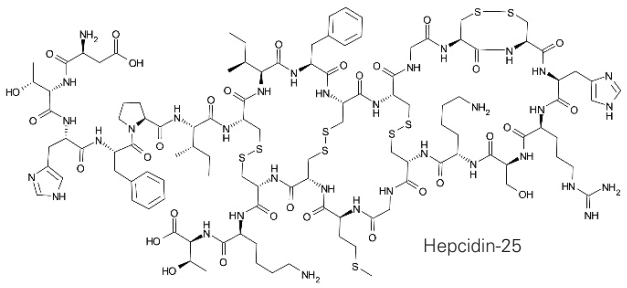
Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Gradient:

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

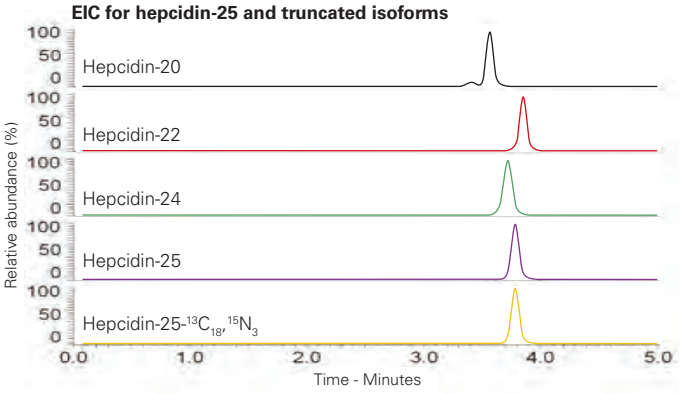
Flow Rate: 0.25 mL/min
Injection: 100 µL
Temperature: 60 °C
Detection: ThermoFisher Scientific Q-Exactive™ high resolution MS
Heated electrospray ionisation (positive mode)
Spray voltage: 4.5 kV
Vaporiser temperature: 200 °C
Capillary temperature: 320 °C
Detection: Full scan *m/z* 400 – 1000
Extracted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

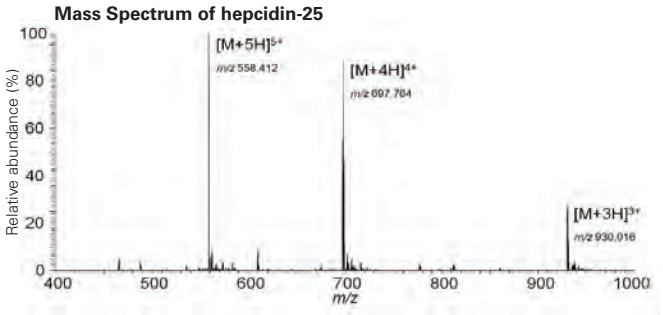
Analyte

1. Hepcidin-25
(MW 2789)



Hepcidin-25





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Herbicide – Benfluralin

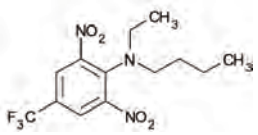
Application #AN2880

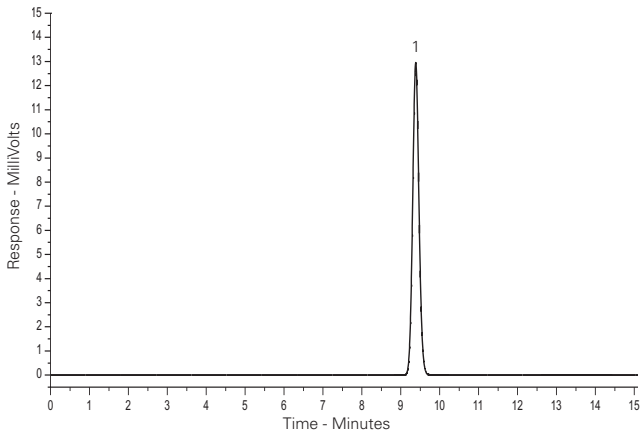
Conditions

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

Analyte

1. Benfluralin





Herbicide – Trifluralin

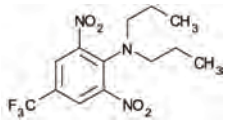
Application #AN2890

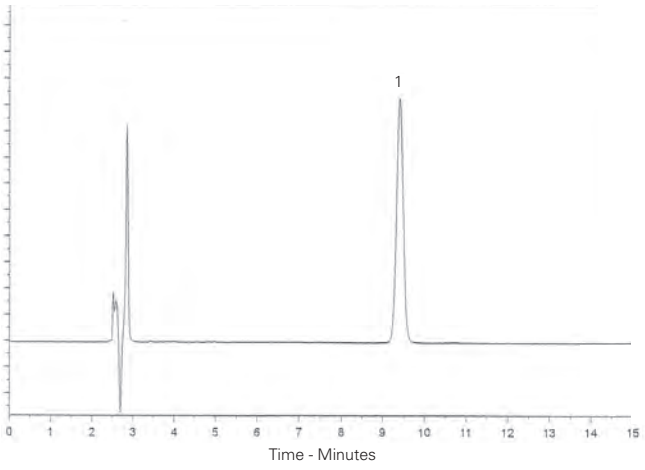
Conditions

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

Analyte

1. Trifluralin





Herbicide Impurity Profile

Application #AN2130

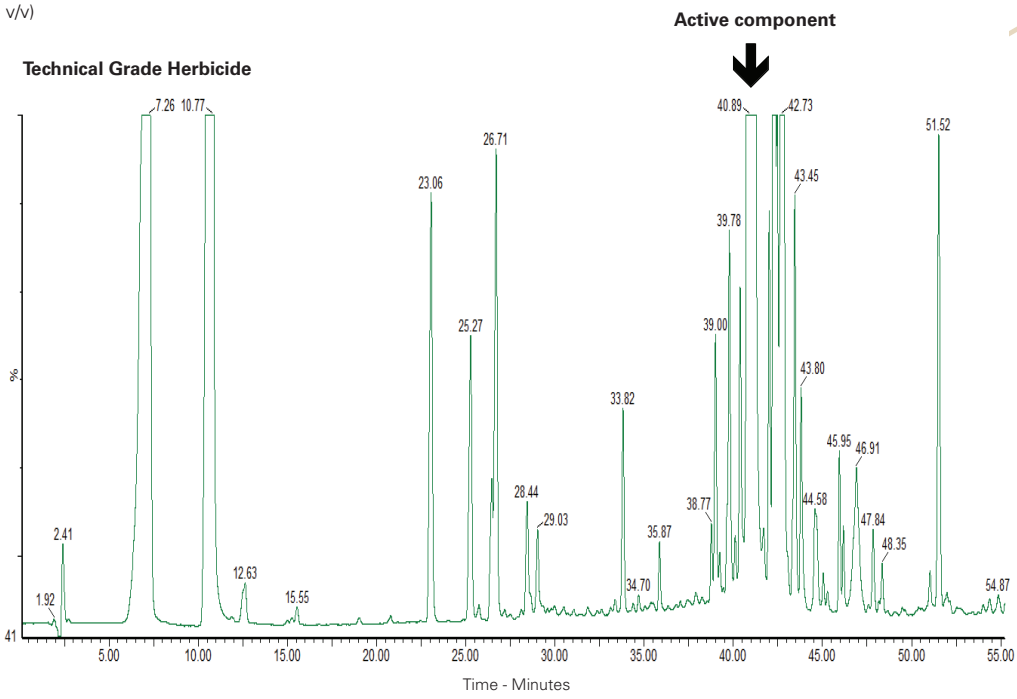
Conditions

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

Gradient:

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

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



Hippuric Acid

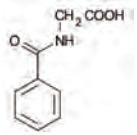
Application #AN2760

Conditions

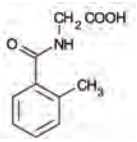
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM KH_2PO_4 pH 3.5 in H_2O/MeCN (15:85 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

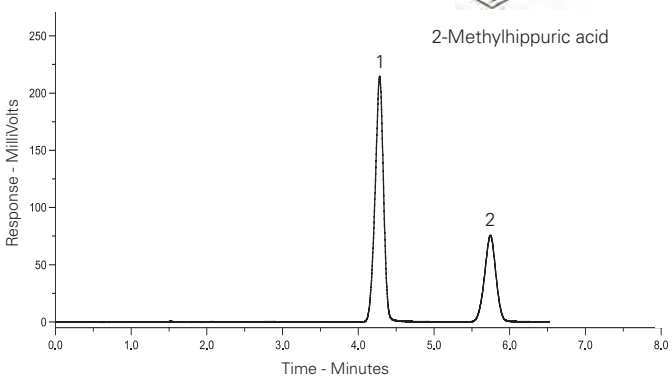
1. Hippuric acid
2. 2-Methylhippuric acid



Hippuric acid



2-Methylhippuric acid



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email: info@ace-hplc.com

Human Urine Metabolite Profiling by LC-MS

Application #AN2600

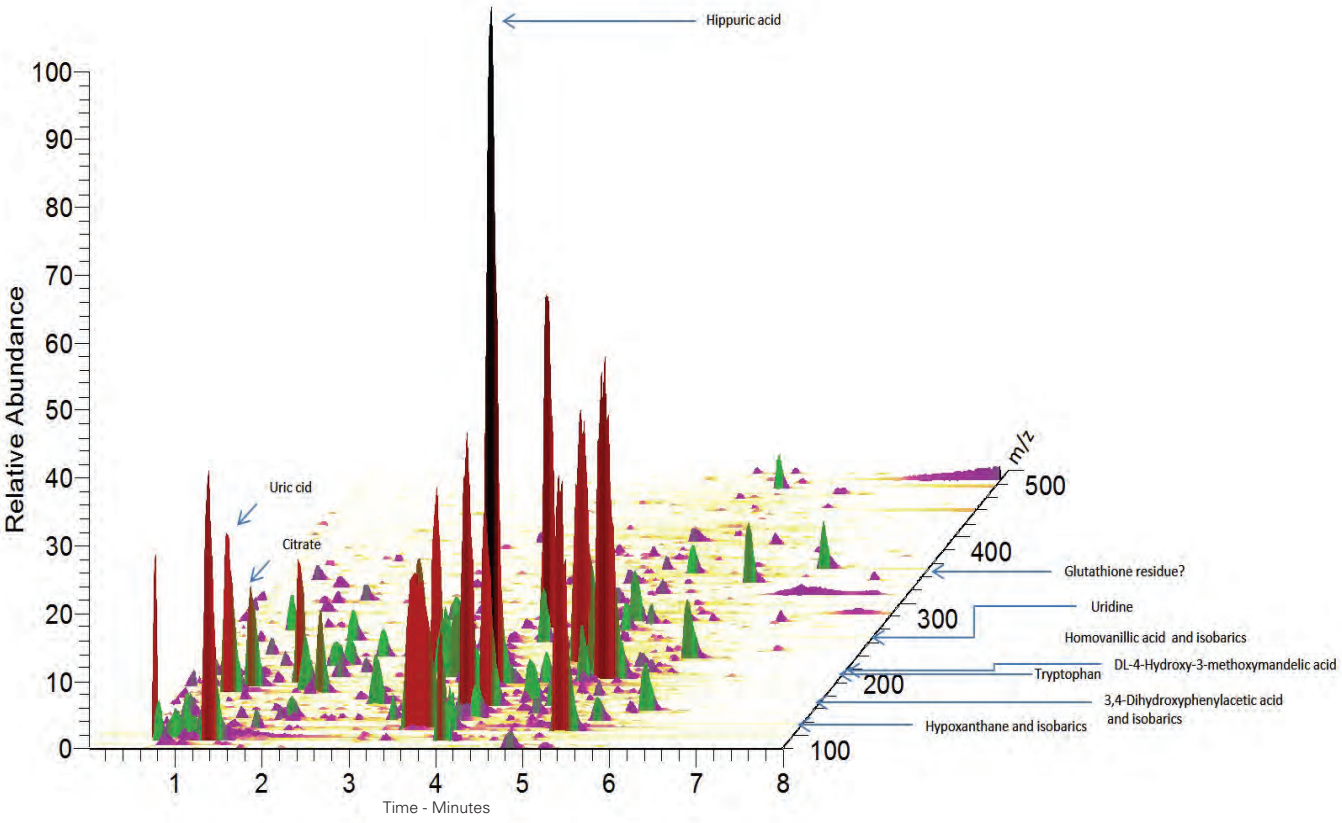
Conditions

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

Gradient:

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

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



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

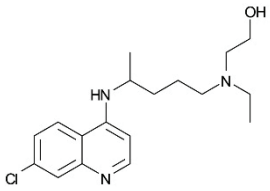
Application #AN1120

Conditions

Column:	ACE Excel 2 SuperC18
Dimensions:	50 x 2.1 mm
Part Number:	EXL-1011-0502U
Mobile Phase:	A: 0.5% Ammonium hydroxide pH 10 in H_2O B: 0.5% Ammonium hydroxide in MeCN
Gradient:	**Time (mins) %B** 0.00 30 1.50 100 2.50 100 2.51 30
Flow Rate:	0.4 mL/min
Injection:	5 µL
Temperature:	40 °C
Detection:	MS/MS detection with Waters TQD ESI +ve ion mode

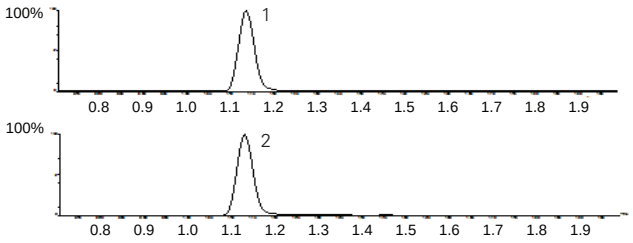
Analytes

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

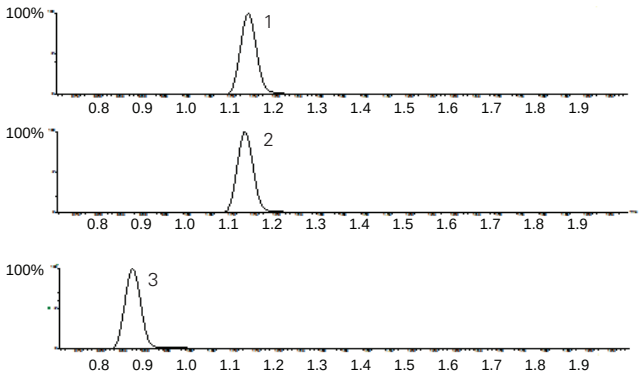


Hydroxychloroquine

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



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





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Combined Hypertension Therapy Drugs

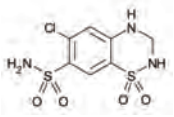
Application #AN4210

Conditions

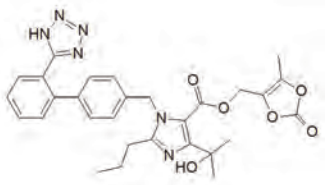
Column:	ACE 5 CN
Dimensions:	200 x 4.6 mm
Part Number:	ACE-124-2046
Mobile Phase:	10 mM phosphoric acid in H_2O, pH 2.5/MeCN/MeOH (80:7:13 v/v/v)
Flow Rate:	1 mL/min
Injection:	20 µL
Temperature:	30 °C
Detection:	UV, 235 nm
Sample:	1 µg/mL each analyte

Analytes

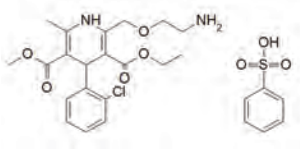
1. Hydrochlorothiazide
2. Olmesartan medoxomil
3. Amlodipine besylate
4. Valsartan



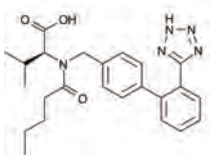
Hydrochlorothiazide



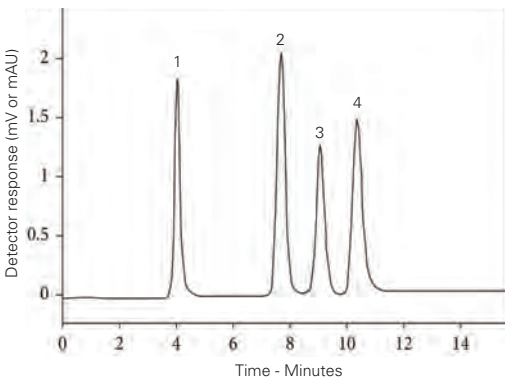
Olmesartan medoxomil



Amlodipine besylate



Valsartan



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

Ibuprofen and Related Impurities

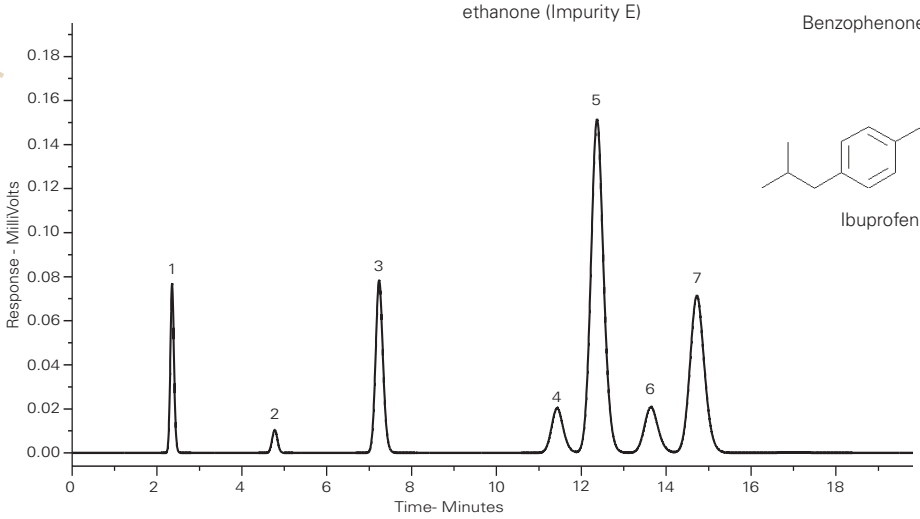
Application #AN4000

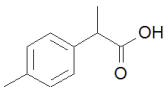
Conditions

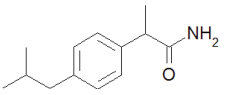
Column: ACE 5 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-121-1503
Mobile Phase: 0.1% TFA in H_2O/MeCN (64:36 v/v)
Flow Rate: 1.5 mL/min
Temperature: 40 °C
Detection: UV, 214 nm

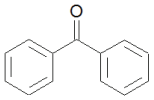
Analytes

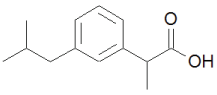
1. 2-(4-Methylphenyl) propanoic acid (Impurity D)
2. 2-(4-Isobutylphenyl) propanamide (Impurity C)
3. Benzophenone (IS)
4. 2-(3-Isobutylphenyl) propanoic acid (Impurity A)
5. Ibuprofen
6. 2-(4-Butylphenyl) propanoic acid (Impurity B)
7. 1-(4-Isobutylphenyl) ethanone (Impurity E)

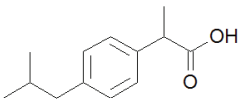


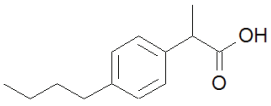

2-(4-Methylphenyl) propanoic acid (Impurity D)

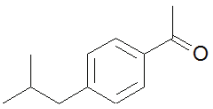

2-(4-Isobutylphenyl) propanamide (Impurity C)


Benzophenone (IS)


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


Ibuprofen


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


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

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Ibuprofen in Combination with Antihistamine and Decongestant

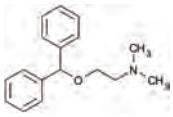
Application #AN2120

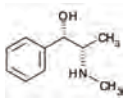
Conditions

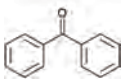
Column: ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: EXL-1112-1546U
Mobile Phase: 0.01% potassium dihydrogen phosphate/MeCN (60:40 v/v)
Flow Rate: 0.6 mL/min
Injection: 0.5 µL
Temperature: 45 °C
Detection: UV, 214 nm

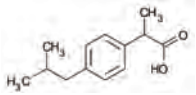
Analytes

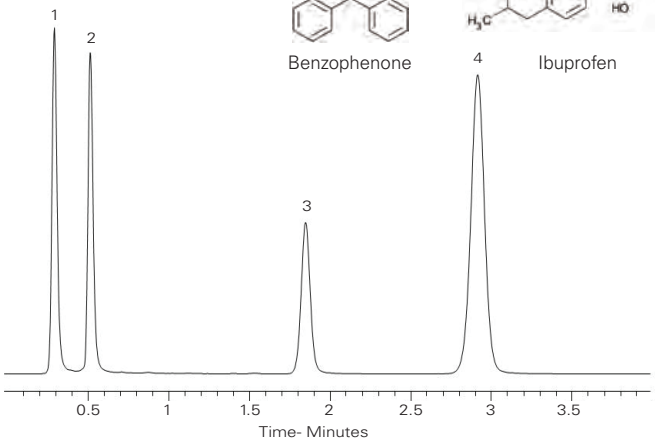
1. Diphenhydramine
2. Pseudoephedrine
3. Benzophenone
4. Ibuprofen


Diphenhydramine


Pseudoephedrine


Benzophenone


Ibuprofen



Alternative column dimensions available

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Illegal Dyes in Spices

Application #AN2910

Conditions

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

Gradient:

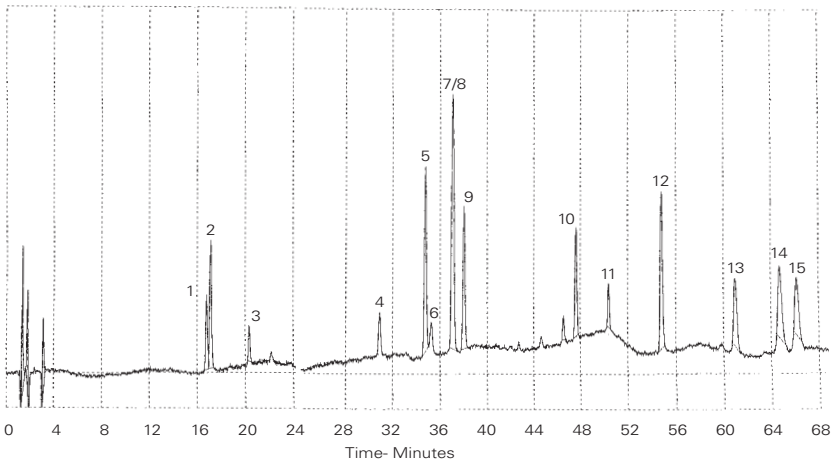
Time (mins)	%A	%B	%C	Curve
0	45	50	5	
45	3	92	5	6
65	3	92	5	11
66	45	50	5	1
75	45	50	5	1

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

Analytes

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





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Insulin Analogues in Clinical and Post-Mortem Analyses

Application #AN3350

Conditions

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

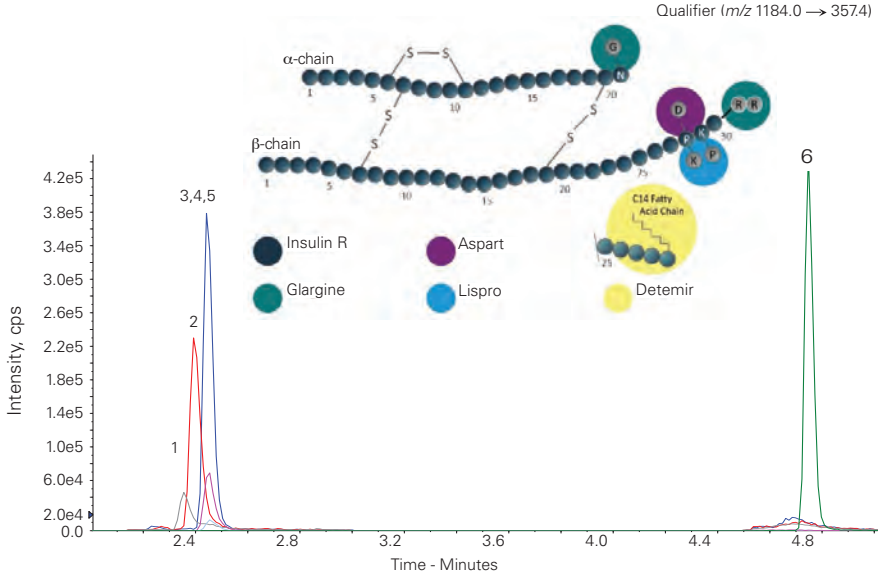
Gradient:

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

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

Analytes

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



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Insulins

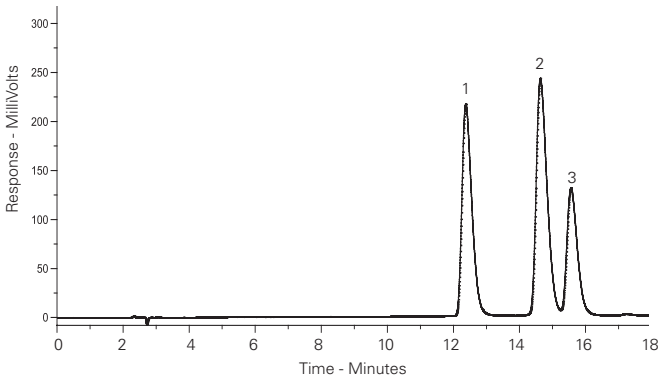
Application #AN2770

Conditions

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

Analytes

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



Isoflavones

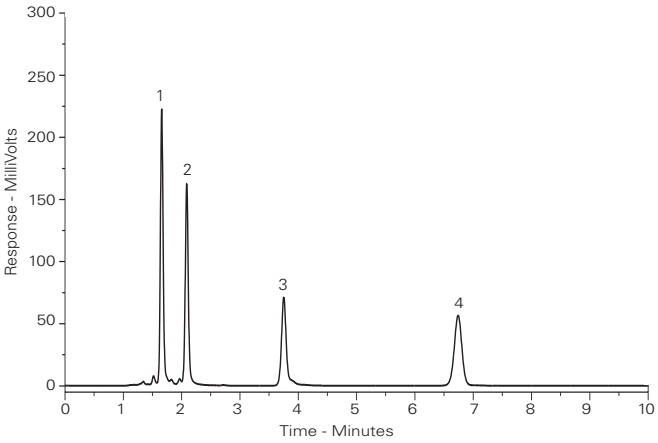
Application #AN2970

Conditions

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

Analytes

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



Isoflavones in Red Clover and Soy Extract

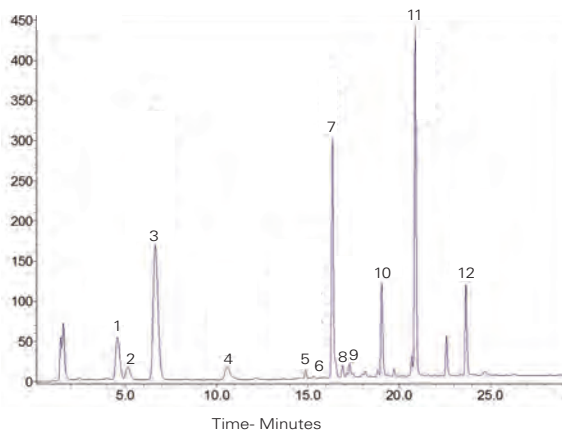
Application #AN1130

Conditions

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

Analytes

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



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



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

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

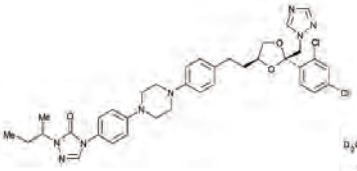
Application #AN3380

Conditions

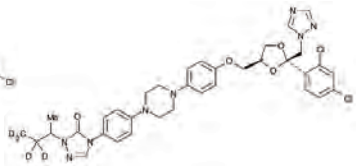
Column:	ACE 3 C18-AR
Dimensions:	50 x 2.1 mm
Part Number:	ACE-119-0502
Mobile Phase:	A: 10 mM ammonium acetate in H_2O
	B: 10 mM ammonium acetate in MeOH
Gradient:	**Time (mins) %B**
	0 75
	2 98
	3 98
Flow Rate:	0.7 mL/min
Temperature:	45 °C
Detection:	AB Sciex 4000
	ESI positive ion mode
Sample:	1.0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

Analytes

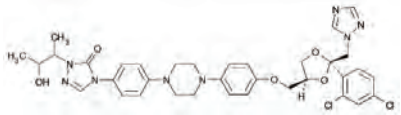
1. Itraconazole
   (*m/z* 705.3 → 392.3)
2. Itraconazole-d5
   (*m/z* 710.4 → 397.4)
3. Hydroxyitraconazole
   (*m/z* 721.3 → 408.2)
4. Hydroxyitraconazole-d5
   (*m/z* 726.4 → 413.3)



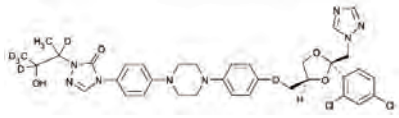
Itraconazole



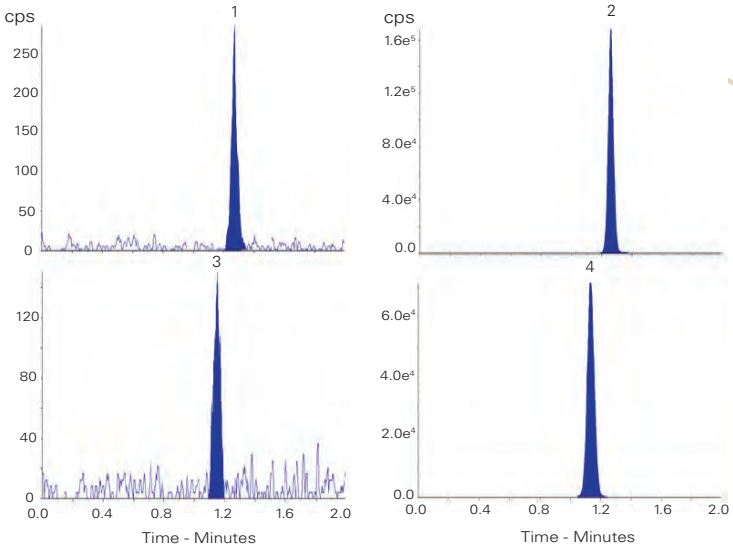
Itraconazole-d5



Hydroxyitraconazole



Hydroxyitraconazole-d5



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Lansoprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl

Application #AN1520

Conditions

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

Gradient:

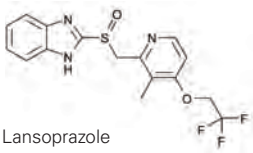
Time 1 (mins)	Time 2 (mins)	Time 3 (mins)	%B
0.0	0.0	0.0	10
15.0	30.0	45.0	90
15.5	30.5	45.5	90
18.0	33.0	48.0	10

Post time 10 minutes

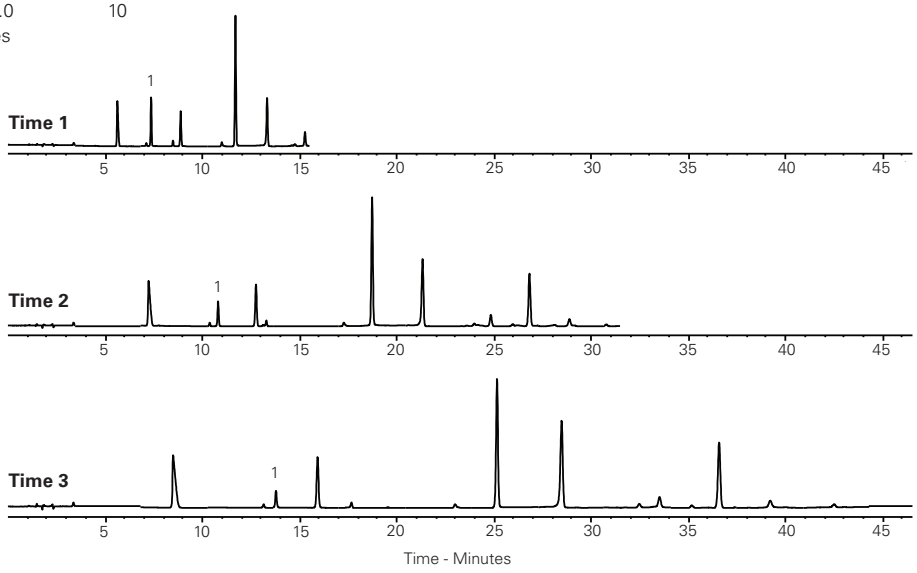
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 280 nm

Analyte

1. Lansoprazole



Lansoprazole



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

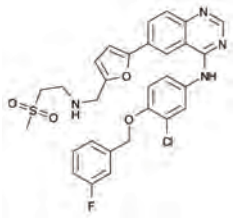
Application #AN3360

Conditions

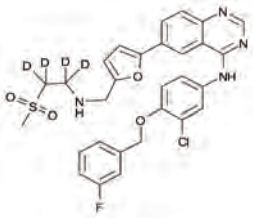
Column: ACE 5 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-121-1046
Mobile Phase: 10 mM ammonium formate pH 3.5/MeCN (10:90 v/v)
Flow Rate: 1 mL/min
Injection: 0.5 µL
Temperature: 40 °C
Detection: API 4000 triple quad MS
Positive ion mode ESI
Ion spray voltage: 5500 V
Temperature: 400 °C
Sample: Extracted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

Analytes

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

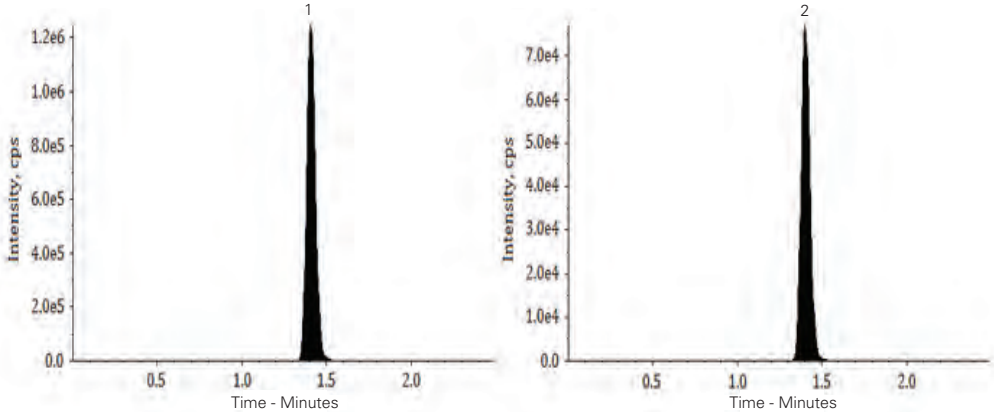


Lapatinib



Lapatinib-d4 (IS)

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



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Lidocaine in Saliva by LC-MS/MS

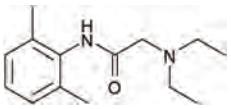
Application #AN2570

Conditions

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

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

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

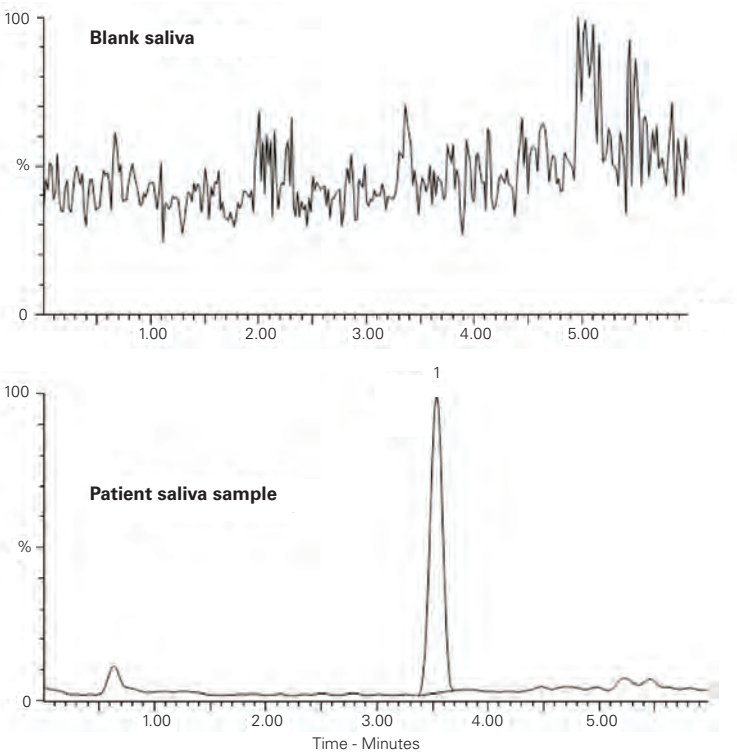


1. Lidocaine

Analyte

1. Lidocaine

(*m/z* 235 → 86)



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

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Lincosamide Antibiotics

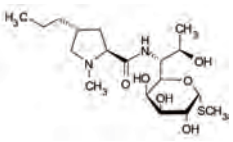
Application #AN2650

Conditions

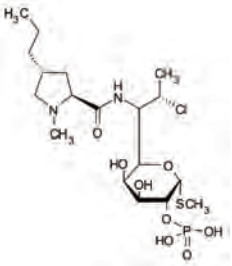
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	0.02 M sodium phosphate dibasic pH 3.0/MeCN (70:30 v/v)
Flow Rate:	1 mL/min
Injection:	25 µL
Temperature:	25 °C
Detection:	UV, 205 nm

Analytes

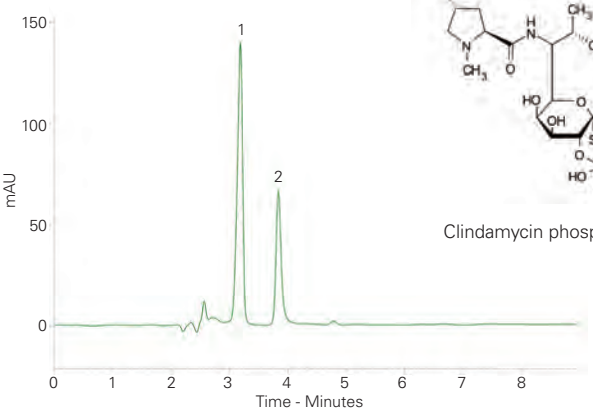
1. Lincomycin HCl
2. Clindamycin phosphate



Lincomycin HCl



Clindamycin phosphate



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Lipid Classes Separation from *Drosophila Melanogaster*

Application #AN1530

Conditions

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

Gradient:

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

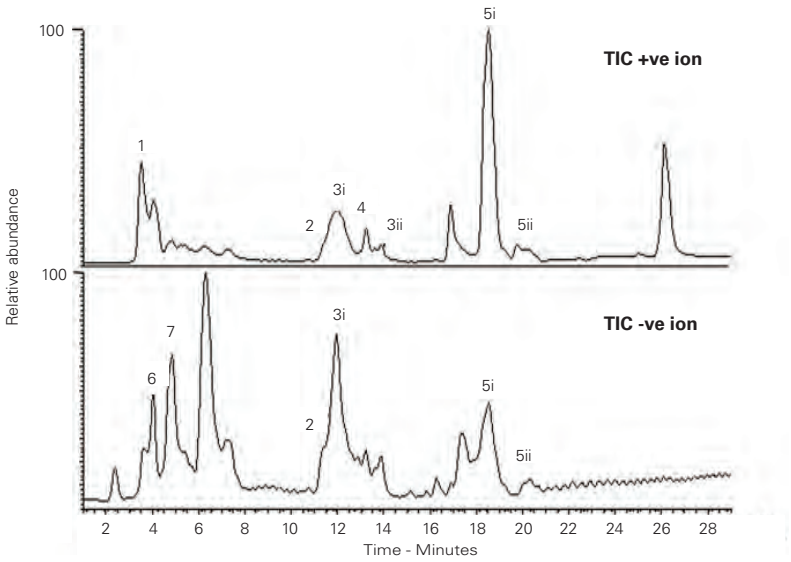
Flow Rate: 0.3 mL/min
Detection: LTQ Orbitrap MS
Positive and negative ion mode



Drosophila Melanogaster

Analytes

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



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Liquorice Extracts Fingerprint

Application #AN2090

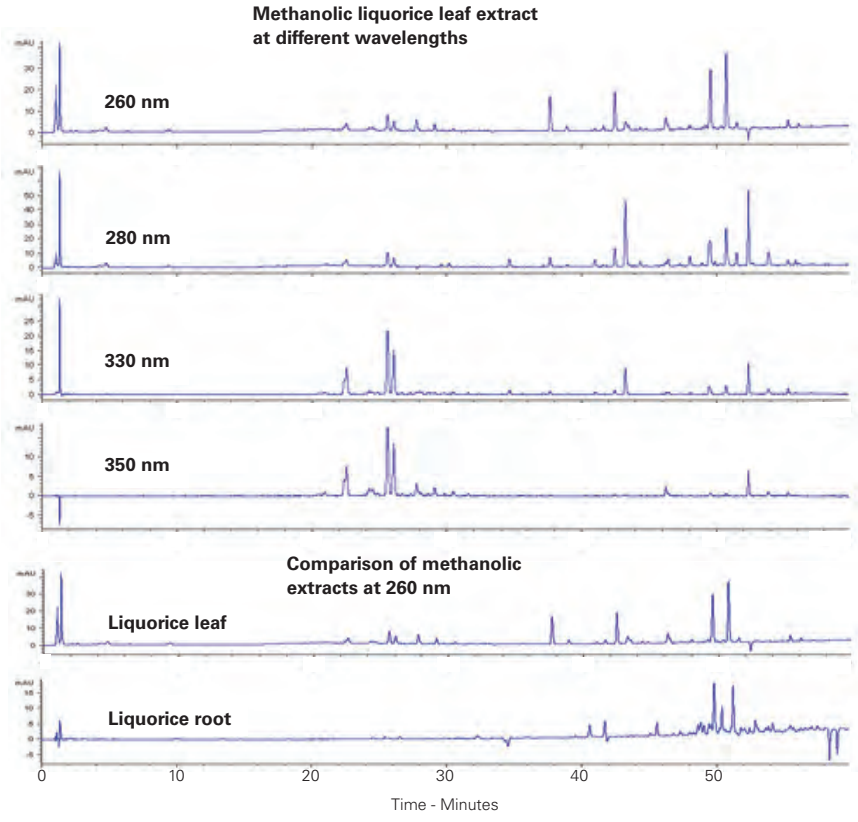
Conditions

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

Gradient:

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

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



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Local Anaesthetics

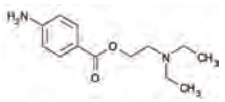
Application #AN3220

Conditions

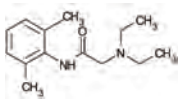
Column: ACE 5 AQ
Dimensions: 250 x 4.6 mm
Part Number: ACE-126-2546
Mobile Phase: MeCN/H_2O/2.5 M H_2SO_4 (21:79:0.1 v/v/v)
Flow Rate: 1.5 mL/min
Detection: UV

Analytes

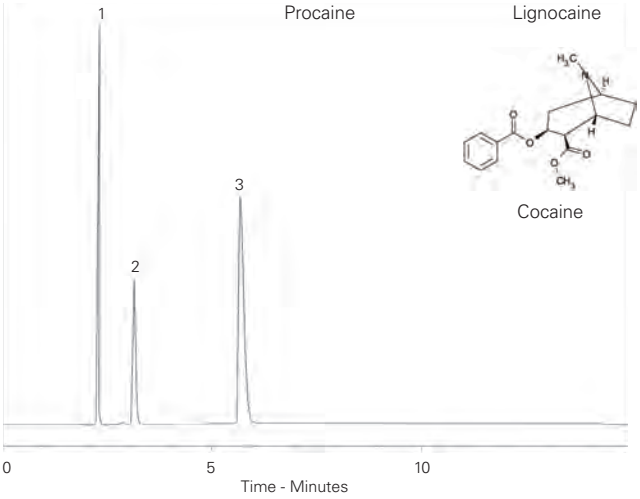
1. Procaine
2. Lignocaine
3. Cocaine



Procaine



Lignocaine



Cocaine

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15-Hydroxy Lubiprostone in Human Plasma

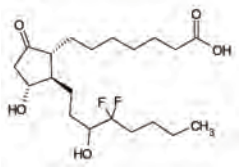
Application #AN1900

Conditions

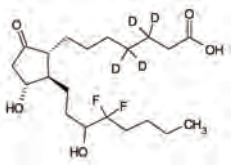
Column: ACE Excel 2 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-101-0503U
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeCN
Flow Rate: 0.65 mL/min
Injection: 15 µL
Temperature: 35 °C
Detection: MDS Sciex API 5000
TurbolonSpray negative mode
IonSpray voltage -4500 V
Source Temperature 450 °C

Analytes

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

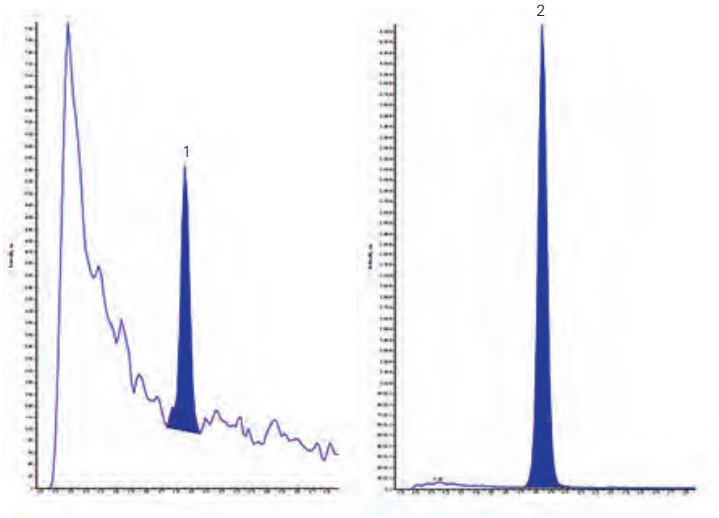


15-Hydroxy lubiprostone



15-Hydroxy lubiprostone-d4

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



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Lubricant Additives: ADPA/OPNA Antioxidants

Application #AN1170

Conditions

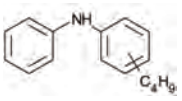
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	CORE-25A-1546U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN/IPA (1:2 v/v)

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

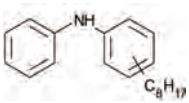
Flow Rate:	1 mL/min
Temperature:	60 °C
Detection:	UV, 220 nm

Analytes

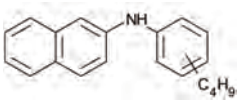
1. C4-ADPA
2. C8-ADPA
3. C4-OPNA
4. C12-ADPA
5. C16-ADPA



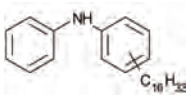
C4-ADPA



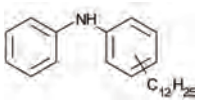
C8-ADPA



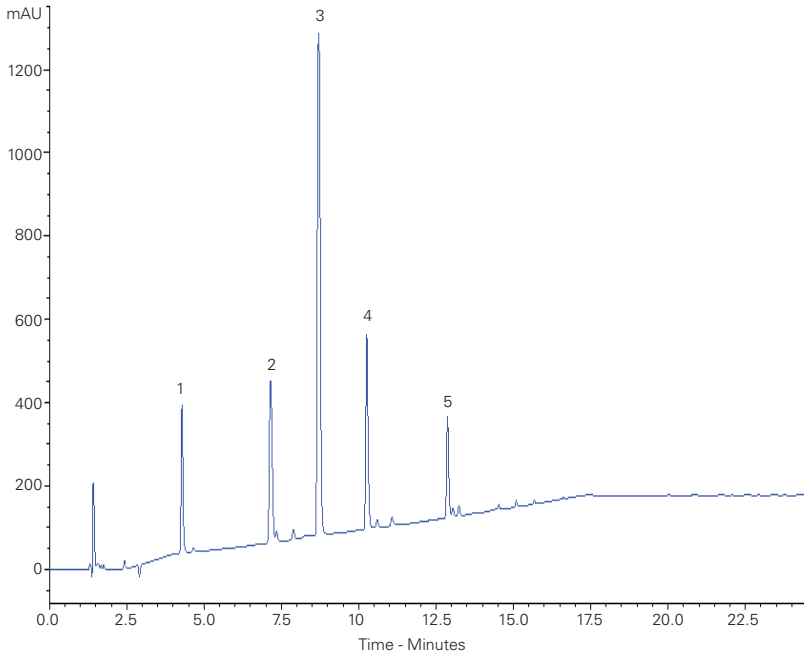
C4-OPNA



C16-ADPA



C12-ADPA



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Lurbinectedin in Plasma by LC-MS/MS

Application #AN3810

Conditions

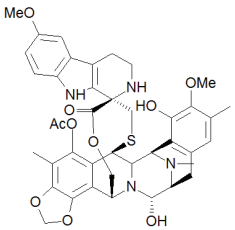
Column:	ACE 3 C18-PFP
Dimensions:	30 x 2.1 mm
Part Number:	ACE-1110-0302
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

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

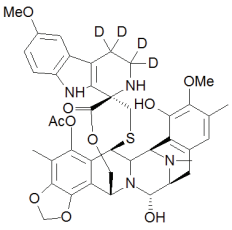
Flow Rate:	0.6 mL/min
Injection:	5 µL
Temperature:	50 °C
Detection:	API 4000 triple quad
	TurbolonSpray, ESI positive ion mode
	Turbo Temperature: 650 °C
	Ion Spray Potential: 5000 V

Analytes

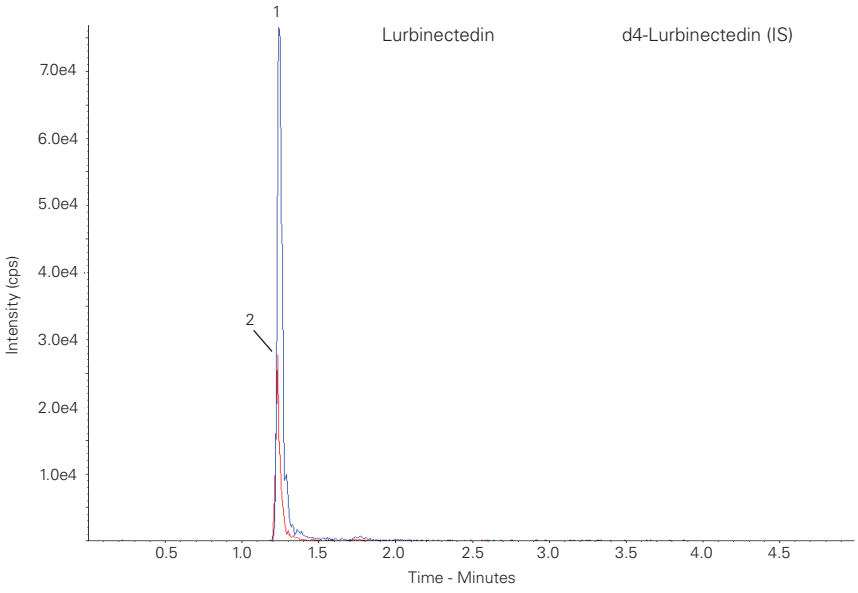
1. Lurbinectedin
   (*m/z* 767.3 → 273.0)
   (LLOQ 0.1 ng/mL)
2. d4-Lurbinectedin (IS)
   (*m/z* 771.4 → 277.0)



Lurbinectedin



d4-Lurbinectedin (IS)



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Malachite Green

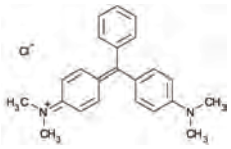
Application #AN2860

Conditions

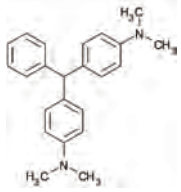
Column:	ACE 5 C18
Dimensions:	150 x 3.0 mm
Part Number:	ACE-121-1503
Mobile Phase:	10 mM oxalic acid pH 2.9 in H_2O/MeCN (80:20 v/v)
Flow Rate:	0.4 mL/min
Temperature:	Ambient
Detection:	UV-Vis, 618 nm

Analytes

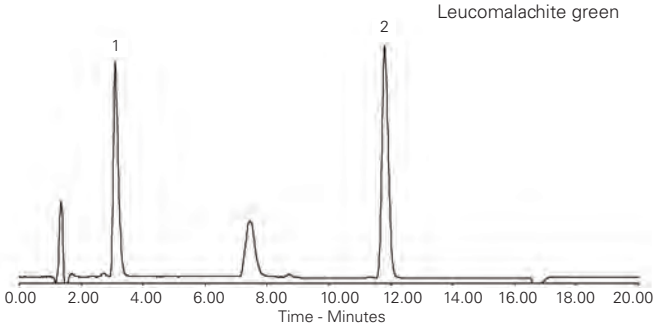
1. Malachite green
2. Leucomalachite green



Malachite green



Leucomalachite green



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Maleic and Fumaric Acids

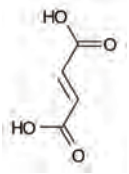
Application #AN3230

Conditions

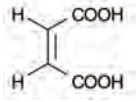
Column:	ACE 5 AQ
Dimensions:	250 x 4.6 mm
Part Number:	ACE-126-2546
Mobile Phase:	50 mM KH_2PO_4 pH 7.0 in H_2O
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 210 nm

Analytes

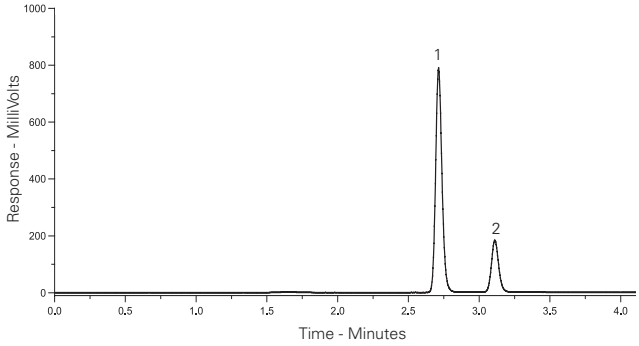
1. Fumaric acid
2. Maleic acid



Fumaric acid



Maleic acid



MDMA (Ecstasy) and PMA (Dr Death) Separation

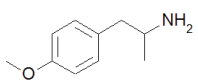
Application #AN4220

Conditions

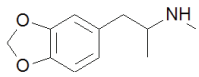
Column:	ACE 3 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-111-1546
Mobile Phase:	0.05 M KH_2PO_4 pH 3.2 in H_2O/MeCN (90:10 v/v)
Flow Rate:	1.2 mL/min
Injection:	10 µL
Temperature:	22 °C
Detection:	UV, 210 nm

Analytes

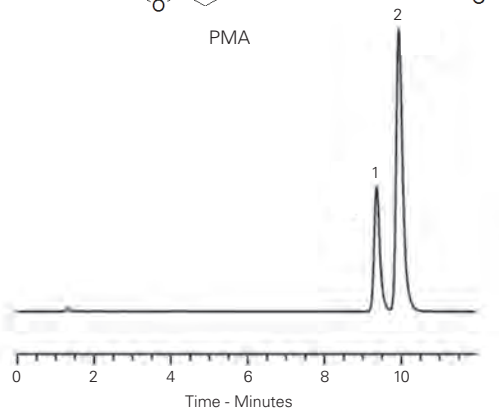
1. PMA
   (4-Methoxyamphetamine)
   LOD 0.08 µg/mL
   LOQ 0.26 µg/mL
2. MDMA
   (3,4-Methylenedioxy methamphetamine)
   LOD 0.04 µg/mL
   LOQ 0.12 µg/mL



PMA



MDMA



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

Melamine using Ion-Pairing Reagent

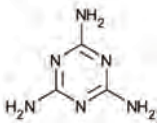
Application #AN2510

Conditions

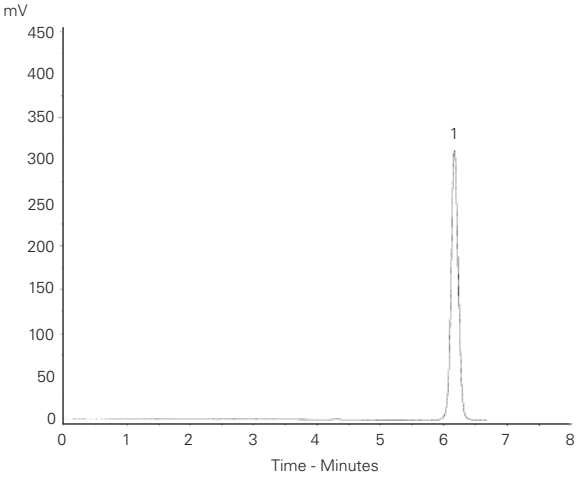
Column:	ACE 5 C8
Dimensions:	150 x 4.6 mm
Part Number:	ACE-122-1546
Mobile Phase:	5 mM heptafluorobutyric acid/MeCN (95:5 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	Ambient
Detection:	UV, 240 nm

Analyte

1. Melamine



Melamine



Metabolomic Analysis of Extracted Jurkat T Cells by LC-HRMS

Application #AN3980

Conditions

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

Gradient:

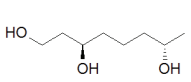
Time (mins)	%B
0	0
1	0
11	65
13	65
18	95
20	95

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

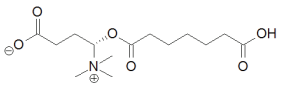
TIC overlay for Jurkat T-lymphocyte cells rinsed with either 0.3% ammonium formate (darker line) or 0.3% ammonium acetate.

Analytes

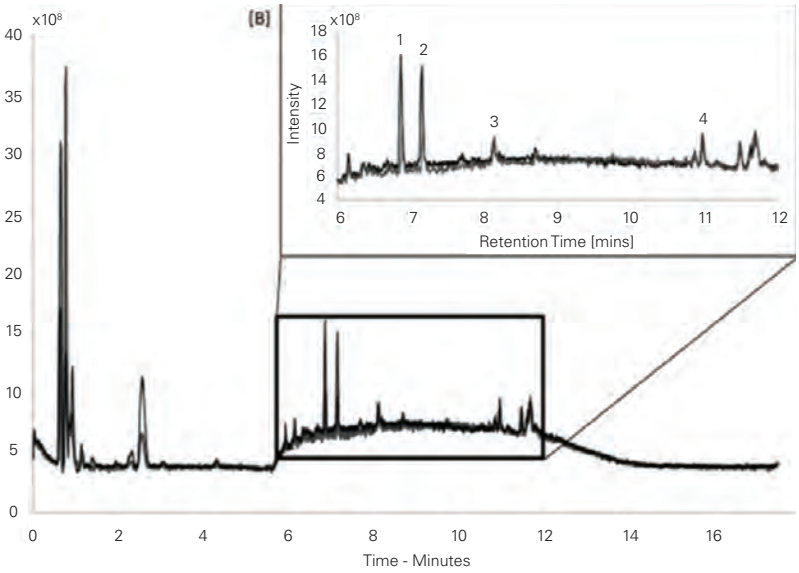
1. Caffeine-d3 (IS)
2. Tryptophan-d3 (IS)
3. 1,3,7-Octanetriol
4. Pimelylcarnitine



1,3,7-Octanetriol



Pimelylcarnitine



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

Metabolomic Biomarkers in Ethylmalonic Encephalopathy

Application #AN4130

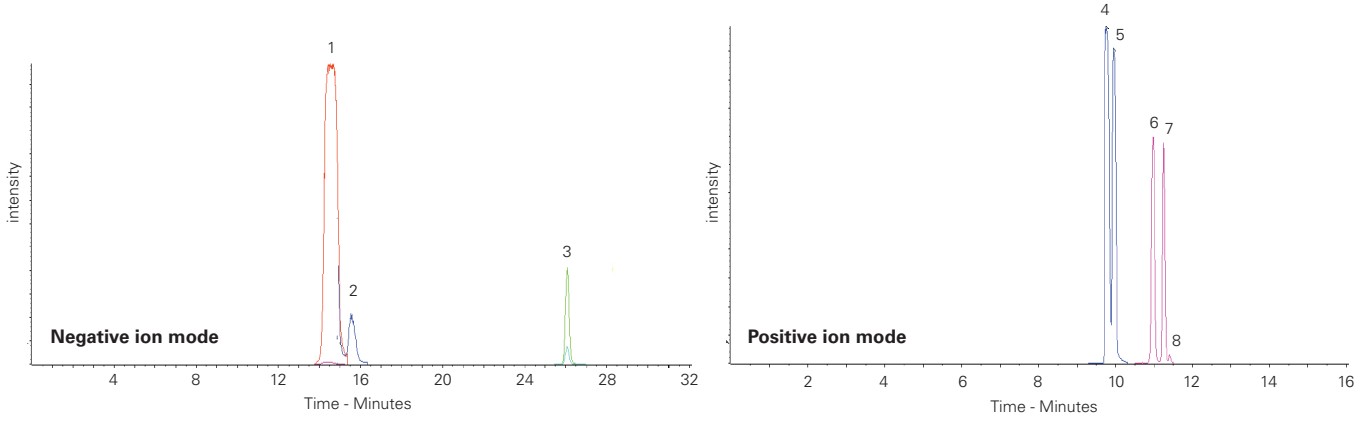
Conditions

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

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

Analytes

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



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Metabolomics and Biochemical Genetics - Acylglycines

Application #AN4080

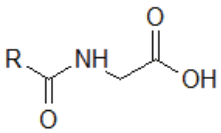
Conditions

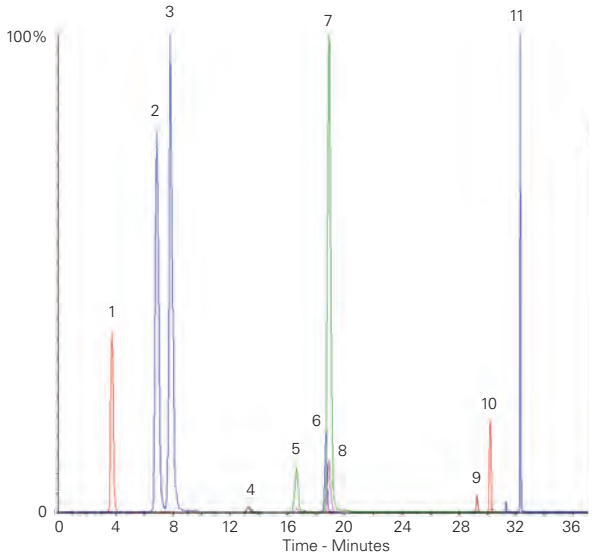
Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
ESI in negative ion mode
Sample: Urine / plasma sample is filtered and extracted with ice-cold methanol, evaporated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

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

Analytes

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





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Metabolomics – C4 & C5 Hydroxy and Dicarboxylic Acids

Application #AN4110

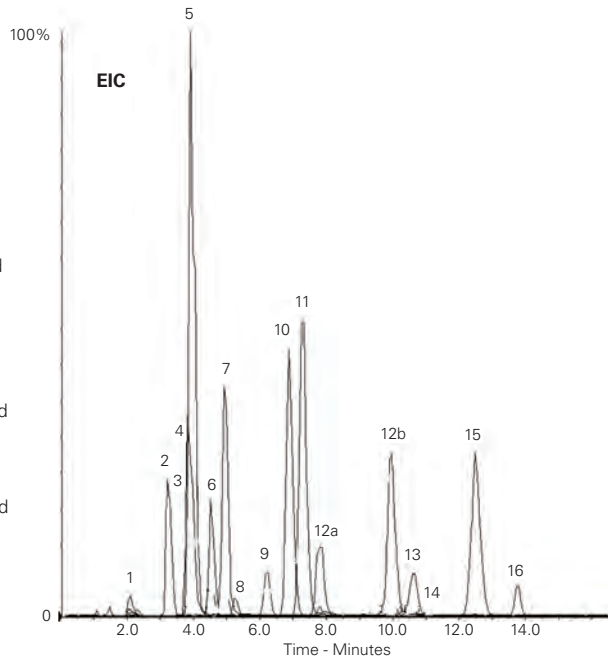
Conditions

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

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

Analytes

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



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Metabolomics – C4 Hydroxy Acids

Application #AN4120

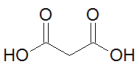
Conditions

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

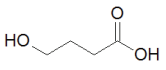
Please contact info@ace-hplc.com for additional information on the chromatographic conditions used for this analysis.

Analytes

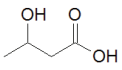
1. Malonic acid (*m/z* 103 → 59)
2. 4-Hydroxybutyric acid (*m/z* 103 → 57)
3. 3-Hydroxybutyric acid (*m/z* 103 → 59)
4. 3-Hydroxyisobutyric acid (*m/z* 103 → 73)
5. 2-Hydroxybutyric acid (*m/z* 103 → 57)



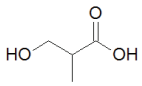
Malonic acid



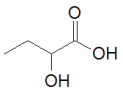
4-Hydroxybutyric acid



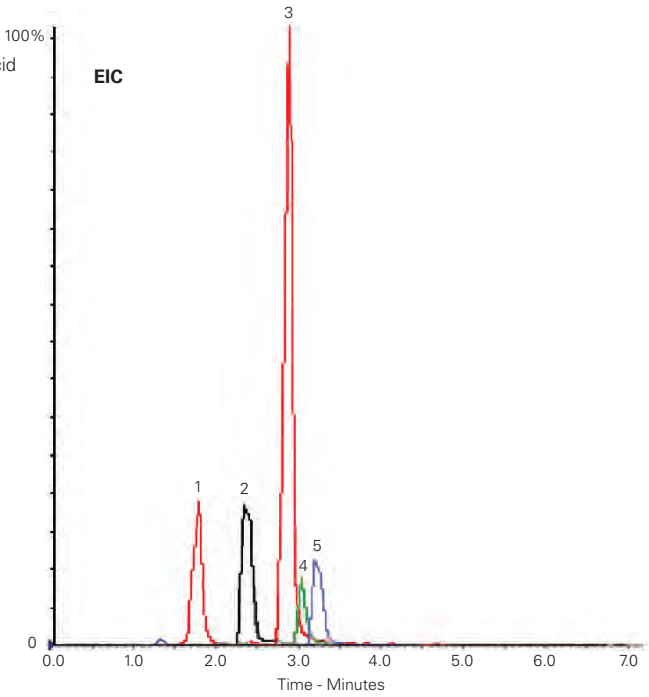
3-Hydroxybutyric acid



3-Hydroxyisobutyric acid



2-Hydroxybutyric acid



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Metabolomics – C6 & C7 Hydroxy and Dicarboxylic Acids

Application #AN4100

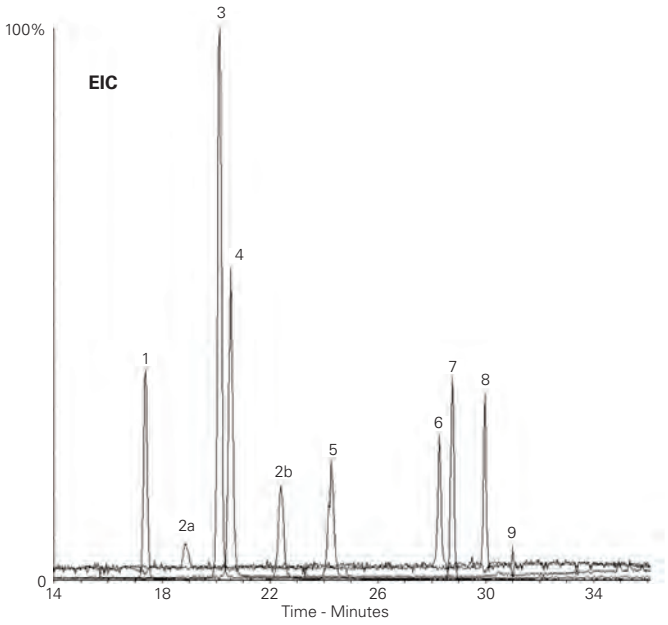
Conditions

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

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

Analytes

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



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Methotrexate in K_3EDTA Human Plasma by LC-MS/MS

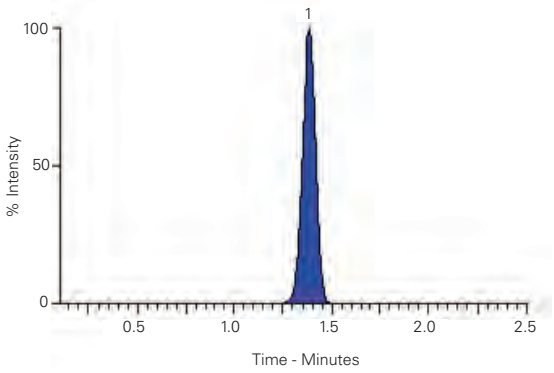
Application #AN3760

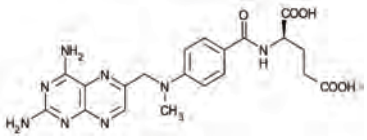
Conditions

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

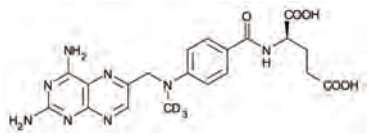
Analytes

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

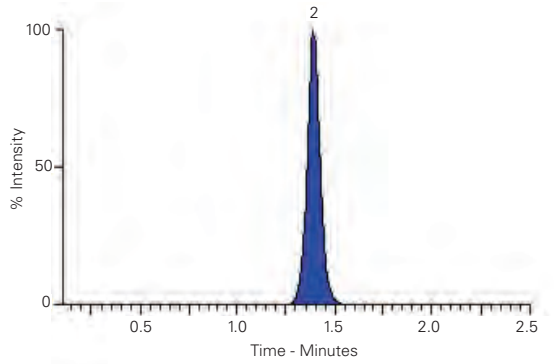




Methotrexate



Methotrexate-d3 (I.S.)



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17α-Methyltestosterone in Freshwater Tilapia Aquaculture

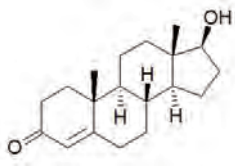
Application #AN4340

Conditions

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

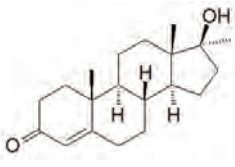
Analytes

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

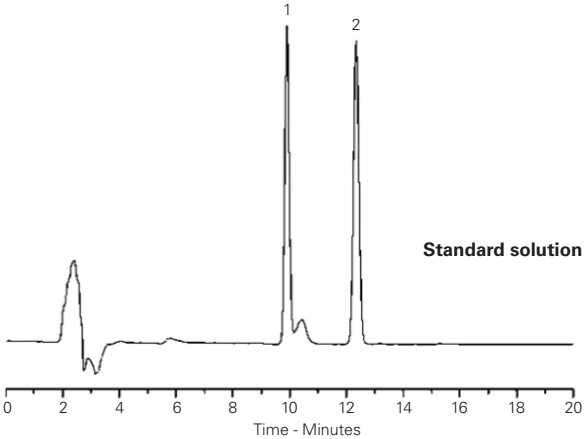


Testosterone (IS)

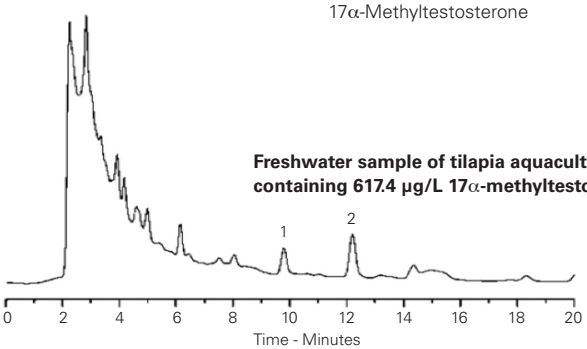
17α-Methyltestosterone is used for sex reversal of tilapia fish in order to avoid overpopulation in ponds. It therefore has to be monitored in aqueous matrices to prevent release into the environment.



17α-Methyltestosterone



Standard solution (600 µg/L)



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

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

mGluR5 PET Tracer by Radio HPLC Analysis

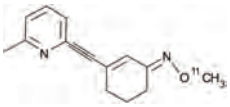
Application #AN2700

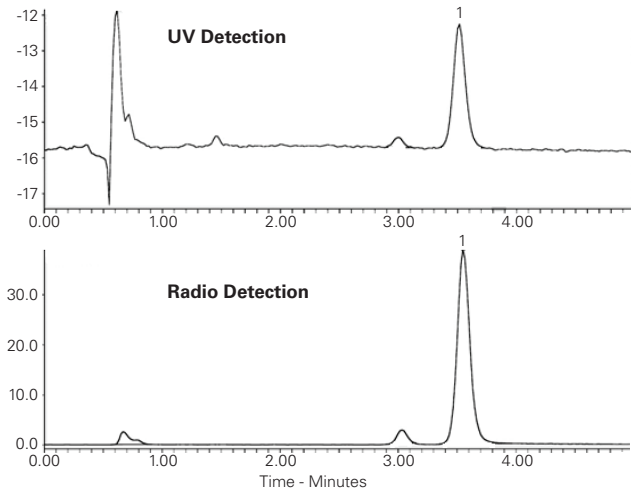
Conditions

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

Analyte

1. ^{11}C-ABP688





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For additional column dimensions

Please enquire
email: info@ace-hplc.com

Microbial Extract by LC-MS

Application #AN1180

Conditions

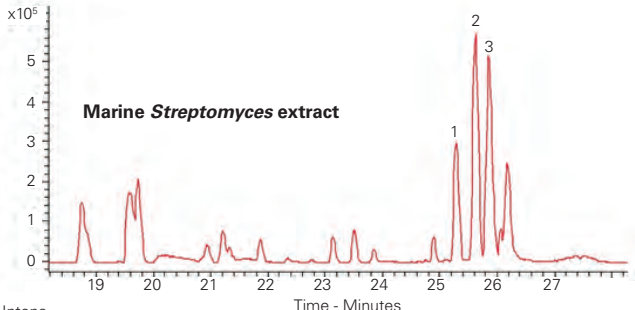
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: CORE-25A-1502U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Gradient:

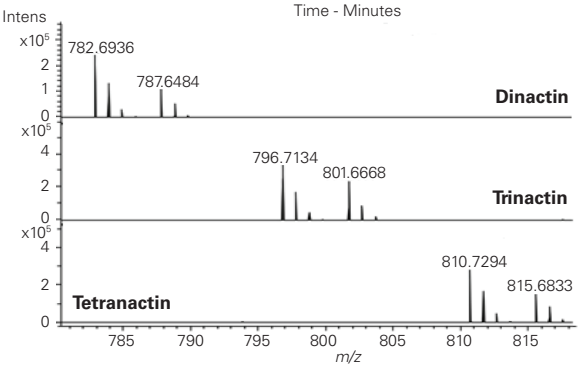
Time (mins)	%B
0.0	5
5.0	5
20.0	100
25.0	100

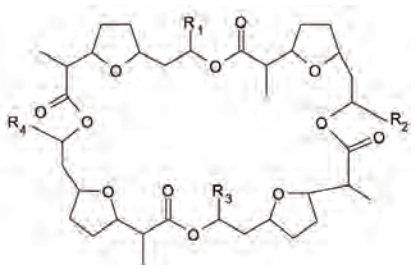
Flow Rate: 0.2 mL/min
Detection: Dionex 3000RS UHPLC system
coupled with Bruker MaXis Q-TOF MS
Electrospray MS positive mode
Source end plate offset -500 V
Nebuliser gas (N_2) 1.6 bar
Drying gas (N_2) temp 180 °C
Collision energy 5.0 eV
Collision RF 600 Vpp

Analytes

Macrotetralides
1. Dinactin $R_1 = R_3 = CH_2CH_3$, $R_2 = R_4 = CH_3$
2. Trinactin $R_1 = R_2 = R_3 = CH_2CH_3$, $R_4 = CH_3$
3. Tetranactin $R_1 = R_2 = R_3 = R_4 = CH_2CH_3$







Macrotetralides

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Microcystins from Blue/Green Algae in Drinking Water

Application #AN1190

Conditions

Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeCN

Gradient:

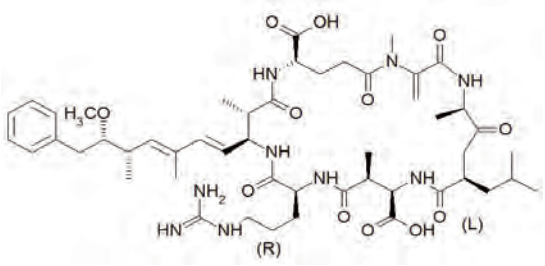
Time (mins)	%B
0.0	30
1.0	30
7.0	95
7.1	30
10.0	30

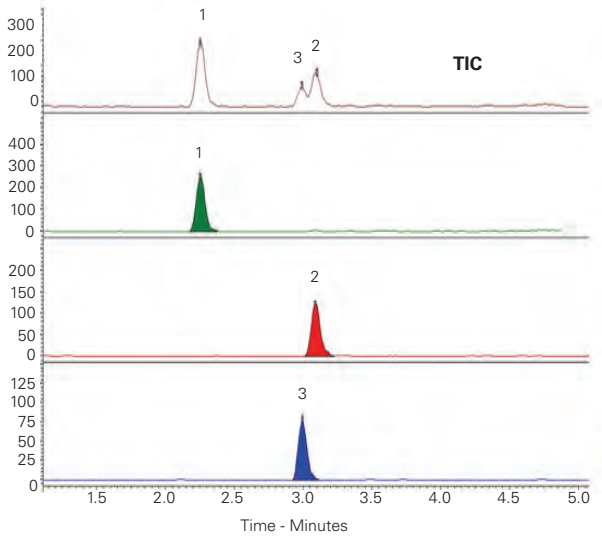
Flow Rate: 0.4 mL/min
Injection: 50 µL
Temperature: 40 °C
Sample: 0.05 ppb
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 350 °C
Cone gas temperature: 200 °C
Spray voltage: 4500 V (+)
Collision gas: argon 1.5 mTorr

Analytes

1. Microcystin RR (MW 1038)
   (*m/z* 520 → 135)
2. Microcystin LR (MW 995)
   (*m/z* 498 → 135)
3. Microcystin YR (MW 1045)
   (*m/z* 523 → 135)

Variants	R	L
Microcystin-LR	Leucine	Arginine
Microcystin-RR	Arginine	Arginine
Microcystin-YR	Tyrosine	Arginine





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Milk Proteins

Application #AN1540

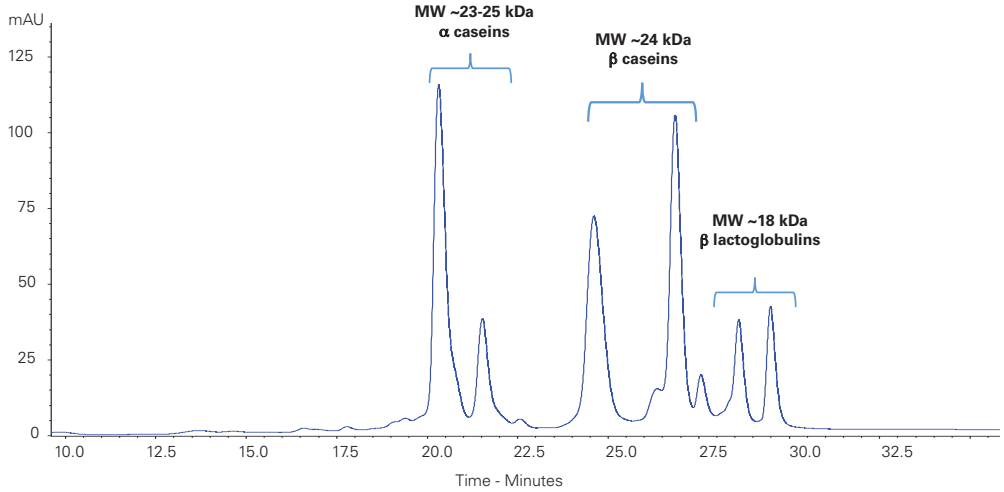
Conditions

Column: ACE 5 C18-300
Dimensions: 150 x 2.1 mm
Part Number: ACE-221-1502
Mobile Phase: A: 0.01% TFA in H_2O
B: 0.01% TFA in MeCN

Gradient:

Time (mins)	%B
0.0	33
5.0	33
9.0	35
18.0	37
22.0	40
27.5	41
28.0	41
43.0	43

Flow Rate: 0.2 mL/min
Temperature: 45 °C
Detection: UV, 214 nm



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Mycotoxins by LC-MS/MS

Application #AN2330

Conditions

Column: ACE Excel 2 C18-AR
Dimensions: 50 x 2.1 mm
Part Number: EXL-109-0502U
Mobile Phase: A: 1 mM ammonium acetate, 0.5% acetic acid in H_2O
B: 1 mM ammonium acetate, 0.5% acetic acid in 95% MeOH

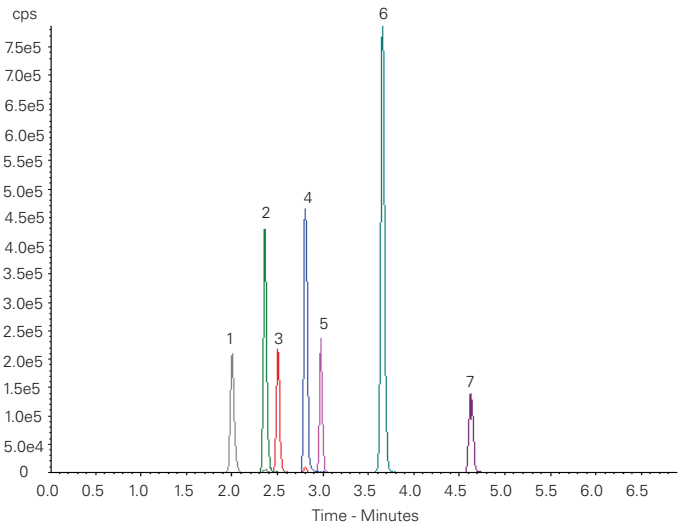
Gradient:

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

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

Analytes

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



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Mycotoxins/Aflatoxins from Peppers

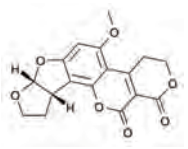
Application #AN1200

Conditions

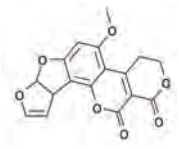
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: H_2O/MeOH (60:40 v/v)
Flow Rate: 1 mL/min
Injection: 100 µL
Temperature: 45 °C
Detection: Fluorescence, λ_{Ex} 362 nm, λ_{Em} 425 nm

Analytes

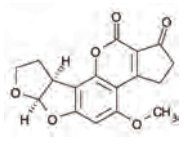
1. Aflatoxin G2
2. Aflatoxin G1
3. Aflatoxin B2
4. Aflatoxin B1



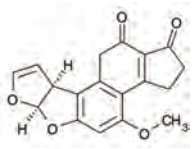
Aflatoxin G2



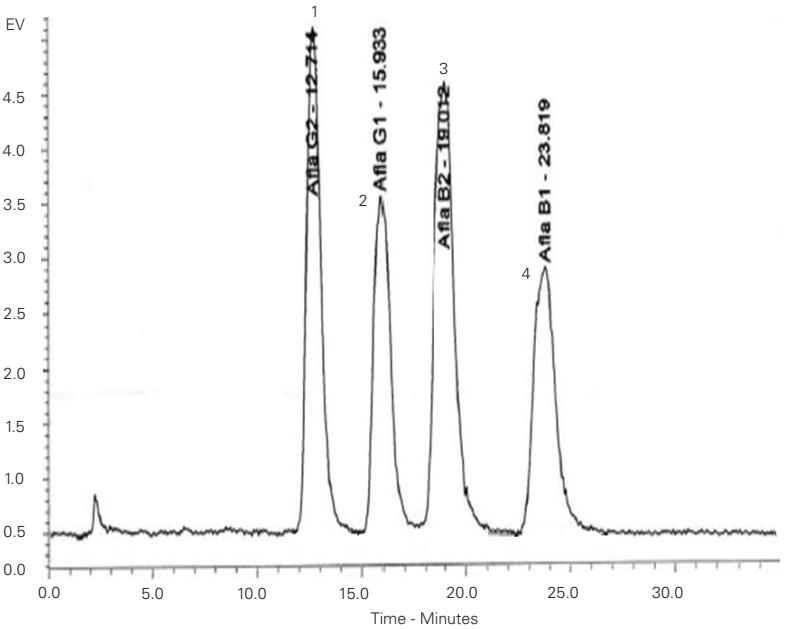
Aflatoxin G1



Aflatoxin B2



Aflatoxin B1



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Naphthalenes (Substituted)

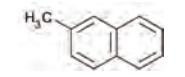
Application #AN3690

Conditions

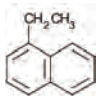
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	MeCN/H_2O (51:49 v/v)
Flow Rate:	1.5 mL/min
Temperature:	18 °C
Detection:	UV, 225 nm

Analytes

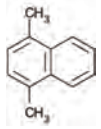
1. 2-Methylnaphthalene
2. 1-Ethylnaphthalene
3. 1,4-Dimethylnaphthalene
4. 2-Ethylnaphthalene
5. n-Butylbenzene



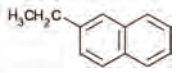
2-Methylnaphthalene



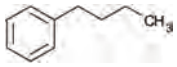
1-Ethylnaphthalene



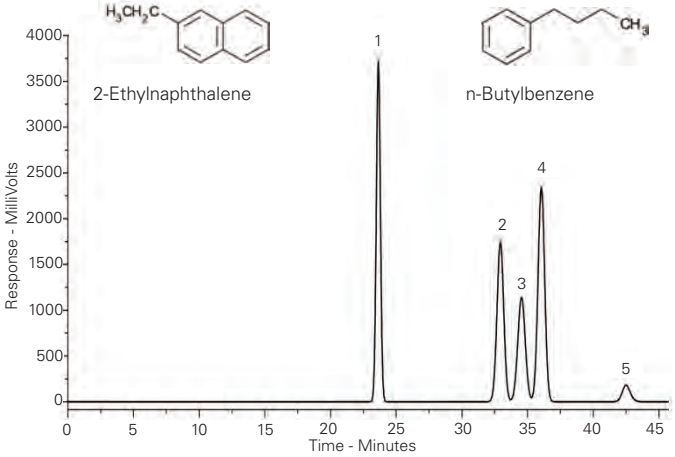
1,4-Dimethylnaphthalene



2-Ethylnaphthalene



n-Butylbenzene



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ACE columns are available in an extensive range of phases, particle sizes and dimensions

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email: info@ace-hplc.com

Neonicotinoids in Honey by LC-MS/MS

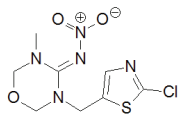
Application #AN4050

Conditions

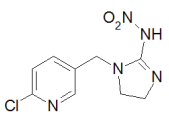
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	100 x 2.1 mm
Part Number:	CORE-25A-1002U
Mobile Phase:	A: 0.05% ammonia in H_2O
	B: 0.05% ammonia in MeOH
Gradient:	**Time (mins) %B**
	0 5
	3 100
Flow Rate:	0.6 mL/min
Injection:	1 µL (POISe mode)
Temperature:	30 °C
Detection:	Shimadzu LCMS-8060
	Positive ion mode HESI
Sample:	Honey spiked at 0.1 ppb
	(QuEChERS extract)

Analytes

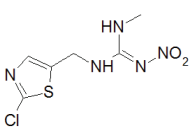
1. Thiamethoxam
   (*m/z* 292 → 211)
2. Imidacloprid
   (*m/z* 256 → 175)
3. Clothianidin
   (*m/z* 250 → 169)
4. Acetamiprid
   (*m/z* 223 → 126)
5. Thiacloprid
   (*m/z* 253 → 126)



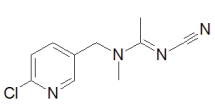
Thiamethoxam



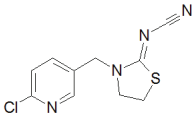
Imidacloprid



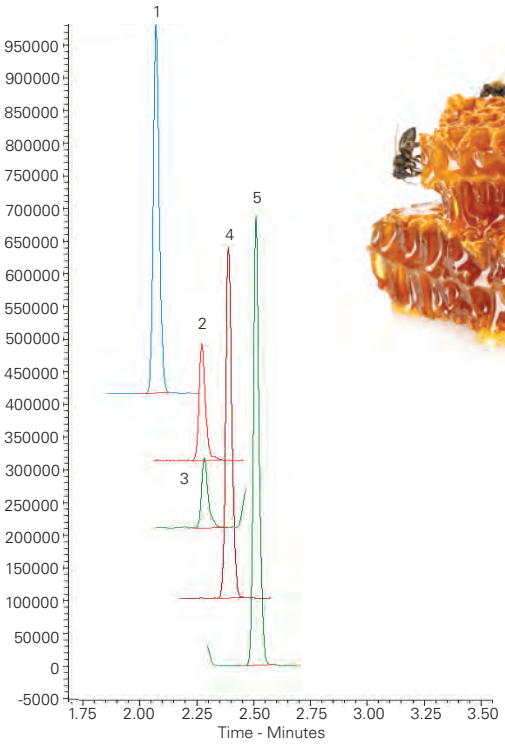
Clothianidin



Acetamiprid



Thiacloprid





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Neurotransmitters and Metabolites from Rat Brain by LC-MS/MS

Application #AN3870

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: A: 0.2% formic acid in H_2O
B: MeCN

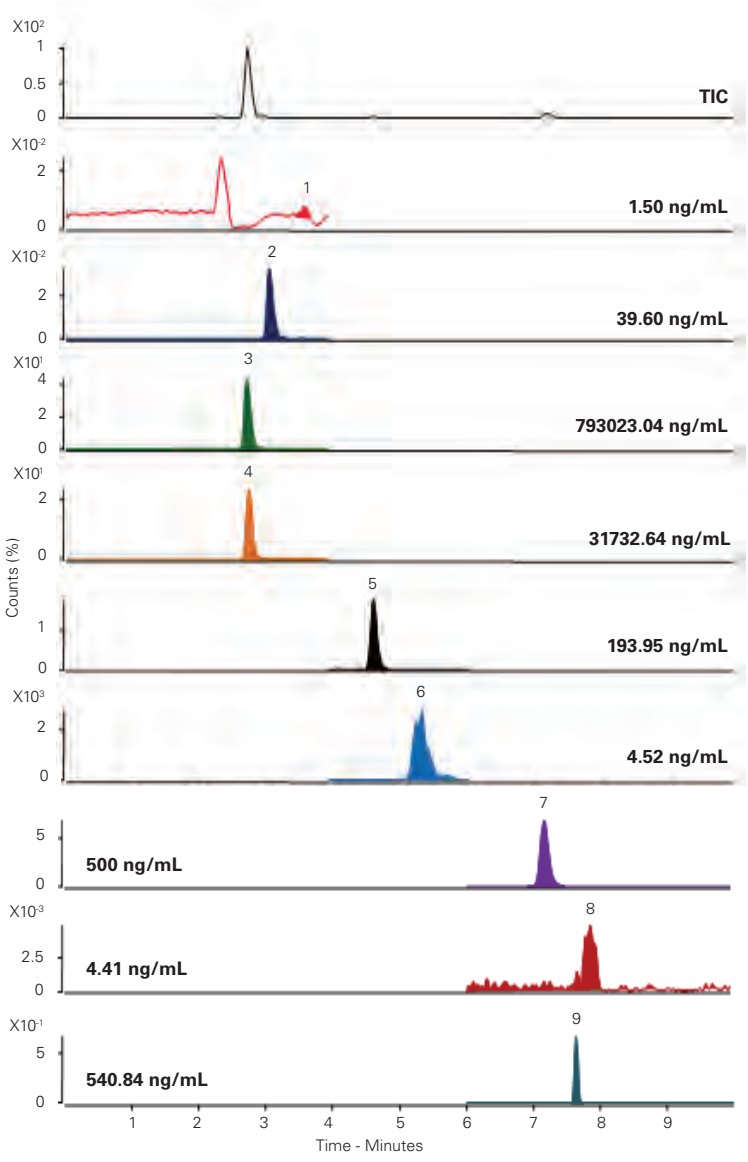
Gradient:

Time (mins)	%B
0	5
2	5
5	90
8	90
10	5
14	5

Flow Rate: 0.6 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: Agilent 6410 triple quad
ESI in positive ion mode (negative ion mode for MHPG)
Capillary Voltage: 1950 kV
Sample: Rat brain samples homogenised in aqueous formic acid, centrifuged and proteins removed by precipitation with acetonitrile

Analytes

	Quantifier	Qualifier	LLOQ (ng/mL)
1. Adrenaline	*m/z* 184.2 → 166.2	*m/z* 184.2 → 57.1	0.25
2. Noradrenaline	*m/z* 170.2 → 107.1	*m/z* 170.2 → 152.1	0.5
3. Glutamic acid	*m/z* 148.1 → 84.1	*m/z* 148.1 → 130.1	250
4. GABA	*m/z* 104 → 45	*m/z* 104 → 87	250
5. Dopamine	*m/z* 154.1 → 137.1	*m/z* 154.1 → 91.1	0.25
6. MHPG (3-Methoxy-4-hydroxyphenylglycol)	*m/z* 263 → 165.1	*m/z* 263 → 165.1	1
7. Isoprenaline (IS)	*m/z* 212.2 → 194.1		
8. 5-Hydroxyindoleacetic acid	*m/z* 192 → 145.9	*m/z* 192 → 90.9	1
9. Serotonin	*m/z* 177.2 → 160.2	*m/z* 177.2 → 132.1	10



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Nitroanilines (I)

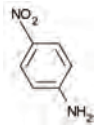
Application #AN3240

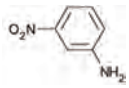
Conditions

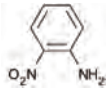
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM KH_2PO_4 pH 3.15/ MeCN (50:50 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

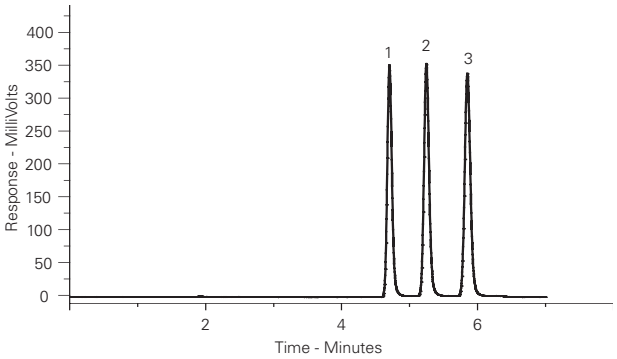
Analytes

1. p-Nitroaniline
2. m-Nitroaniline
3. o-Nitroaniline


p-Nitroaniline


m-Nitroaniline


o-Nitroaniline



Nitroanilines (II)

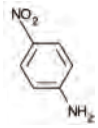
Application #AN3250

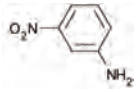
Conditions

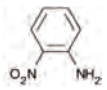
Column: ACE 5 CN
Dimensions: 250 x 4.6 mm
Part Number: ACE-124-2546
Mobile Phase: Heptane/Ethyl acetate (90:10 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

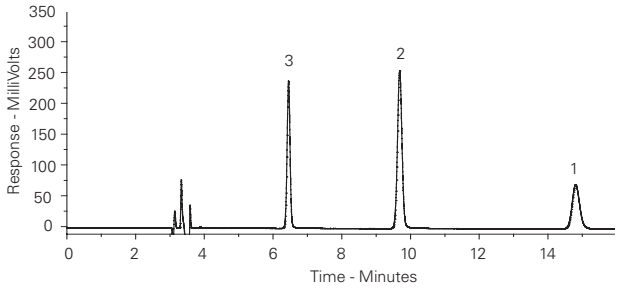
Analytes

1. p-Nitroaniline
2. m-Nitroaniline
3. o-Nitroaniline


p-Nitroaniline


m-Nitroaniline


o-Nitroaniline



Nitrofuran Metabolites by LC-MS/MS

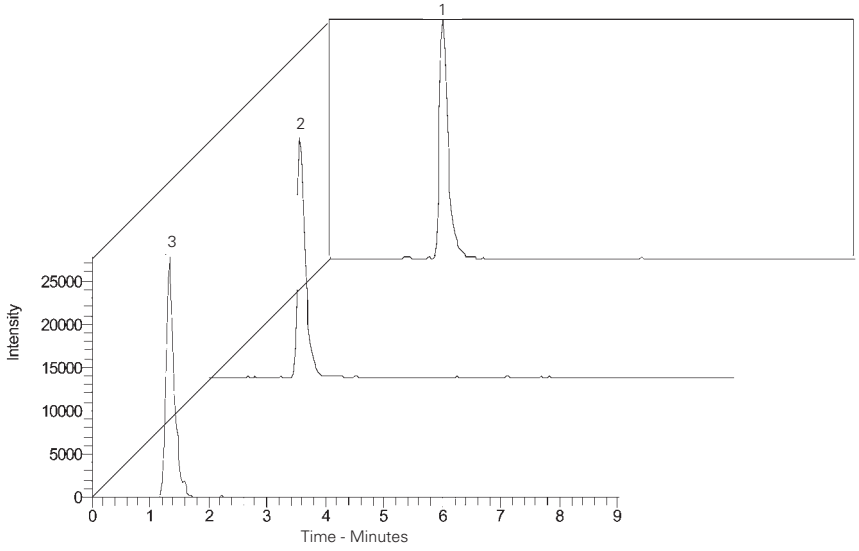
Application #AN3050

Conditions

Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: MeOH/0.5 mM ammonium acetate in H_2O (50:50 v/v)
Flow Rate: 0.2 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: ESI MS/MS (+ve mode)
Sample: Metabolites derivatised with 2-nitrobenzaldehyde to form nitrophenyl derivatives, prior to LC-MS analysis

Analytes

1. 5-Methylmorpholino-3-amino-2-oxazolidinone derivative (NBAMOZ)
   (metabolite of furaltadone)
   (*m/z* 335 → 291)
2. 3-Amino-2-oxazolidinone derivative (NBAOZ)
   (metabolite of furazolidone)
   (*m/z* 236 → 134)
3. 1-Aminohydantoin derivative (NBAHD)
   (metabolite of nitrofurazone)
   (*m/z* 249 → 134)



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Nitrosamines European Toy Standard Method by LC-MS/MS

Application #AN1110

Conditions

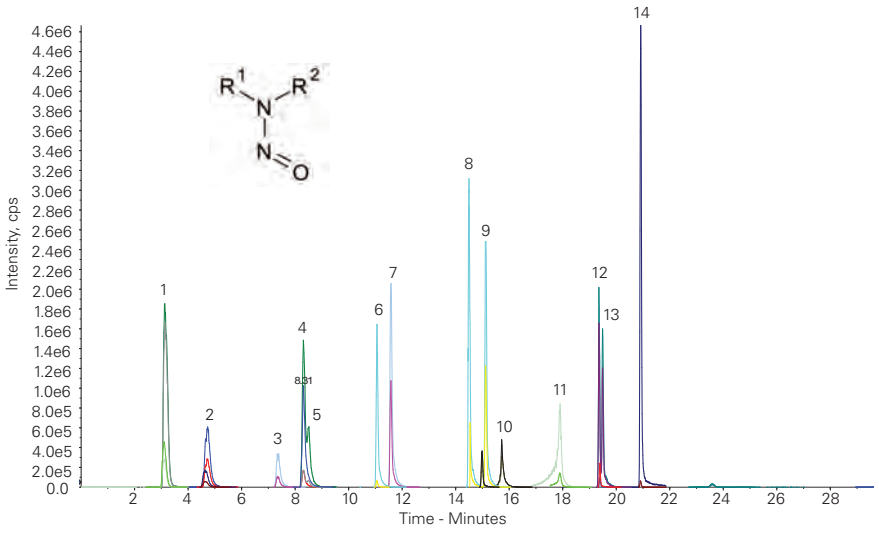
Column:	ACE Excel 2 C18-PFP
Dimensions:	150 x 3.0 mm
Part Number:	EXL-1010-1503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH

Gradient:	**Time (mins)**	**%B**
	0.0	5
	1.0	5
	10.0	65
	14.0	65
	15.0	90
	20.0	90
	21.0	5
	30.0	5

Flow Rate:	0.35 mL/min
Injection:	20 µL
Temperature:	40 °C
Sample Temperature:	4 °C
Detection:	Applied Biosystems 4000 Q-Trap MS
	Source: APCI (positive mode)
	Collision energy: 10-30 V
	Source temperature: 300 °C

Analytes

1. NDELA
   (*m/z* 135.2 → 74.2, 135.2 → 104.2)
2. NDMA
   (*m/z* 74.9 → 43.2, 74.9 → 58.2)
3. Nmorph
   (*m/z* 117.1 → 86.3, 117.1 → 73.3)
4. Npyrr
   (*m/z* 101.2 → 55.3, 101.2 → 59.2)
5. NMEA
   (*m/z* 89.2 → 61.1, 89.2 → 43.3)
6. NDEA
   (*m/z* 103.1 → 75.2, 103.1 → 47.2)
7. NPIP
   (*m/z* 115.1 → 69.1, 115.1 → 41.2)
8. NDnPA
   (*m/z* 131.2 → 89.2, 131.2 → 43.3)
9. NdiPA
   (*m/z* 131.2 → 89.2, 131.2 → 43.3)
10. NMPhA
    (*m/z* 137.2 → 107.2, 137.2 → 66.1)
11. NEPhA
    (*m/z* 151.1 → 77.1, 151.1 → 95.3)
12. NDiBA
    (*m/z* 159.3 → 57.2, 159.3 → 103.2)
13. NDnBA
    (*m/z* 159.3 → 103.2, 159.3 → 57.2)
14. NDBzA
    (*m/z* 227.2 → 91.1, 227.2 → 181.2)



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

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Non-Steroidal Anti-Inflammatory Drugs (I)

Application #AN1210

Conditions

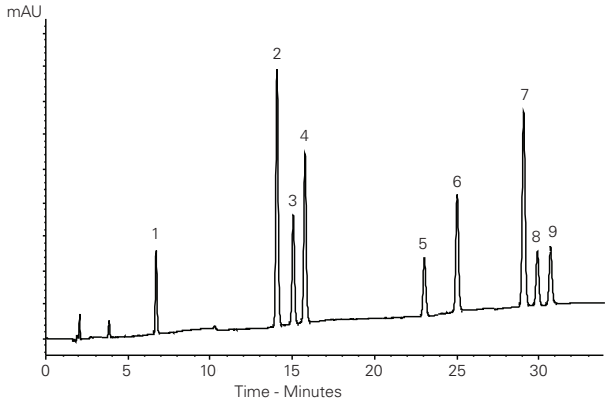
Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH

Gradient:	**Time (mins)**	**%B**
	0	52
	28	74
	33	74
	38	52
	48	52

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

Analytes

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



Non-Steroidal Anti-Inflammatory Drugs (II)

Application #AN1220

Conditions

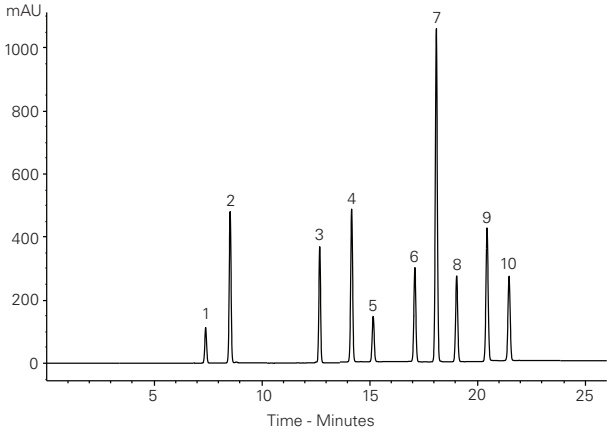
Column:	ACE Excel 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1211-1546U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0	20
	20	70
	25	70
	36	20

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

Analytes

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



Non-Steroidal Anti-Inflammatory Drugs (III)

Application #AN3570

Conditions

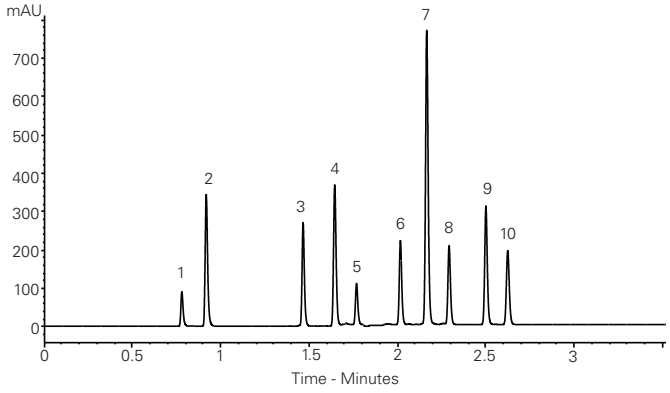
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 3.0 mm
Part Number:	CORE-25A-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0.02	20
	2.71	70
	3.39	70
	3.52	20

Flow Rate:	0.85 mL/min
Injection:	1.04 µL
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

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



Non-Steroidal Anti-Inflammatory Drugs – Fast Analysis

Application #AN2080

Conditions

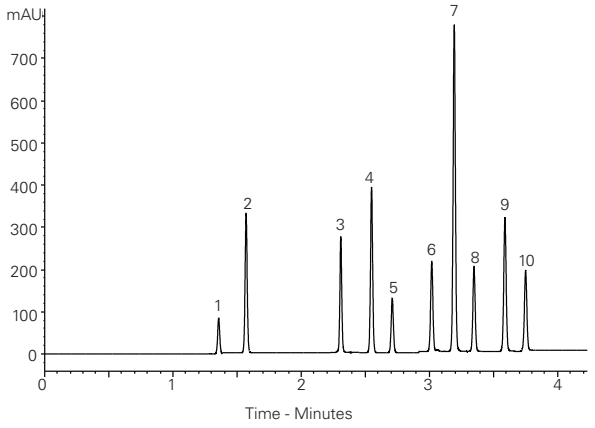
Column:	ACE Excel 2 SuperC18
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1011-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0.00	20
	0.25	20
	3.50	70
	4.00	20
	4.25	20

Flow Rate:	0.86 mL/m
Injection:	1.4 µL
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

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



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

Application #AN2630

Conditions

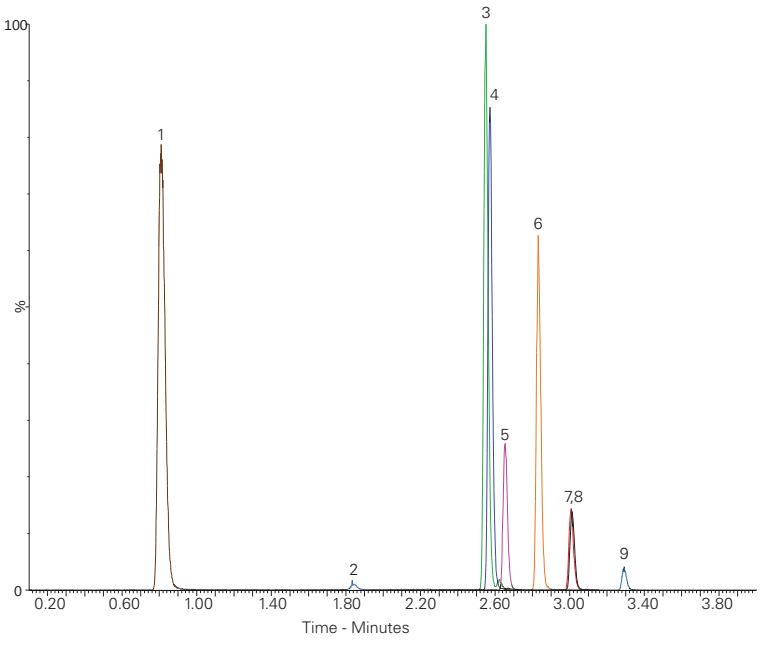
Column:	ACE Excel 2 C18
Dimensions:	50 x 2.1 mm
Part Number:	EXL-101-0502U
Mobile Phase:	A: 2 mM ammonium acetate, 0.1% formic acid in H_2O
	B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

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

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

Analytes

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)

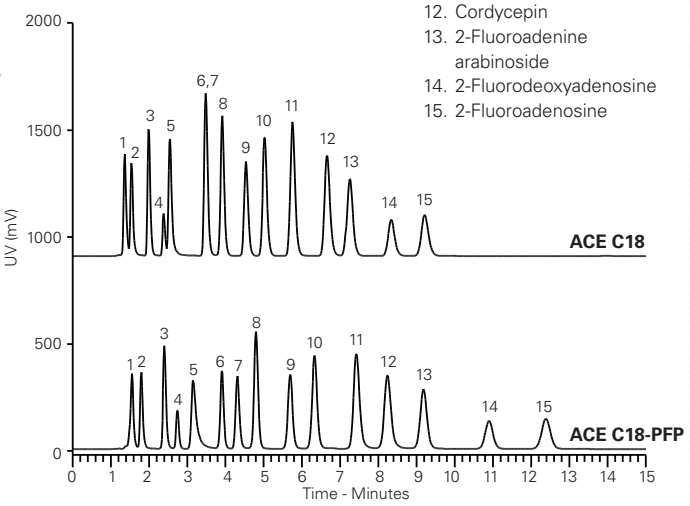
Application #AN1080

Conditions

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

Analytes

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



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Nucleosides and Vitamins

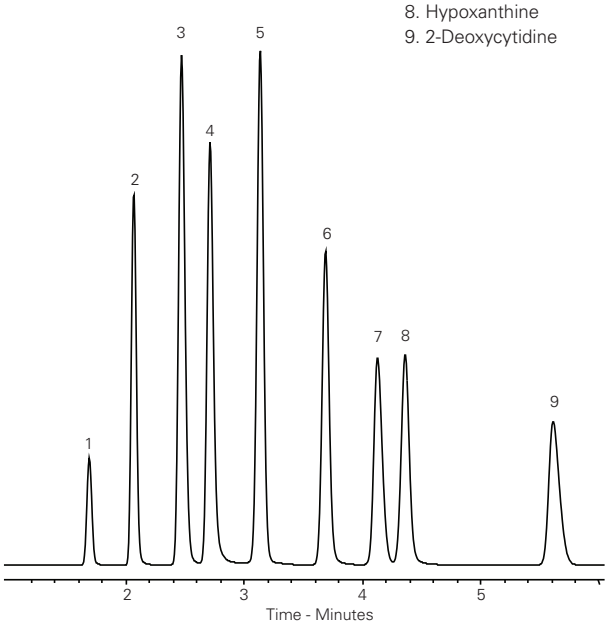
Application #AN1330

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: 20 mM H_3PO_4 in H_2O
Flow Rate: 1 mL/min
Temperature: 22 °C
Detection: UV, 254 nm

Analytes

1. Pyridoxamine (Vitamin B6)
2. Cytosine
3. Thiamine (Vitamin B1)
4. Nicotinamide
5. L-Ascorbic acid (Vitamin C)
6. Uracil
7. Cytidine
8. Hypoxanthine
9. 2-Deoxycytidine



Nucleic Acids / Disease Biomarker Profiling (II)

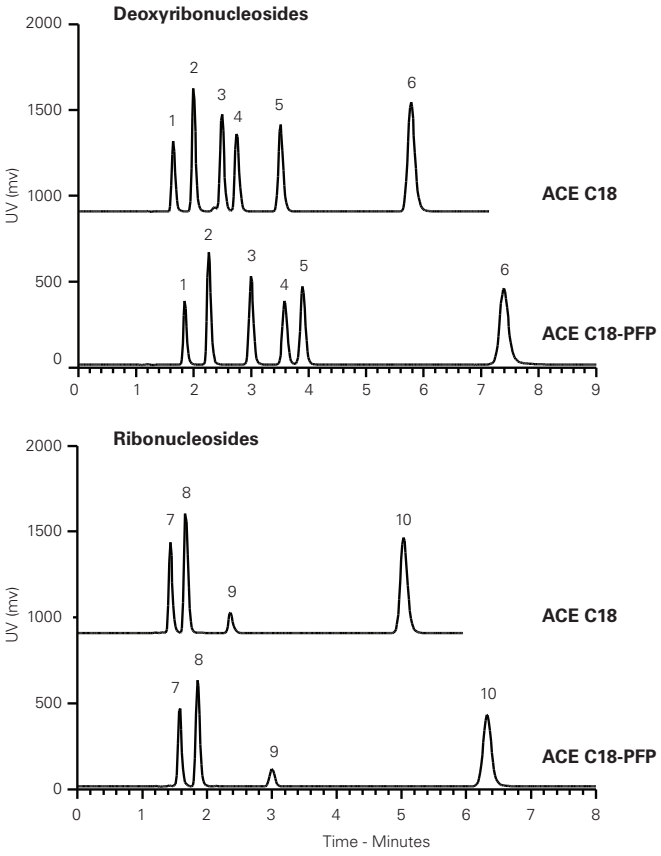
Application #AN1090

Conditions

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

Analytes

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



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Ochratoxin A

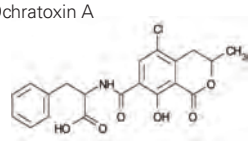
Application #AN2870

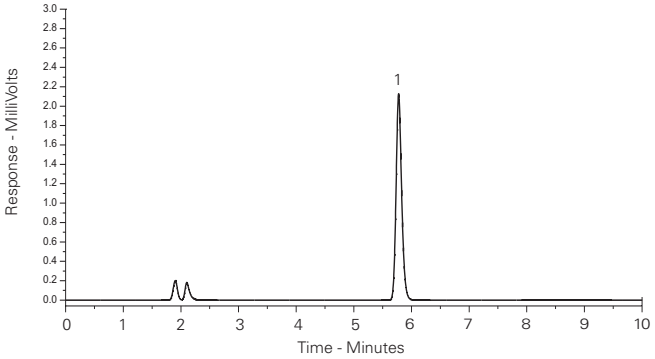
Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/H_2O/Acetic acid (51:47:2 v/v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: Fluorescence – λ_{ex} 333 nm, λ_{em} 443 nm

Analyte

1. Ochratoxin A





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Olanzapine in Human Plasma by LC-MS/MS

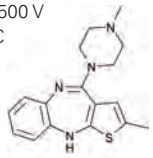
Application #AN2520

Conditions

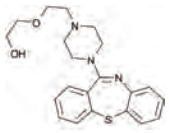
Column: ACE 5 C18-300
Dimensions: 100 x 4.6 mm
Part Number: ACE-221-1046
Mobile Phase: MeCN/0.01% ammonia in 2 mM ammonium formate pH 6.6 (85:15 v/v)
Flow Rate: 0.9 mL/min
Injection: 5 µL
Detection: API 4000 triple quad MS
Turbo Ion Spray in positive mode
Ion Spray voltage: 5500 V
Temperature: 550 °C

Analytes

1. Olanzapine (*m/z* 313.2 → 256.2)
2. Quetiapine (IS) (*m/z* 384.2 → 253.2)

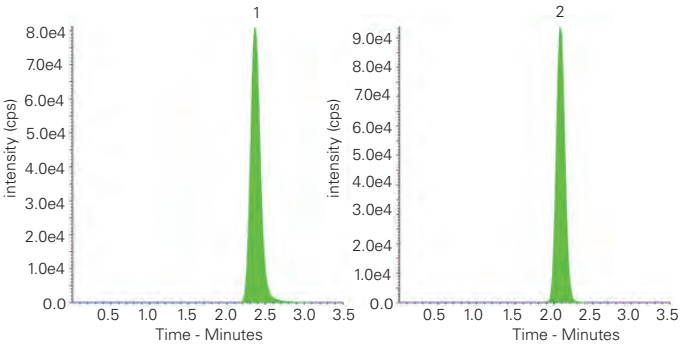


Olanzapine



Quetiapine (IS)

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



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Omeprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl

Application #AN1560

Conditions

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

Gradient:

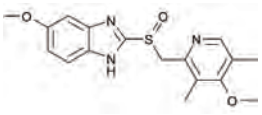
Time 1 (mins)	Time 2 (mins)	Time 3 (mins)	%B
0.0	0.0	0.0	10
15.0	30.0	45.0	90
15.5	30.5	45.5	90
18.0	33.0	48.0	10

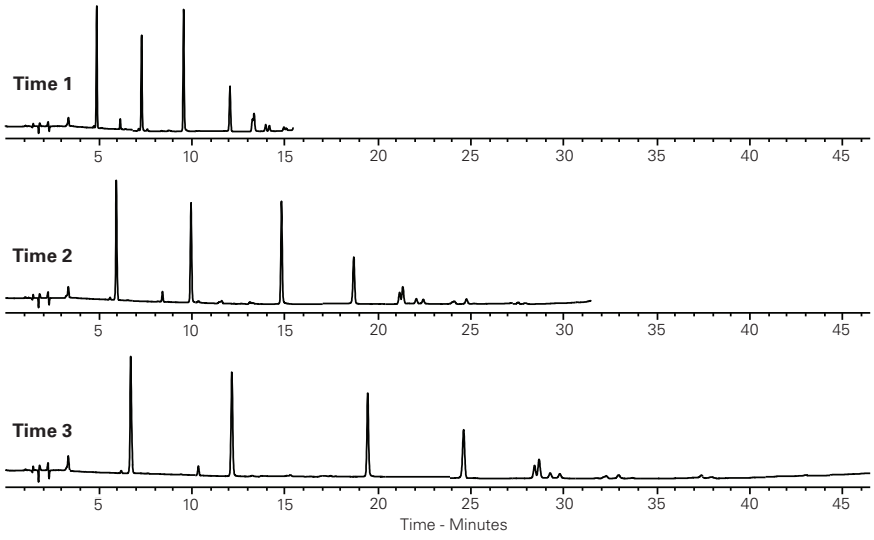
Post time 10 minutes

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

Analyte

Omeprazole





Opiates from Drugs of Abuse Screen (#AN2190)

Application #AN2340

Conditions

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

Gradient:

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

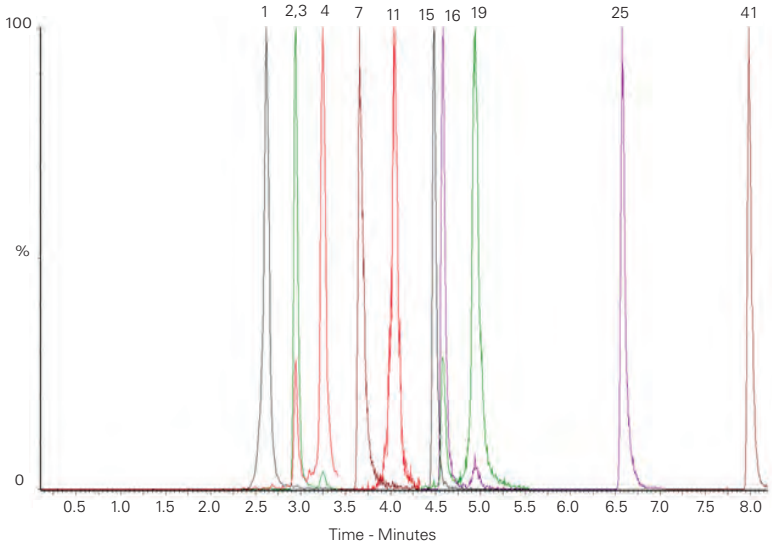
Flow Rate: 0.3 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: MS Quattro Premier XE triple quad
MRM, positive and negative ESI mode
Desolvation temperature: 450 °C
IonSource temperature: 150 °C
Collision gas pressure: 3.5 x 10^{-3} mbar



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Analytes

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



Opiates in Urine by LC-MS/MS

Application #AN1230

Conditions

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

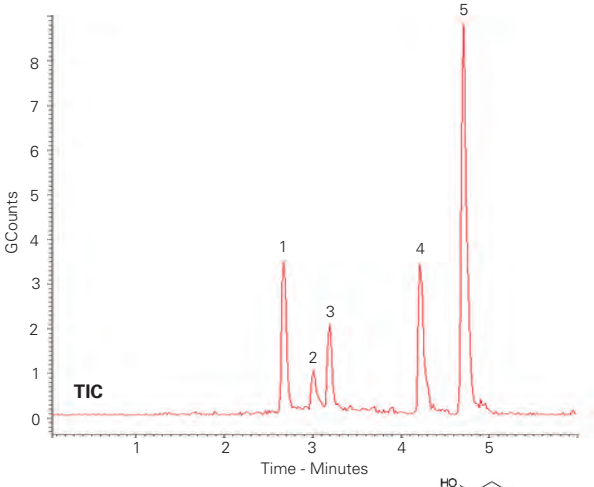
Gradient:

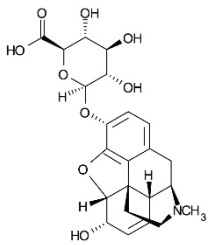
Time (mins)	%B
0	30
5	95

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

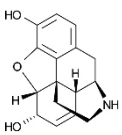
Analytes

1. Morphine 3-β-D-glucuronide
LOD (est) 100 ppb
(*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)

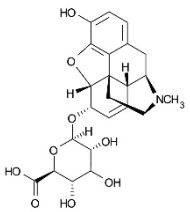




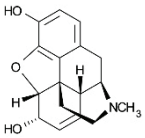
Morphine 3-β-D-glucuronide



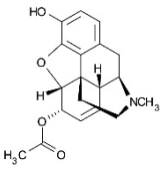
Normorphine



Morphine 6-β-D-glucuronide



Morphine



6-Acetylmorphine

Organic Acids

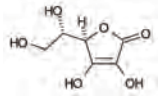
Application #AN2780

Conditions

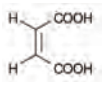
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	50 mM KH_2PO_4 pH 5.7 in H_2O/MeOH (70:30 v/v)
Flow Rate:	1 mL/min
Temperature:	22 °C
Detection:	UV, 220 nm

Analytes

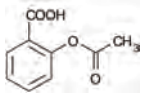
1. L-Ascorbic acid
2. Maleic acid
3. Acetylsalicylic acid
4. Benzoic acid
5. Salicylic acid



L-Ascorbic acid



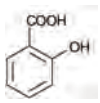
Maleic acid



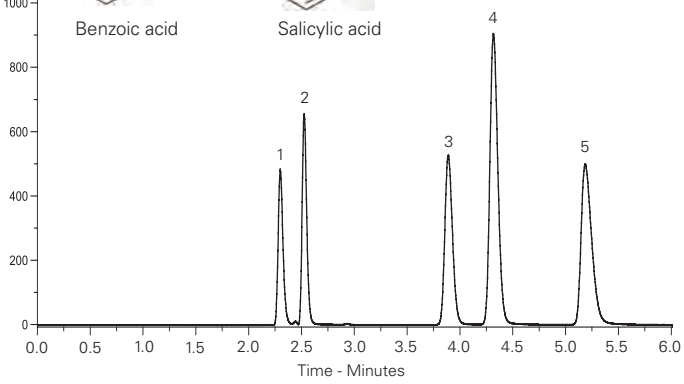
Acetylsalicylic acid



Benzoic acid



Salicylic acid



For further applications

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

Organic Acids – Fast Separation

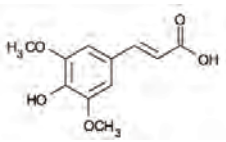
Application #AN2200

Conditions

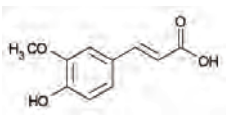
Column:	ACE Excel 3 C18-Amide ACE Excel 1.7 C18-Amide
Dimensions:	250 x 2.1 mm, 50 x 3.0 mm
Part Number:	250 x 2.1 mm (EXL-1112-2502U), 50 x 3 mm (EXL-1712-0503U)
Mobile Phase:	20 mM H_3PO_4 in MeOH/H_2O (40:60 v/v)
Flow Rate:	0.21 mL/min (250 x 2.1 mm) 0.8 mL/min (50 x 3.0 mm)
Injection:	5 µL (250 x 2.1 mm) 2 µL (50 x 3.0 mm)
Temperature:	20 °C
Detection:	UV, 210 nm

Analytes

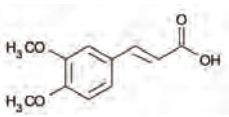
1. Sinapic acid
2. Ferulic acid
3. 3,4-Dimethoxycinnamic acid
4. Cinnamic acid
5. 4-Methoxycinnamic acid



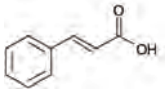
Sinapic acid



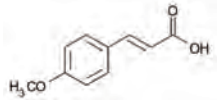
Ferulic acid



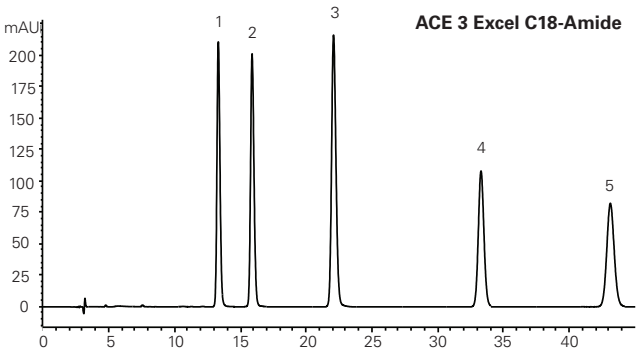
3,4-Dimethoxycinnamic acid

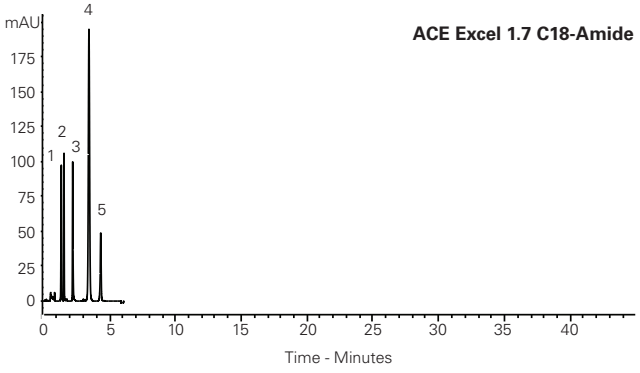


Cinnamic acid



4-Methoxycinnamic acid





Organophosphorus Flame Retardants in Water by LC-MS/MS

Application #AN1240

Conditions

Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.05 mM ammonium formate + 0.005% formic acid in H_2O
B: MeOH/MeCN (95:5 v/v)

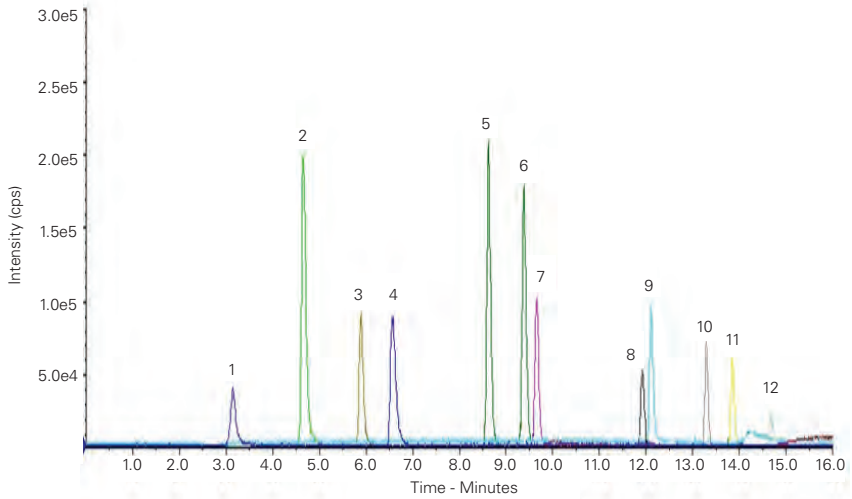
Gradient:

Time (mins)	%B
0.1	50
12.0	90
13.0	100
15.0	100
15.1	50
20.0	50

Flow Rate: 0.25 mL/min
Injection: 80 µL
Temperature: 25 °C
Detection: MS/MS

Analytes

		Q1 Mass	Q3 Mass
1.	Trimethyl phosphate (TMP)	141	109
2.	Triethyl phosphate (TEP)	183	127
3.	Tris(2-chloroethyl) phosphate (TCEP)	285	223
4.	Bis(1,3-dichloro-2-propyl) phosphate (BDCP)	321	99
5.	Triiso-propyl phosphate (TiPP)	225	99
6.	Tri-n-propyl phosphate (TPrP)	225	99
7.	Tris((2R)-1-chloro-2-propyl) phosphate (TCPP)	327	99
8.	Tris(1,3-dichloro-2-propyl) phosphate (TDCPP)	431	99
9.	Triphenyl phosphate (TPP)	327	215
10.	Tri-n-butyl phosphate (TBP)	267	211
11.	Tris(2-butoxyethyl) phosphate (TBEP)	399	299
12.	Bis(2-ethylhexyl) phosphate (BEHP)	323	99



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Organophosphorus (Isomeric) Flame Retardants in Water

Application #AN1140

Conditions

Column: ACE 3 C18
ACE 3 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002, ACE-1110-1002
Mobile Phase: A: 0.05 mM ammonium formate + 0.005% formic acid in H_2O
B: MeOH/MeCN (95:5 v/v)

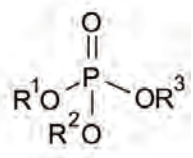
Gradient:

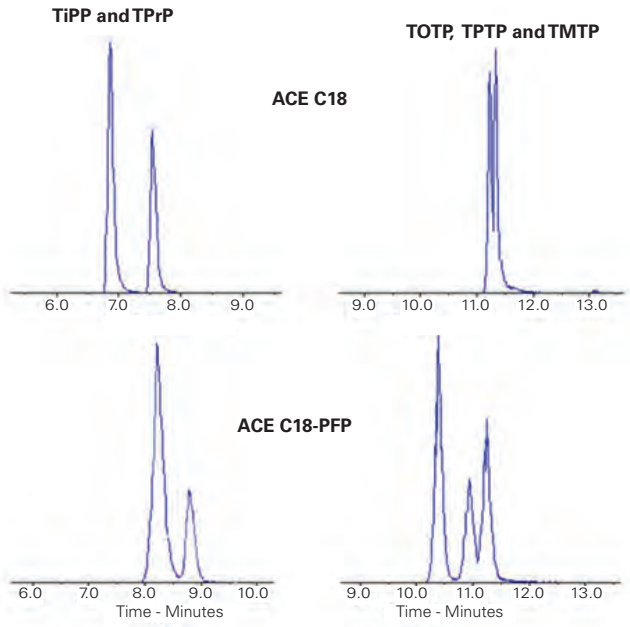
Time (mins)	%B
0.1	50
12.0	90
13.0	100
15.0	100
15.1	50
20.0	50

Flow Rate: 0.25 mL/m
Injection: 80 µL
Temperature: 25 °C
Detection: MS/MS

Analytes

Triiso-propyl phosphate (TiPP)
(*m/z* 225 → 99)
Tri-n-propyl phosphate (TPrP)
(*m/z* 225 → 99)
Tri-o-tolyl phosphate (TOTP)
(*m/z* 369 → 91)
Tri-p-tolyl phosphate (TPTP)
(*m/z* 369 → 91)
Tri-m-tolyl phosphate (TMTP)
(*m/z* 369 → 91)





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Organotin Compounds

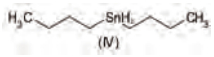
Application #AN3650

Conditions

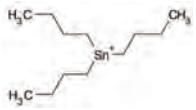
Column: ACE 3 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-111-1502
Mobile Phase: H_2O/MeCN/acetic acid/TEA (23:65:12:0.05 v/v/v/v)
Flow Rate: 0.2 mL/min
Detection: ICP-MS

Analytes

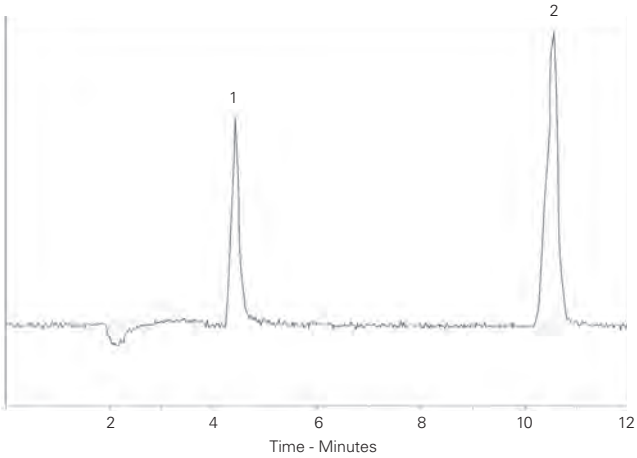
1. Dibutyltin
2. Tributyltin



Dibutyltin



Tributyltin



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OTC Gastric Drugs

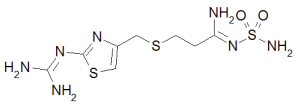
Application #AN3940

Conditions

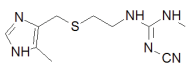
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/10 mM ammonium bicarbonate pH 8.0 in H_2O (18:82)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

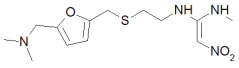
1. Famotidine
2. Cimetidine
3. Ranitidine



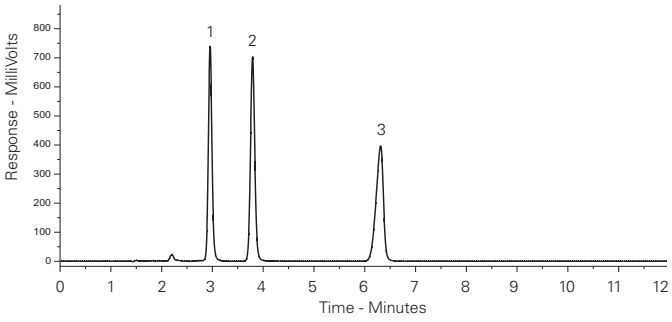
Famotidine



Cimetidine



Ranitidine



Oxysterols by LC-MS/MS

Application #AN2380

Conditions

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

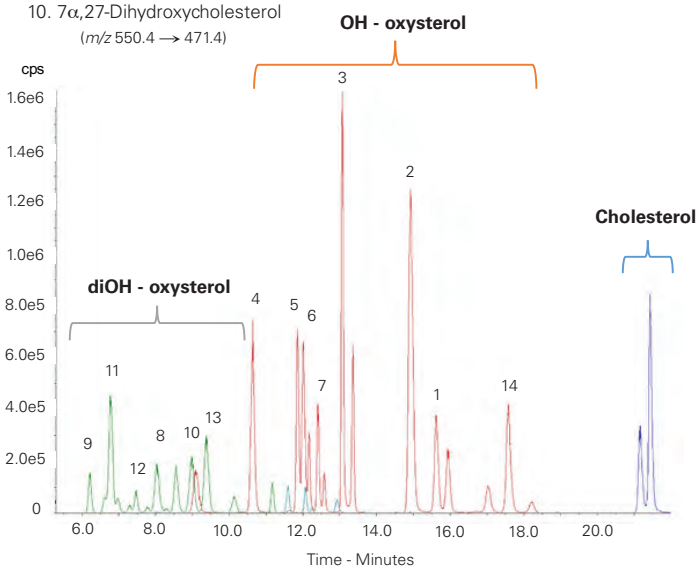
Gradient:

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

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

Analytes

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)

Oxymetazoline in Nasal Spray Formulation

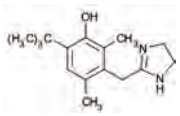
Application #AN3660

Conditions

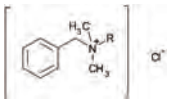
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: aq. Na_2HPO_4 pH 7.0/MeCN (50:50 v/v)
Flow Rate: 1.5 mL/min
Temperature: 30 °C
Detection: UV, 214 nm

Analytes

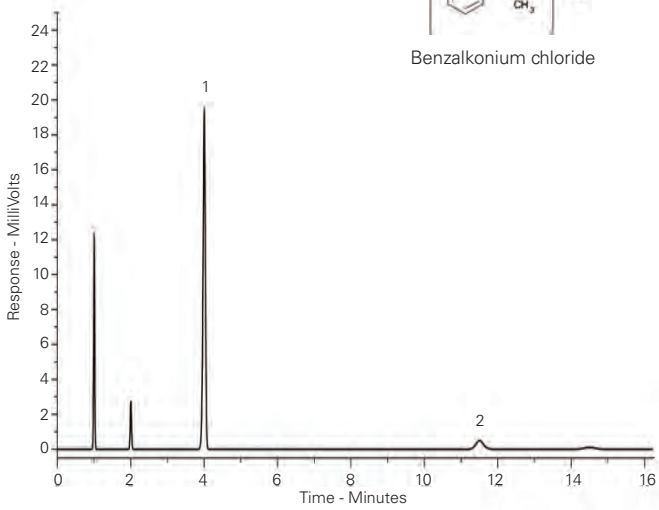
1. Oxymetazoline
2. Benzalkonium chloride



Oxymetazoline



Benzalkonium chloride



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Paclitaxel

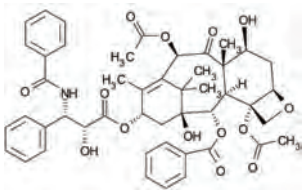
Application #AN3670

Conditions

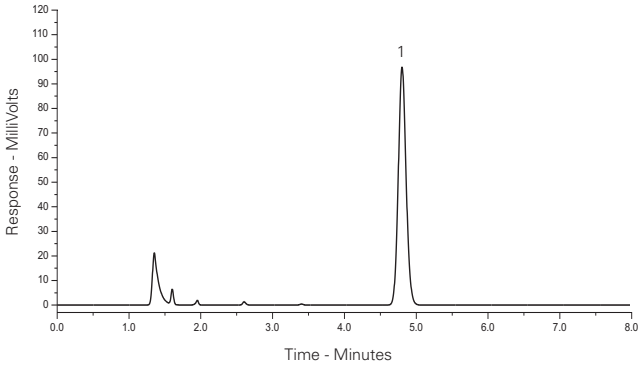
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: H_2O/MeCN (45:55 v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: UV, 227 nm

Analyte

1. Paclitaxel



Paclitaxel



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Paeonia Lactiflora Extract HPLC Fingerprint

Application #AN3820

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% phosphoric acid in H_2O
B: MeCN

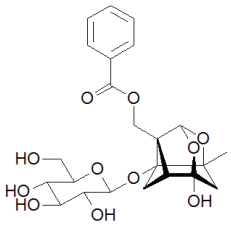
Gradient:

Time (mins)	%B
0	10
5	15
25	22
45	70
46	80
50	80

Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 25 °C
Detection: UV, 254 nm
Sample: *P. lactiflora* root extracted with boiling water and polysaccharides removed by precipitation

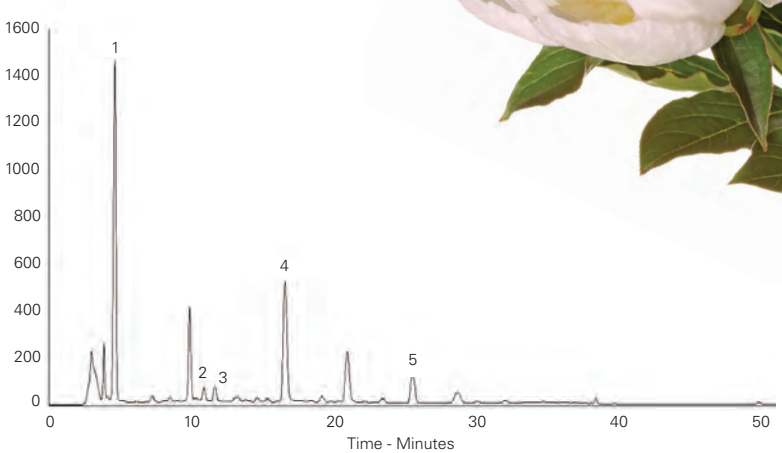
Analytes

1. Gallic acid
2. Catechin hydrate
3. Methyl gallate
4. Paeoniflorin
5. Benzoic acid



Paeoniflorin





Choi H-J, Chung T-W, Park M-J, Lee KS, Yoon Y, Kim HS, Lee JH, Kwon S-M, Lee S-O, Kim K-J, Baek J-H, Ha K-T. (2016) *Paeonia lactiflora* Enhances the Adhesion of Trophoblast to the Endometrium via Induction of Leukemia Inhibitory Factor Expression. PloS ONE 11(2): e0148232. doi:10.137/journal.pone.0148232

Paraben Preservatives

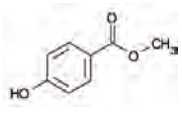
Application #AN1250

Conditions

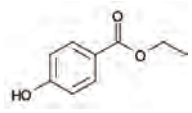
Column:	ACE 3 Phenyl
Dimensions:	150 x 2.1 mm
Part Number:	ACE-115-1502
Mobile Phase:	25 mM ammonium acetate pH 6.8 in H_2O/MeOH (50:50 v/v)
Flow Rate:	0.2 mL/min
Injection:	2 µL
Temperature:	40 °C
Detection:	UV, 240 nm

Analytes

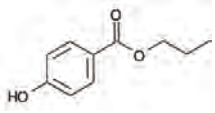
1. Methyl paraben
2. Ethyl paraben
3. n-Propyl paraben
4. i-Butyl paraben
5. n-Butyl paraben
6. Benzyl paraben



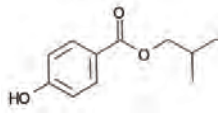
Methyl paraben



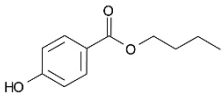
Ethyl paraben



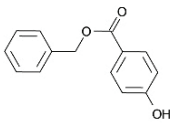
n-Propyl paraben



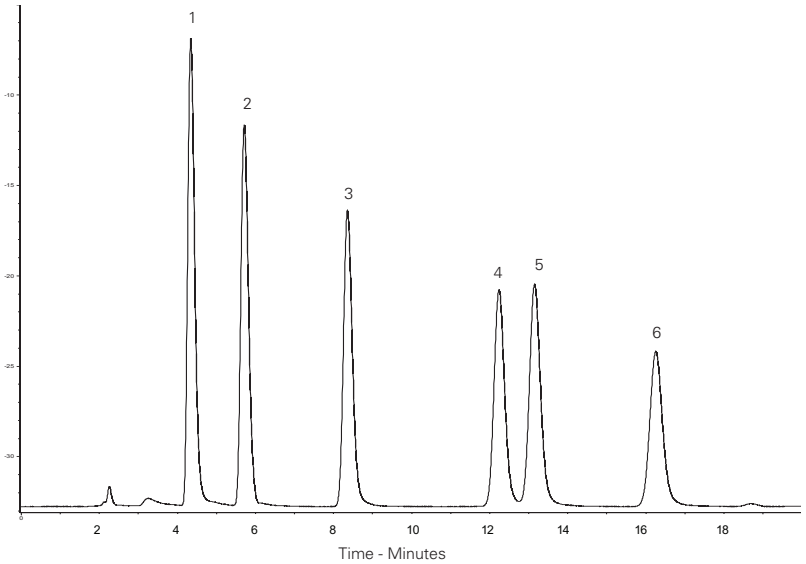
i-Butyl paraben



n-Butyl paraben



Benzyl paraben



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Paracetamol and Related Compounds

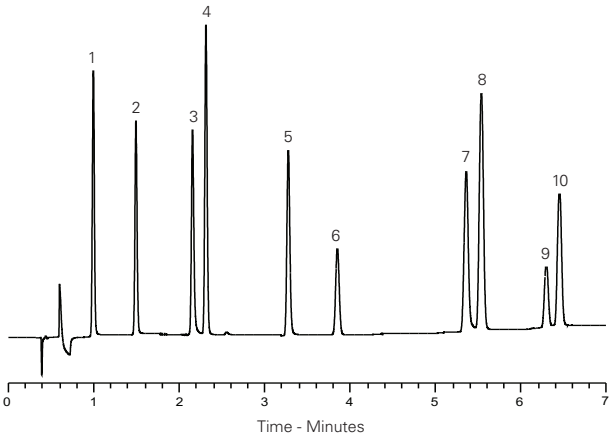
Application #AN1260

Conditions

Column:	ACE Excel 2 C18-PFP	
Dimensions:	100 x 3.0 mm	
Part Number:	EXL-1010-1003U	
Mobile Phase:	A: 20 mM ammonium acetate pH 6.0 in H_2O	
	B: 20 mM ammonium acetate pH 6.0 in MeOH/H_2O (90:10 v/v)	
Gradient:	**Time (mins)**	**%B**
	0.0	6
	5.5	63
Flow Rate:	1.2 mL/min	
Injection:	2 µL	
Temperature:	27 °C	
Detection:	UV, 220 nm	

Analytes

1. 4-Aminophenol
2. Hydroquinone
3. 2-Aminophenol
4. Paracetamol
5. 2-Acetamidophenol
6. Phenol
7. 4-Nitrophenol
8. 2-Nitrophenol
9. 4-Chloroacetanilide
10. 4-Chlorophenol



Paracetamol and Related Substances – Fast Analysis (I)

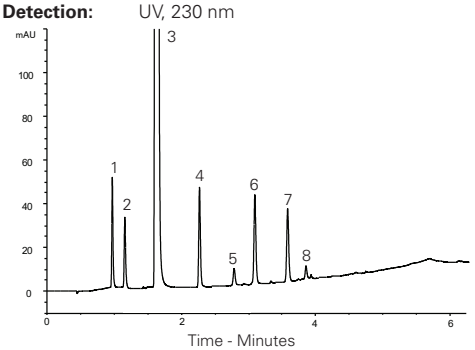
Application #AN2210

Conditions

Column:	ACE Excel 1.7 C18	
Dimensions:	50 x 3.0 mm	
Part Number:	EXL-171-0503U	
Mobile Phase:	A: 10 mM ammonium acetate pH 6.0 in H_2O	
	B: 10 mM ammonium acetate pH 6.0 in MeOH/H_2O (90:10 v/v)	
Gradient:	**Time (mins)**	**%B**
	0.00	5
	0.08	5
	5.08	95
	6.76	95
	7.09	5
	10.00	5
Flow Rate:	0.51 mL/min	
Injection:	0.7 µL	
Temperature:	40 °C	
Detection:	UV, 230 nm	

Analytes

1. 4-Aminophenol
2. Hydroquinone
3. Paracetamol
4. 2-Acetamidophenol
5. Phenol
6. 4-Nitrophenol
7. 2-Nitrophenol
8. 4-Chloroacetanilide



For enhanced resolution of paracetamol and related compounds, see AN2220.

Paracetamol and Related Substances – Enhanced Resolution

Application #AN2220

Conditions

Column:	ACE Excel 1.7 C18
Dimensions:	100 x 3.0 mm
Part Number:	EXL-171-1003U
Mobile Phase:	A: 10 mM ammonium acetate pH 6.0 in H_2O
	B: 10 mM ammonium acetate pH 6.0 in MeOH/H_2O (90:10 v/v)

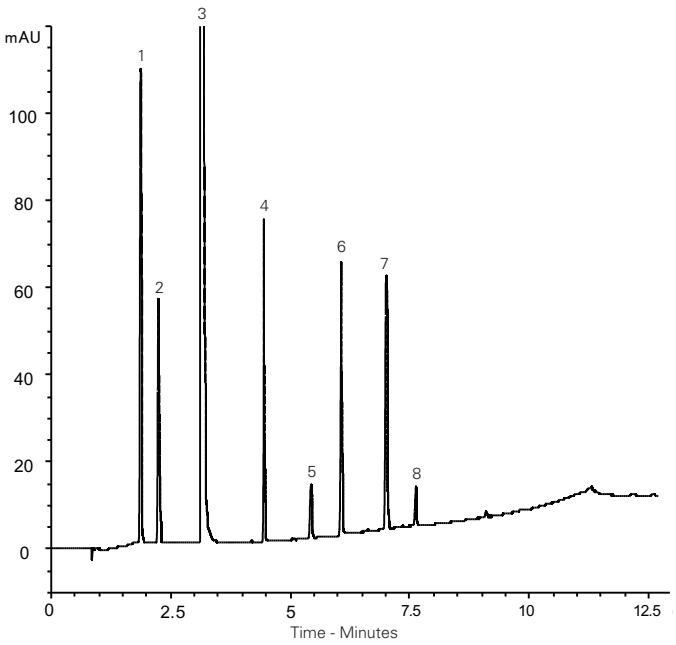
Gradient:	**Time (mins)**	**%B**
	0.00	5
	0.21	5
	10.23	95
	13.56	95
	14.16	5
	20.24	5

Flow Rate:	0.51 mL/min
Injection:	1.4 µL
Temperature:	40 °C
Detection:	UV, 230 nm

Analytes

1. 4-Aminophenol
2. Hydroquinone
3. Paracetamol
4. 2-Acetamidophenol
5. Phenol
6. 4-Nitrophenol
7. 2-Nitrophenol
8. 4-Chloroacetanilide





For enhanced speed of paracetamol and related compounds, see AN2210.

Paracetamol and Related Substances – Phase Selectivity

Application #AN3580

Conditions

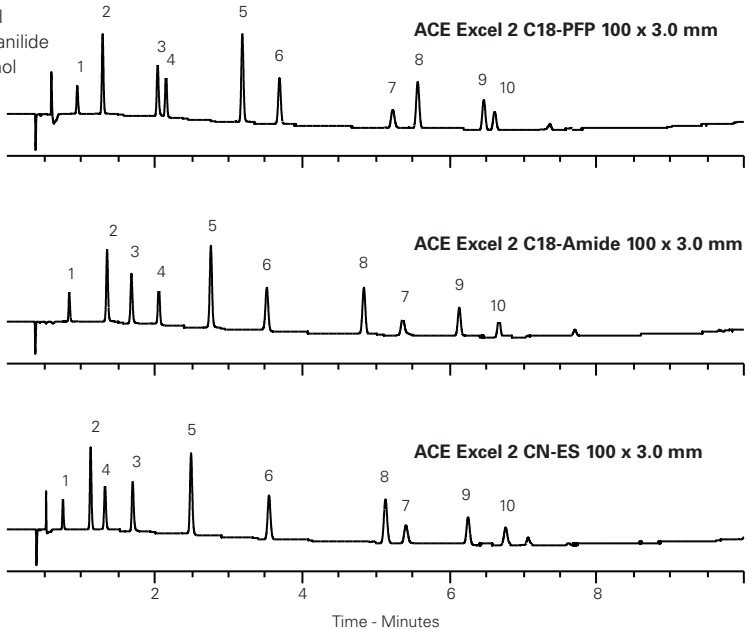
Column:	ACE Excel 2 C18-PFP, ACE Excel 2 C18-Amide, ACE Excel 2 CN-ES
Dimensions:	100 x 3.0 mm
Part Number:	EXL-1010-1003U, EXL-1012-1003U, EXL-1013-1003U
Mobile Phase:	A: 20 mM ammonium acetate pH 6.0 in H_2O
	B: 20 mM ammonium acetate pH 6.0 in MeOH/H_2O (90:10 v/v)

Gradient:	**Time (mins)**	**%B**
	0.0	5
	10.0	95
	12.5	95
	13.0	5

Flow Rate:	1.2 mL/min
Injection:	2 µL
Temperature:	40 °C
Detection:	UV, 210 nm

Analytes

1. 4-Aminophenol
2. Hydroquinone
3. 2-Aminophenol
4. Paracetamol
5. 2-Acetamidophenol
6. Phenol
7. 4-Nitrophenol
8. 2-Nitrophenol
9. 4-Chloroacetanilide
10. 4-Chlorophenol



Paralytic Shellfish Poisoning (PSP) Toxins

Application #AN3180

Conditions

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

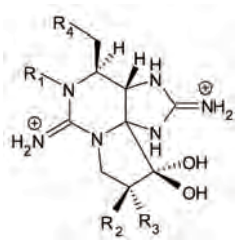
Gradient:

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

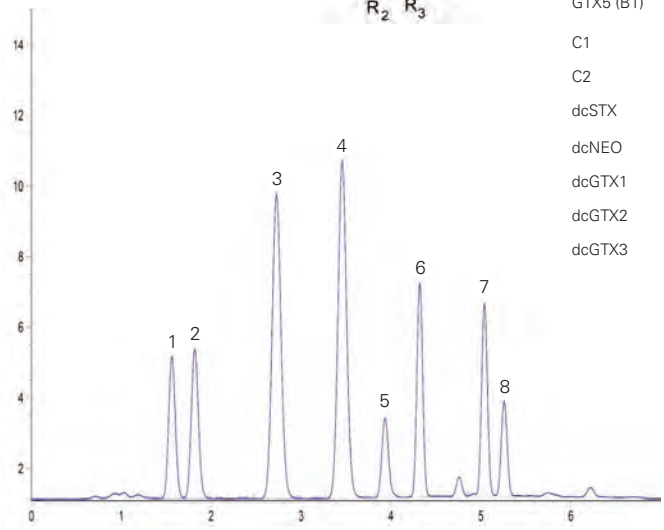
Flow Rate: 2 mL/min
Injection: 30 µL
Temperature: 20 °C
Detection: Fluorescence λ_{Ex} 340 nm, λ_{Em} 395 nm
Sample: Prechromatographic oxidation with hydrogen peroxide and periodate

Analytes

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



PST Variant	R1	R2	R3	R4
STX	H	H	H	H_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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Parotoid Macrogland Secretions from South American Toads

Application #AN3970

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% TFA in H_2O
B: 0.1% TFA in MeCN/H_2O (90:10 v/v)

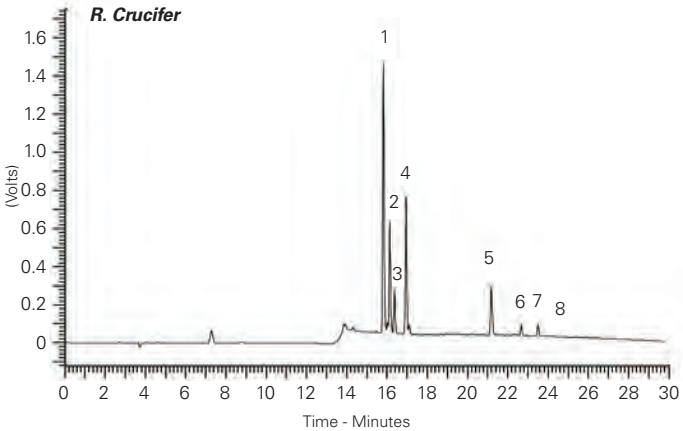
Gradient:

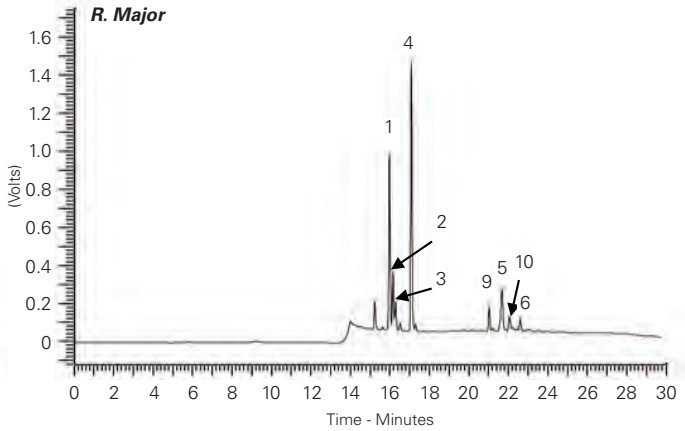
Time (mins)	%B
0	0
5	0
25	100

Flow Rate: 1 mL/min
Detection: PDA, 214 nm (Scanning 200-500 nm)

Analytes

1. Serotonin
2. N-Methylserotonin
3. N,N-Dimethylserotonin (bufotenine)
4. Dehydrobufotenine
5. Hellebrigenin
6. Marinobufagin
7. Telocinobufagin
8. Bufalin
9. Hellebrigenol-3-O-sulphate
10. Desacetylcinobufagin





Sciani JM, Angeli CB, Antoniazzi MM, Jared C, Pimenta DC. Differences and Similarities among Parotoid Macrogland Secretions in South American Toads: A Preliminary Biochemical Delineation.The Scientific World Journal 2013, http://dx.doi.org/10.1155/2013/937407

Paroxetine and Desfluoro Analogue

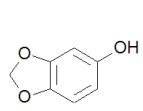
Application #AN3890

Conditions

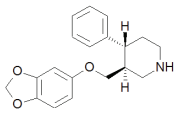
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: 20 mM ammonium formate pH 3.0/MeOH (60:40 v/v)
Flow Rate: 2 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV, 295 nm

Analytes

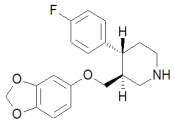
1. Sesamol
2. Desfluoroparoxetine
3. Paroxetine



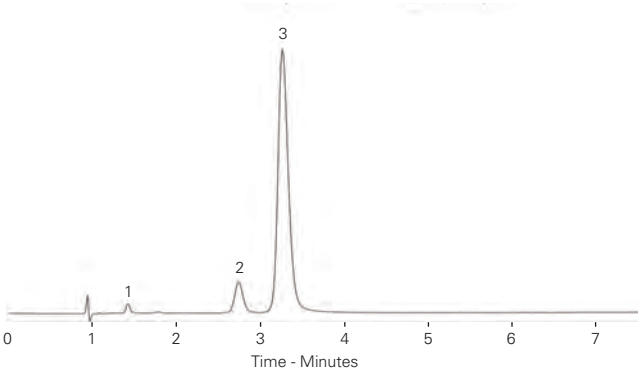
Sesamol



Desfluoroparoxetine



Paroxetine



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Peptide Test Mix

Application #AN3930

Conditions

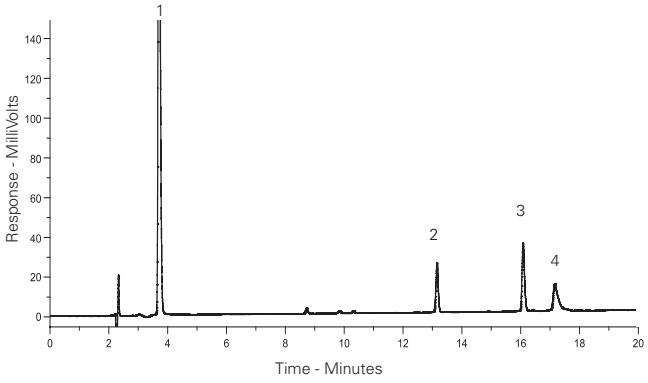
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H_2O
B: 0.1% TFA in MeCN

Gradient:	**Time (mins)**	**%B**
	0	10
	25	40

Flow Rate: 2 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 220 nm

Analytes

1. Gly-Tyr (MW: 238.34)
2. Oxytocin (MW: 1007)
3. Angiotensin II (MW: 1046.18)
4. Neurotensin (MW: 1672.92)



Peptides – Varying pH

Application #AN3990

Conditions

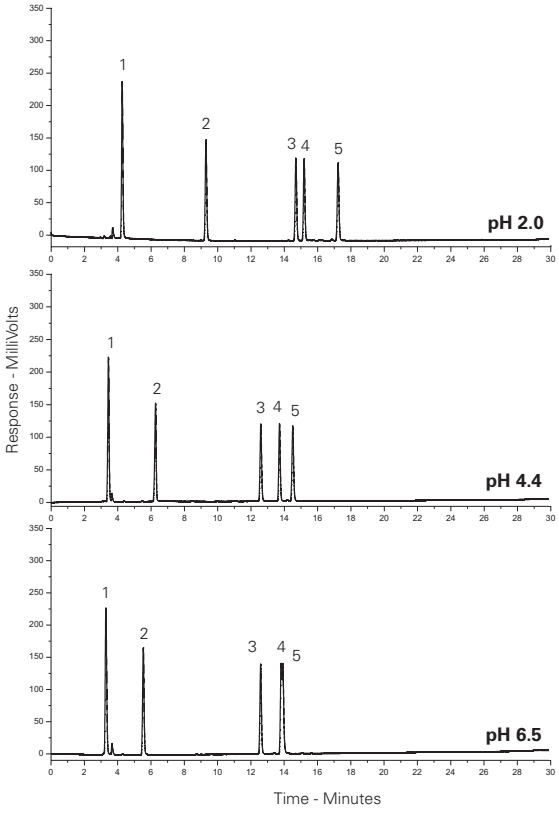
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 20 mM KH_2PO_4 in H_2O (pH as indicated)
B: MeCN

Gradient:	**Time (mins)**	**%B**
	0	10
	25	40

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 220 nm

Analytes

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



Peptides – Selectivity Changes with Bonded Phase and Mobile Phase

Application #AN3430

Conditions

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

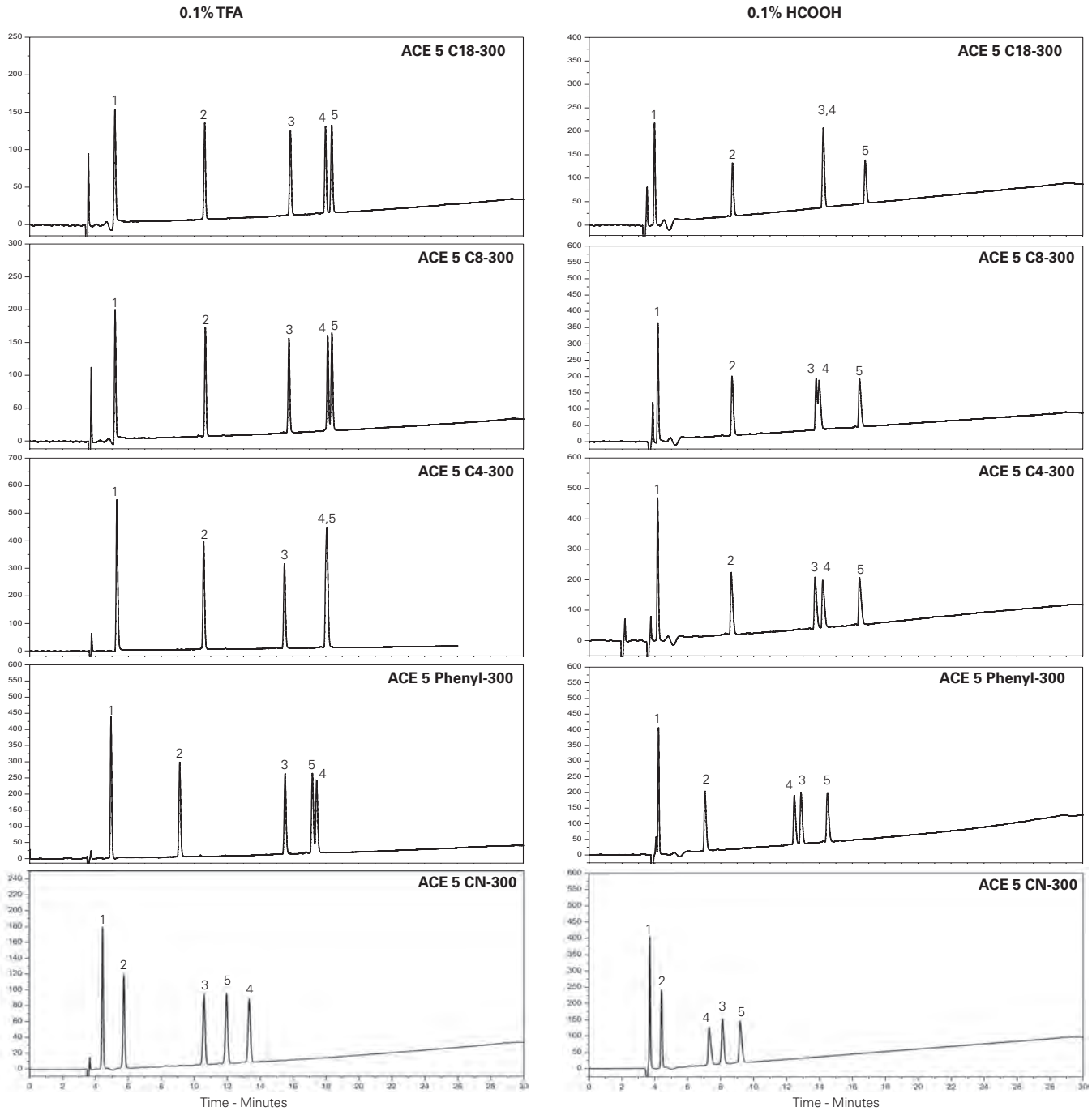
Gradient:

Time (mins)	%B
0.0	10
25.0	40

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 220 nm

Analytes

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



Perfluoro Acids by LC-MS/MS

Application #AN1280

Conditions

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

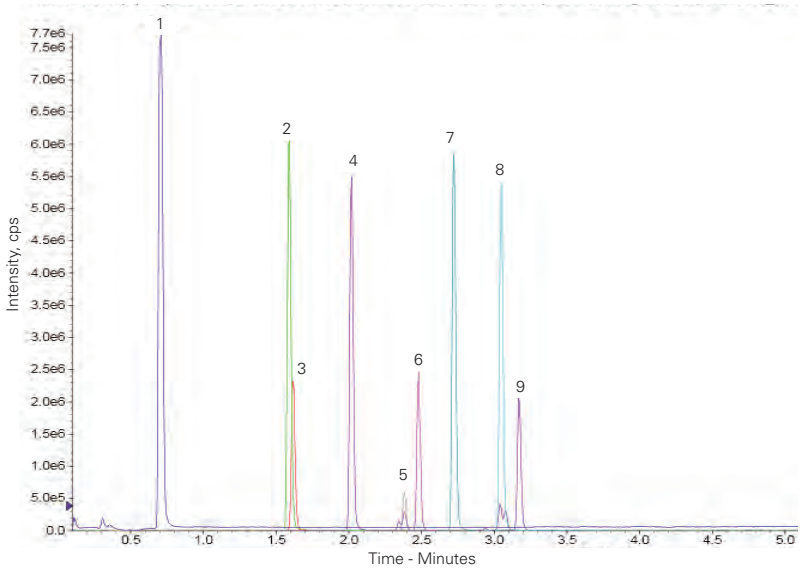
Gradient:

Time (mins)	%B
0.0	25
0.5	25
5.5	95
7.5	95
8.0	25
10.0	25

Flow Rate: 0.5 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: AB SCIEX triple quad 5500
Negative ESI MRM
Source temperature: 450 °C
IonSpray voltage: -2400 V

Analytes

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



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Perfluoroalkyl Substances by Ion-Pairing LC-MS/MS

Application #AN2560

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 2 mM ammonium acetate + 5 mM 1-methylpiperidine in MeOH/H_2O (5:95 v/v)
B: 2 mM ammonium acetate + 5 mM 1-methylpiperidine in MeOH/H_2O (95:5 v/v)

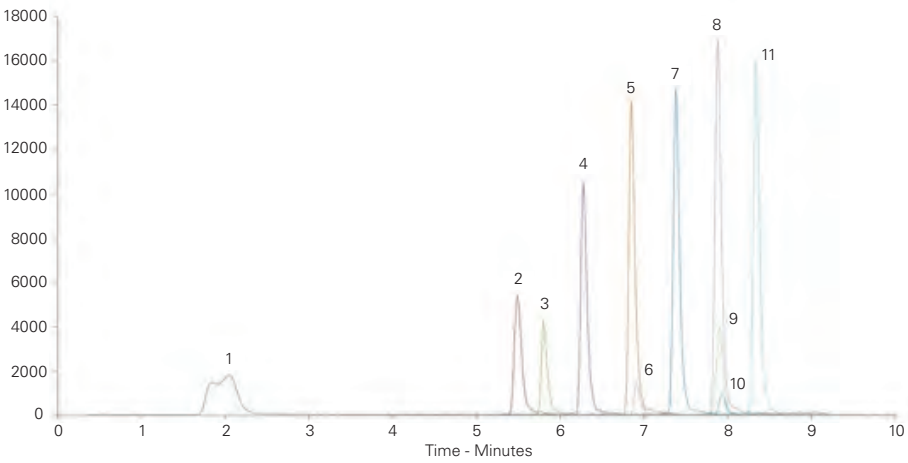
Gradient:

Time (mins)	%B
0.0	10
0.3	10
1.0	20
1.5	50
5.0	80
10.0	80
13.0	100
16.0	100

Flow Rate: 0.3 mL/min
Injection: 5 µL
Temperature: 35 °C
Detection: Agilent 6430 triple quad MS
ESI in negative ion mode
Capillary voltage: 3000 V
Nebulizer pressure: 50 psi

Analytes

1. PFBA (*m/z* 213 → 169)
2. PFPeA (*m/z* 263 → 219) (*m/z* 263 → 175)
3. PFBS (*m/z* 299 → 99) (*m/z* 299 → 80)
4. PFHxA (*m/z* 313 → 269) (*m/z* 313 → 119)
5. PFHpA (*m/z* 363 → 319) (*m/z* 363 → 169)
6. PFHxS (*m/z* 399 → 99) (*m/z* 399 → 80)
7. PFOA (*m/z* 413 → 369) (*m/z* 413 → 169)
8. PFNA (*m/z* 463 → 419) (*m/z* 463 → 169)
9. PFOS (*m/z* 499 → 99) (*m/z* 499 → 80)
10. FOSA (*m/z* 498 → 498) (*m/z* 498 → 78)
11. PFDA (*m/z* 513 → 469) (*m/z* 513 → 269)



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Perfluorinated Compounds in Water by LC-MS/MS

Application #AN2260

Conditions

Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H_2O/MeCN (90:10 v/v)
B: 2 mM ammonium acetate, 0.1% formic acid in H_2O/MeCN (10:90 v/v)

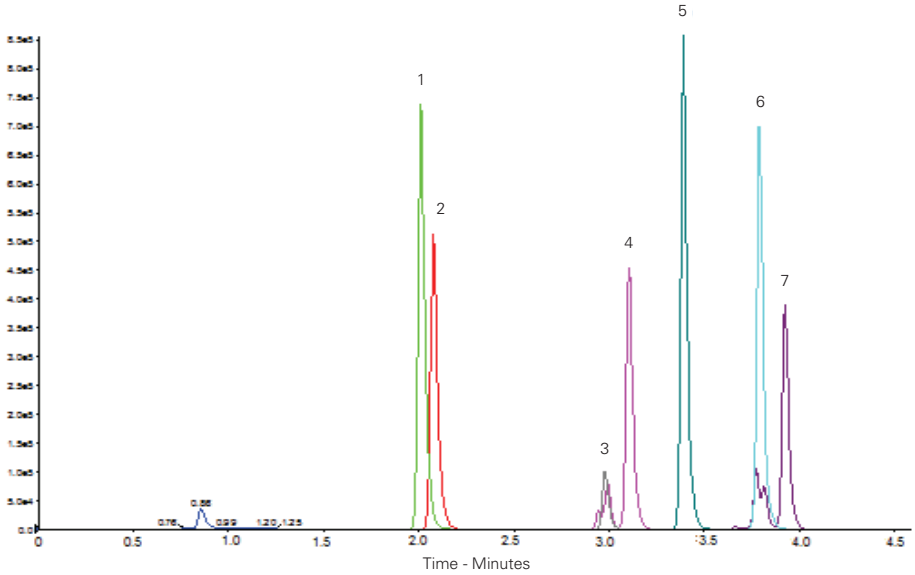
Gradient:

Time (mins)	%B
0.0	25
0.5	25
3.5	70
4.0	100
5.5	100
6.0	25
9.0	25

Flow Rate: 0.5 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: AB SCIEX triple quad 5500
Negative ESI MRM
Source temperature: 450 °C
IonSpray voltage: -2400 V

Analytes

1. Perfluorohexanoic acid (*m/z* 313.0 ⟶ 268.9)
2. Perfluorobutanesulfonic acid (*m/z* 299.0 ⟶ 79.9)
3. Perfluorooctanoic acid (*m/z* 413.0 ⟶ 368.9)
4. Perfluorohexanesulfonic acid (*m/z* 399.0 ⟶ 80.0)
5. Perfluorononanoic acid (*m/z* 463.0 ⟶ 419.0)
6. Perfluorodecanoic acid (*m/z* 513.0 ⟶ 469.0)
7. Perfluorooctanesulfonic acid (*m/z* 499.0 ⟶ 80.0)



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250 Pesticide Screen by LC-MS/MS

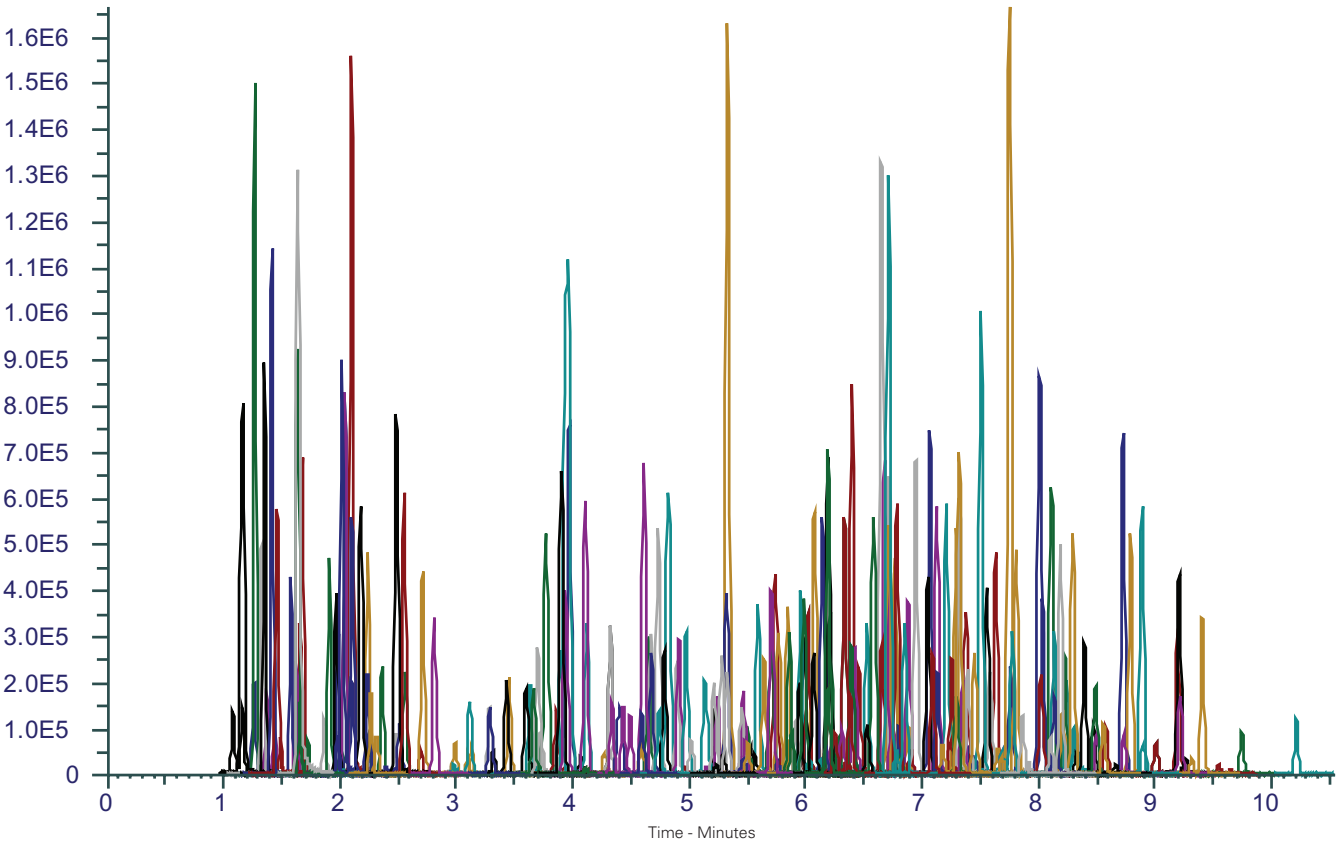
Conditions

Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 10 mM ammonium formate + 0.05% formic acid in H_2O
B: 10 mM ammonium formate + 0.05% formic acid in MeOH

Gradient:

Time (mins)	%B
0.00	2
0.25	30
10.00	100
12.00	100
12.50	2
14.50	2

Flow Rate: 0.5 mL/min
Temperature: 50 °C
Detection: TSQ Quantiva triple quad MS
Positive mode HESI
Spray voltage: 3500 V
Ion transfer tube temperature: 350 °C
Vaporizer temperature: 300 °C



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250 Pesticide Screen by LC-MS/MS

Analyte	R_t (mins)	Adduct	Precusor Ion *m/z*	Quant Ion *m/z*	Conf Ion *m/z*
3-OH Carbofuran	2.25	$[M+H]^+$	238.1	181.2	163.1
5-OH Thiabendazole	1.66	$[M+H]^+$	218.0	147.2	191.1
Abamectin	9.45	$[M+NH_4]^+$	890.5	305.3	567.5
Acephate	1.26	$[M+H]^+$	184.0	143.1	125.1
Acetamiprid	2.24	$[M+H]^+$	223.1	126.1	90.1
Aldicarb	2.95	$[M+NH_4]^+$	208.1	116.1	89.0
Aldicarb sulfone	1.44	$[M+NH_4]^+$	240.1	148.0	86.0
Aldicarb sulfoxide	1.37	$[M+NH_4]^+$	224.1	132.0	89.1
Allethrin	8.33	$[M+H]^+$	303.2	135.1	123.1
Ametoctradin	7.64	$[M+H]^+$	276.2	149.1	176.2
Atrazine	4.64	$[M+H]^+$	216.1	174.0	104.0
Azinphos ethyl	6.30	$[M+H]^+$	346.0	132.1	223.0
Azinphos methyl	5.14	$[M+H]^+$	318.0	132.0	124.9
Azinphos methyl OA	2.98	$[M+H]^+$	302.0	132.2	160.0
Azoxystrobin	5.59	$[M+H]^+$	404.1	372.1	344.1
Bendiocarb	3.72	$[M+H]^+$	224.1	167.1	109.1
Benoxacor	5.23	$[M+H]^+$	260.1	134.1	120.1
Bifenazate	6.27	$[M+H]^+$	301.1	198.0	170.1
Bitertanol	7.41	$[M+H]^+$	338.2	269.3	99.1
Boscalid	5.85	$[M+H]^+$	343.0	307.0	140.0
Bupirimate	6.68	$[M+H]^+$	317.2	210.2	237.3
Buprofezin	8.24	$[M+H]^+$	306.1	201.1	106.1
Cadusafos	7.58	$[M+H]^+$	271.1	159.0	131.0
Carbaryl	4.07	$[M+NH_4]^+$	219.1	145.1	127.0
Carbendazim	2.10	$[M+H]^+$	192.1	160.1	132.1
Carbofuran	3.77	$[M+H]^+$	222.1	165.2	123.2
Carboxin	3.97	$[M+H]^+$	236.1	143.0	93.0
Carfentrazone ethyl	6.88	$[M+H]^+$	412.0	346.1	366.0
Chlorantraniliprole	5.24	$[M+H]^+$	484.0	286.0	194.0
Chlorfenvinphos	7.21	$[M+H]^+$	359.0	170.0	99.1
Chlorimuron ethyl	5.73	$[M+H]^+$	415.1	186.0	83.0
Chlorpyrifos	8.47	$[M+H]^+$	349.9	198.0	97.0
Chlorpyrifos OA	6.65	$[M+H]^+$	334.0	278.0	197.9
Clethodim	7.71	$[M+H]^+$	360.3	164.1	136.1
Clofentezine	7.38	$[M+H]^+$	303.0	138.1	102.0
Cloransulam methyl	4.13	$[M+H]^+$	430.0	398.1	370.0
Clothianidin	1.99	$[M+H]^+$	250.0	169.1	132.0
Coumaphos	7.07	$[M+H]^+$	363.0	227.1	307.1
Crotoxyphos	5.86	$[M+NH_4]^+$	332.1	127.1	193.1
Crufomate	6.77	$[M+H]^+$	292.1	236.1	108.1
Cyantraniliprole	4.33	$[M+2+H]^+$	475.0	286.0	444.1
Cyazofamid	6.52	$[M+H]^+$	325.1	108.1	261.2
Cyflufenamid	7.42	$[M+H]^+$	413.1	295.1	203.0
Cymoxanil	2.48	$[M+H]^+$	199.1	128.1	111.1
Cyphenothrin	9.27	$[M+NH_4]^+$	393.2	151.2	123.2

Analyte	R_t (mins)	Adduct	Precusor Ion *m/z*	Quant Ion *m/z*	Conf Ion *m/z*
Cyprosulfamide	3.30	$[M+H]^+$	375.1	135.1	254.1
Cyromazine	1.15	$[M+H]^+$	167.1	125.2	68.2
DEF	9.20	$[M+H]^+$	315.1	169.0	113.0
Demeton-S sulfone	2.55	$[M+H]^+$	291.1	235.1	263.1
Dialifos	7.46	$[M+H]^+$	394.0	208.1	181.0
Diazinon	7.12	$[M+H]^+$	305.1	169.1	153.2
Diazinon OA	5.32	$[M+H]^+$	289.1	153.2	233.1
Dichlormid	3.85	$[M+H]^+$	208.0	140.0	81.2
Dichlorvos	3.63	$[M+H]^+$	221.0	109.1	127.0
Dicrotophos	1.87	$[M+H]^+$	238.1	112.2	193.1
Diethofencarb	5.53	$[M+H]^+$	268.2	124.1	180.2
Diflubenzuron	6.66	$[M+H]^+$	311.0	158.0	141.0
Dimethenamid	5.70	$[M+H]^+$	276.1	244.1	168.2
Dimethoate	2.23	$[M+H]^+$	230.1	199.0	125.0
Dimethomorph	5.76, 6.07	$[M+H]^+$	388.1	301.0	165.1
Dinotefuran	1.36	$[M+H]^+$	203.1	129.1	114.2
Dioxacarb	2.26	$[M+H]^+$	224.1	123.1	167.1
Dioxathion	8.10	$[M-C_4H_{10}O_2PS_2]^+$	271.1	97.0	125.0
Disulfoton sulfone	4.59	$[M+H]^+$	307.0	261.1	125.0
Disulfoton sulfoxide	4.49	$[M+H]^+$	291.0	185.1	213.1
Diuron	4.82	$[M+H]^+$	233.0	72.1	160.0
DMST	3.90	$[M+H]^+$	215.1	106.1	151.0
Dodine	7.56	$[M+H]^+$	228.3	186.3	60.1
Emamectin	8.57	$[M+H]^+$	886.5	158.1	126.1
Ethiofencarb	4.27	$[M+H]^+$	226.1	107.1	169.1
Ethiofencarb sulfone	1.90	$[M+NH_4]^+$	275.1	107.1	201.1
Ethiofencarb sulfoxide	1.98	$[M+H]^+$	242.1	107.1	185.0
Ethion	8.31	$[M+H]^+$	385.0	199.1	143.0
Ethion monoxon	6.73	$[M+H]^+$	369.0	199.0	143.0
Ethiprole	5.77	$[M+NH_4]^+$	413.9	351.0	255.0
Ethofumesate	5.55	$[M+H]^+$	287.1	121.1	241.1
Ethoprop	6.46	$[M+H]^+$	243.1	173.0	131.0
Etofenprox	9.75	$[M+NH_4]^+$	394.2	177.2	107.1
Etoxazole	8.73	$[M+H]^+$	360.2	141.0	304.2
Famoxadone	7.24	$[M+NH_4]^+$	392.2	331.1	238.0
Fenamidone	5.76	$[M+H]^+$	312.1	236.1	92.2
Fenamiphos	6.71	$[M+H]^+$	304.1	217.1	202.0
Fenamiphos sulfone	4.10	$[M+H]^+$	336.1	266.1	188.1
Fenamiphos sulfoxide	3.96	$[M+H]^+$	320.1	233.1	171.1
Fenazaquin	9.21	$[M+H]^+$	307.2	161.2	57.2
Fenhexamid	6.39	$[M+H]^+$	302.1	178.0	97.2
Fenobucarb	5.49	$[M+H]^+$	208.1	95.0	152.0
Fenoxaprop ethyl	8.04	$[M+H]^+$	362.1	288.1	91.1
Fenoxycarb	6.80	$[M+H]^+$	302.1	88.1	116.1
Fenpropimorph	6.42	$[M+H]^+$	304.3	147.2	119.1

250 Pesticide Screen by LC-MS/MS

Analyte	R_t (mins)	Adduct	Precusor Ion *m/z*	Quant Ion *m/z*	Conf Ion *m/z*
Fenpyroximate	8.90	$[M+H]^+$	422.2	366.1	214.2
Fensulfothion	4.89	$[M+H]^+$	309.0	235.0	281.1
Fenuron	2.17	$[M+H]^+$	165.1	72.1	77.1
Flonicamid	1.66	$[M+H]^+$	230.1	203.0	98.0
Fluazifop-p-butyl	8.12	$[M+H]^+$	384.1	282.2	328.2
Fludioxonil	5.76	$[M+NH_4]^+$	266.1	158.1	131.0
Flufenoxuron	8.79	$[M+H]^+$	489.0	158.1	141.1
Flufenpyr ethyl	6.72	$[M+H]^+$	409.1	335.0	307.0
Flumetsulam	2.03	$[M+H]^+$	326.1	129.1	109.0
Flumiclorac pentyl	8.13	$[M+NH_4]^+$	441.1	308.1	354.1
Fluometuron	4.31	$[M+H]^+$	233.1	72.2	46.3
Fluopicolide	6.00	$[M+H]^+$	383.0	173.0	145.0
Fluopyram	6.33	$[M+H]^+$	397.1	173.0	208.0
Fluoxastrobin	6.40	$[M+H]^+$	459.1	427.2	188.1
Fluridone	5.32	$[M+H]^+$	330.1	309.1	290.0
Flusilazole	6.77	$[M+H]^+$	316.1	247.2	165.1
Fluthiacet methyl	6.88	$[M+H]^+$	404.0	344.0	273.9
Flutolanil	5.95	$[M+H]^+$	324.1	262.0	282.0
Flutriafol	4.74	$[M+H]^+$	302.1	70.1	123.1
Fluxapyroxad	6.02	$[M+H]^+$	382.1	342.1	314.1
Forchlorfenuron	4.78	$[M+H]^+$	248.1	129.1	93.1
Formetanate HCl	1.26	$[M+H]^+$	222.0	165.1	120.0
Fosthiazate	4.40	$[M+H]^+$	284.1	104.1	228.1
Hexaconazole	7.29	$[M+H]^+$	314.1	158.9	70.0
Hexythiazox	8.51	$[M+H]^+$	353.1	228.0	168.0
Imazalil	5.14	$[M+H]^+$	297.1	159.1	255.1
Imazosulfuron	5.28	$[M+H]^+$	413.0	153.0	156.1
Imidacloprid	1.96	$[M+H]^+$	256.1	209.1	175.0
Imiprothrin	6.34	$[M+H]^+$	319.2	151.1	123.1
Indaziflam	6.58	$[M+H]^+$	302.2	158.1	145.1
Indoxacarb	7.75	$[M+H]^+$	528.1	249.0	150.1
Ipconazole	7.81	$[M+H]^+$	334.2	70.1	125.0
Iprovalicarb	6.31	$[M+H]^+$	321.2	119.1	186.2
Isofenphos	7.39	$[M+H]^+$	346.1	217.0	245.1
Isoprocarb	4.67	$[M+H]^+$	194.1	95.1	152.2
Isoproturon	4.79	$[M+H]^+$	207.2	72.2	165.2
Kresoxim methyl	6.90	$[M+H]^+$	314.1	267.2	222.1
Lactofen	8.22	$[M+NH_4]^+$	479.1	344.1	223.0
Lenacil	4.67	$[M+H]^+$	235.1	153.1	136.1
Leptophos OA	7.75	$[M+2+H]^+$	396.9	155.1	364.9
Linuron	5.46	$[M+H]^+$	249.0	182.1	160.1
Malathion	5.92	$[M+H]^+$	331.0	127.1	285.1
Malathion OA	3.89	$[M+H]^+$	315.1	127.1	99.0
Mandipropamid	5.94	$[M+H]^+$	412.1	328.2	356.2
Mefenpyr diethyl	7.26	$[M+H]^+$	373.1	327.1	160.0



Analyte	R_t (mins)	Adduct	Precusor Ion *m/z*	Quant Ion *m/z*	Conf Ion *m/z*
Mepanipyrim	6.21	$[M+H]^+$	224.1	106.2	77.1
Mesotrione	2.01	$[M+H]^+$	340.1	228.1	104.1
Metaflumizone	8.30	$[M+H]^+$	507.1	178.0	287.1
Metalaxyl	4.91	$[M+H]^+$	280.1	220.1	192.1
Metaldehyde	2.02	$[M+NH_4]^+$	194.1	62.2	45.3
Metconazole	7.32	$[M+H]^+$	320.2	70.1	125.0
Methamidophos	1.16	$[M+H]^+$	142.0	94.2	125.1
Methidathion	4.97	$[M+NH_4]^+$	320.0	145.1	85.1
Methiocarb	5.64	$[M+H]^+$	226.1	169.2	121.1
Methiocarb sulfone	2.35	$[M+NH_4]^+$	275.0	122.1	201.1
Methiocarb sulfoxide	2.10	$[M+H]^+$	242.1	185.1	122.1
Methomyl	1.61	$[M+H]^+$	163.1	106.1	88.1
Methoxyfenozide	6.04	$[M+H]^+$	369.2	149.1	313.1
Metolcarb	3.28	$[M+H]^+$	166.1	109.1	94.1
Metribuzin	3.59	$[M+H]^+$	215.1	187.1	131.1
Mevinphos	2.70	$[M+NH_4]^+$	242.1	193.1	127.1
Monocrotophos	1.71	$[M+H]^+$	224.1	193.0	127.0
Monolinuron	4.16	$[M+H]^+$	215.1	126.1	148.1
Myclobutanil	6.15	$[M+H]^+$	289.1	125.0	70.1
Nicosulfuron	3.45	$[M+H]^+$	411.1	182.0	213.0
Norflurazon	4.98	$[M+H]^+$	304.0	160.0	140.0
Norflurazon desmethyl	4.43	$[M+H]^+$	290.0	179.0	140.0
Omethoate	1.33	$[M+H]^+$	214.0	183.0	125.0
Oxamyl	1.48	$[M+NH_4]^+$	237.1	72.0	90.0
Oxamyl oxime	1.34	$[M+H]^+$	163.1	72.1	90.1
Oxydemeton methyl	1.57	$[M+H]^+$	247.0	169.1	109.1
Oxydemeton methyl sulfone	1.62	$[M+H]^+$	263.0	169.0	109.0
Parathion methyl OA	3.10	$[M+H]^+$	248.0	202.0	109.1
Parathion OA	4.61	$[M+H]^+$	276.1	220.1	248.1
Pencycuron	7.50	$[M+H]^+$	329.1	125.1	89.1
Penflufen	6.95	$[M+H]^+$	318.2	234.1	141.0
Penthiopyrad	7.05	$[M+H]^+$	360.1	177.1	276.1
Phenothrin	9.56	$[M+H]^+$	351.2	183.1	168.0
Phenthoate	6.81	$[M+H]^+$	321.0	247.1	79.1
Phorate OA	5.10	$[M+H]^+$	245.0	75.2	47.2
Phorate OA Sulfone	2.51	$[M+H]^+$	277.0	155.0	127.0
Phorate OA Sulfoxide	2.31	$[M+H]^+$	261.0	153.0	81.0
Phorate Sulfone	4.61	$[M+H]^+$	293.0	114.9	171.0
Phorate Sulfoxide	4.49	$[M+H]^+$	277.0	170.9	199.0
Phosalone	7.35	$[M+H]^+$	368.0	182.0	111.1
Phosmet	5.21	$[M+H]^+$	318.0	160.1	133.1
Phosmet OA	3.12	$[M+H]^+$	302.0	160.0	133.0
Phosphamidon	3.43	$[M+H]^+$	300.1	127.1	174.1
Phoxim	7.25	$[M+H]^+$	299.1	77.2	129.1
Picoxystrobin	6.79	$[M+H]^+$	368.1	145.0	115.0

250 Pesticide Screen by LC-MS/MS

Analyte	R_t (mins)	Adduct	Precusor Ion *m/z*	Quant Ion *m/z*	Conf Ion *m/z*
Pirimicarb	4.24	$[M+H]^+$	239.2	182.1	72.0
Pirimicarb Desmethyl	2.71	$[M+H]^+$	225.1	168.2	72.1
Pirimiphos Methyl	7.34	$[M+H]^+$	306.1	164.2	108.1
Prallethrin	7.69	$[M+H]^+$	301.2	133.0	151.2
Prochloraz	7.39	$[M+H]^+$	376.0	308.1	70.1
Profoxydim	7.71, 9.00	$[M+H]^+$	466.2	280.0	180.0
Promecarb	5.88	$[M+H]^+$	208.1	109.0	151.1
Propamocarb	1.41	$[M+H]^+$	189.1	102.0	144.0
Propaquizafop	8.21	$[M+H]^+$	444.1	299.2	371.2
Propargite	8.74	$[M+NH_4]^+$	368.2	231.2	175.1
Propetamphos	6.13	$[M+H]^+$	282.1	138.1	156.1
Propoxur(S)	3.69	$[M+H]^+$	210.1	168.2	111.1
Prosulfuron	5.29	$[M+H]^+$	420.1	167.1	141.1
Pymetrozine	1.44	$[M+H]^+$	218.1	105.1	78.1
Pyraclostrobin	7.30	$[M+H]^+$	388.1	163.1	194.1
Pyraflufen Ethyl	7.13	$[M+H]^+$	413.0	339.0	253.1
Pyrazophos	7.31	$[M+H]^+$	374.1	222.2	194.1
Pyridaben	9.22	$[M+H]^+$	365.1	309.0	147.1
Pyridalyl	10.21	$[M+2+H]^+$	492.0	110.9	164.0
Pyrimethanil	5.45	$[M+H]^+$	200.1	107.1	168.1
Pyriproxyfen	8.39	$[M+H]^+$	322.1	96.0	227.1
Quinalphos	6.78	$[M+H]^+$	299.1	163.1	147.1
Quinoxyfen	8.50	$[M+H]^+$	308.0	197.1	214.1
Quizalofop Ethyl	8.01	$[M+H]^+$	373.1	299.2	255.1
Resmethrin	9.40	$[M+H]^+$	339.2	128.1	171.1
Rimsulfuron	3.94	$[M+H]^+$	432.1	182.1	139.0
Rotenone	6.71	$[M+H]^+$	395.2	213.2	192.1
Saflufenacil	5.32	$[M+H]^+$	501.1	349.1	198.0
Sedaxane	6.20, 6.54	$[M+H]^+$	332.2	159.0	139.0
Sethoxydim	8.03	$[M+H]^+$	328.2	178.0	220.1
Simazine	3.66	$[M+H]^+$	202.1	104.1	132.1
Spinetoram	8.14	$[M+H]^+$	748.5	142.1	203.1
Spinosad A	7.69	$[M+H]^+$	732.5	142.1	98.0
Spinosad D	8.10	$[M+H]^+$	746.5	142.1	98.0
Spirodiclofen	8.91	$[M+H]^+$	411.1	313.1	71.1
Spiromesifen	8.66	$[M+NH_4]^+$	388.1	273.1	187.0
Spiromesifen Alcohol	5.01	$[M+H]^+$	273.2	187.1	179.1
Spirotetramat	6.38	$[M+H]^+$	374.2	302.3	216.2
Spiroxamine	5.95	$[M+H]^+$	298.3	144.2	100.2
Sulfoxaflor	2.39	$[M+NH_4]^+$	295.2	174.1	154.1
Sulprofos	8.56	$[M+H]^+$	323.0	219.1	139.1
TCMTB	5.48	$[M+H]^+$	239.0	180.0	136.0
Tebufenozide	6.78	$[M+H]^+$	353.2	133.0	104.8
Tebufenpyrad	8.19	$[M+H]^+$	334.2	117.1	145.1
Tebuthiuron	3.89	$[M+H]^+$	229.1	172.0	116.0
Tepraloxydim	4.10, 6.19	$[M+H]^+$	342.2	250.1	166.1
Terbufos Sulfone	5.46	$[M+H]^+$	321.0	115.0	143.0
Terbufos Sulfoxide	5.49	$[M+H]^+$	305.1	97.0	187.0
Terbuthylazine	5.71	$[M+H]^+$	230.1	174.1	104.1
Tetrachlorvinphos	6.86	$[M+2+H]^+$	366.9	127.1	206.0
Tetramethrin	7.91, 8.10	$[M+H]^+$	332.2	164.1	135.1
Thiabendazole	2.48	$[M+H]^+$	202.0	175.0	131.1
Thiacloprid	2.55	$[M+H]^+$	253.0	126.1	99.1
Thiamethoxam	1.65	$[M+H]^+$	292.0	211.1	181.1
Thifensulfuron Methyl	3.28	$[M+H]^+$	388.0	167.1	205.0
Thiobencarb	7.46	$[M+H]^+$	258.1	125.0	89.0
Thiodicarb	4.34	$[M+H]^+$	355.1	163.2	88.1
Thionazin	4.74	$[M+H]^+$	249.1	193.1	97.0
Topramezone	1.63	$[M+H]^+$	364.1	334.1	125.1
Triadimefon	6.07	$[M+H]^+$	294.1	197.0	225.0
Triadimenol	6.25	$[M+H]^+$	296.1	70.2	99.0
Triazophos	6.19	$[M+H]^+$	314.1	162.1	119.1
Tribenuron Methyl	4.59	$[M+H]^+$	396.1	155.1	181.1
Trichlorfon	2.26	$[M+H]^+$	256.9	109.0	221.0
Tricyclazole	2.80	$[M+H]^+$	190.0	163.1	136.1
Trifloxystrobin	7.78	$[M+H]^+$	409.1	186.2	206.2
Triflumizole	7.87	$[M+H]^+$	346.1	278.0	73.0
Triforine	5.23	$[M+2+H]^+$	434.9	213.0	98.2
Zoxamide	7.09	$[M+H]^+$	336.0	187.0	159.0

300 Pesticide Screen by LC-MS/MS

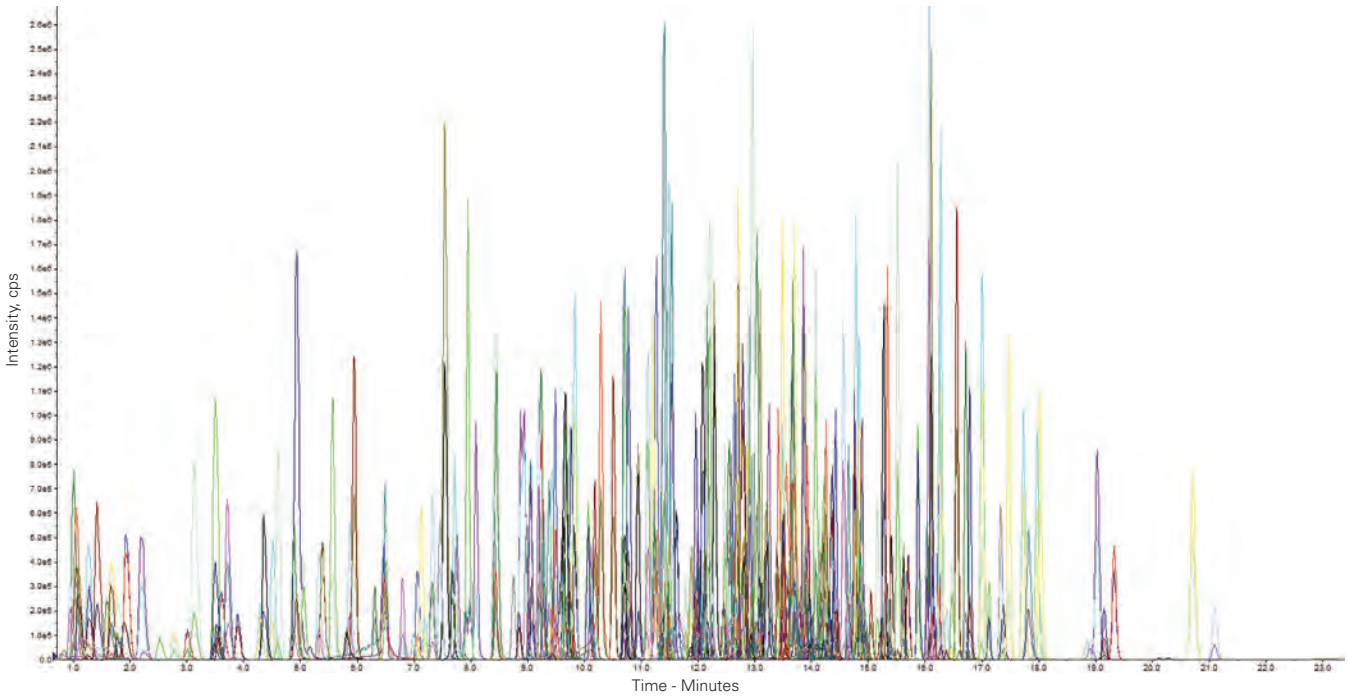
Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 5 mM ammonium formate in H_2O/MeOH (9:1 v/v)
B: 5 mM ammonium formate in H_2O/MeOH (1:9 v/v)

Gradient:

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

Flow Rate: 0.3 mL/min
Injection: 6 µL
Temperature: 24 °C
Detection: AB SCIEX 4000 QTRAP
TurbolonSpray ESI positive mode
Capillary voltage: 5000 V
Heater gas temperature: 450 °C
Sample: Sample prepared using QuEChERs methodology
Method validated using cucumber matrix spiked at 0.01 mg/kg. 265 analytes successfully validated
(Analytes in black)



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300 Pesticide Screen by LC-MS/MS

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
3-Hydroxycarbofuran	3.5	238.1 → 163.1, 238.1 → 181.1
Acephate	1.0	184.1 → 142.9, 184.1 → 124.8
Acetamiprid	3.6	223.2 → 126.1, 225.2 → 128.1
Aclonifen	13.9	265.0 → 248.0, 267.0 → 250.0
Alachlor	12.9	270.2 → 238.2, 270.2 → 162.1
Aldicarb	5.4	208.0 → 89.0, 208.0 → 116.0
Aldicarb sulfone	1.2	240.0 → 86.0, 223.0 → 148.0
Aldicarb sulfoxide	1.1	207.0 → 132.0, 207.2 → 88.9
Ametryn	11.1	228.2 → 186.1, 228.2 → 68.0
Aminopyralid	0.8	207.0 → 160.9, 207.0 → 133.9
Amitrole	0.8	85.1 → 58.1, 85.1 → 57.1
Atrazine	9.3	216.2 → 174.0, 218.1 → 176.1
Atrazine-desethyl	4.4	188.2 → 146.0, 190.1 → 148.0
Atrazine-desisopropyl	2.4	174.1 → 104.1, 174.1 → 132.1
Avermectin B1a	18.2	876.5 → 553.0, 876.5 → 291.0
Avermectin B1b	19.1	890.5 → 305.0, 890.5 → 567.0
Azamethiphos	6.9	325.0 → 183.0, 325.0 → 138.9
Azinphos-ethyl	13.0	346.0 → 132.1, 346.0 → 160.1
Azinphos-methyl	10.9	318.1 → 132.1, 318.1 → 260.8
Aziprotryne	11.8	226.0 → 156.0, 226.0 → 125.0
Azoxystrobin	11.4	404.2 → 372.3, 404.2 → 344.1
Benalaxyl	14.0	326.2 → 148.1, 326.2 → 294.1
Benfuracarb	15.7	411.2 → 252.1, 411.2 → 195.1
Benthiavalicarb-isopropyl	12.0	382.3 → 116.0, 382.3 → 197.0
Bifenazate	12.5	301.2 → 198.1, 301.2 → 170.2
Bifenox	14.9	359.0 → 342.0, 359.0 → 310.0
Bifenthrin	21.0	440.0 → 181.1, 440.0 → 166.1
Bitertanol	14.6	338.2 → 269.0, 338.2 → 99.1
Bixafen	13.6	414.0 → 393.9, 416.1 → 395.9
Boscalid	11.7	343.1 → 306.8, 343.1 → 139.9
Bromfenvinfos-ethyl	14.3	405.0 → 155.0, 403.0 → 155.0
Bromuconazole A	12.2	378.0 → 159.1, 378.0 → 161.0
Bromuconazole B	13.5	378.1 → 159.1, 378.1 → 161.0
Bupirimate	13.5	317.2 → 166.2, 317.2 → 107.9
Buprofezin	16.1	306.3 → 201.1, 306.3 → 116.1
Cadusafos	14.8	271.1 → 158.9, 271.1 → 214.9
Carbaryl	8.3	202.2 → 145.1, 202.2 → 127.1
Carbendazim	4.7	192.2 → 160.1, 192.0 → 132.0
Carbofuran	7.4	222.2 → 165.1, 222.2 → 122.9
Carbosulfan	19.3	381.2 → 160.1, 381.2 → 118.1
Carboxin	8.3	236.1 → 143.1, 236.1 → 87.0
Carfentrazone-ethyl	13.8	412.2 → 345.9, 412.2 → 383.9
Chlorantraniliprole	10.7	484.0 → 452.9, 484.0 → 285.9
Chlorbromuron	11.7	295.1 → 205.9, 293.1 → 182.0
Chlorfenvinfos A	14.3	359.0 → 155.0, 358.9 → 99.0
Chloridazon	3.7	222.1 → 104.0, 222.1 → 77.1
Chlorpyrifos	16.8	349.9 → 198.1, 349.9 → 115.0

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
Chlorpyrifos-methyl	15.2	322.0 → 124.9, 324.0 → 125.1
Chlortoluron	9.1	213.2 → 72.0, 215.1 → 72.1
Cinidon-ethyl	16.3	394.0 → 348.0, 394.0 → 366.0
Clethodim A	12.8	360.1 → 164.1, 360.1 → 268.1
Clethodim B	10.2	360.1 → 164.1, 360.1 → 268.1
Clofentezine	15.1	303.1 → 137.9, 305.1 → 102.0
Clomazone	10.7	240.1 → 124.9, 242.2 → 127.1
Cloquintocet-mexyl	16.1	336.2 → 238.0, 336.2 → 192.1
Clothianidin	2.9	250.1 → 169.0, 250.1 → 132.0
Coumaphos	14.3	363.0 → 227.0, 363.0 → 211.1
Cyanazine	6.7	241.1 → 214.1, 243.1 → 216.1
Cyazofamid	13.2	325.2 → 107.9, 327.2 → 107.9
Cycloate	14.9	216.2 → 83.1, 216.2 → 154.1
Cycloxydim A	13.1	326.3 → 280.0, 326.3 → 180.0
Cycloxydim B	8.4	326.3 → 280.0, 326.3 → 180.0
Cymoxanil	4.2	199.2 → 128.0, 199.2 → 111.1
Cyproconazole A	12.5	292.0 → 70.0, 292.0 → 125.0
Cyproconazole B	12.0	292.0 → 70.0, 292.0 → 125.0
Cyprodinil A	14.1	226.2 → 93.0, 226.2 → 77.0
Demeton-S-methyl	7.7	231.1 → 88.8, 231.1 → 61.0
Demeton-S-methyl sulfone	1.6	263.0 → 168.9, 263.0 → 120.8
Desmedipham	10.6	318.1 → 182.1, 318.1 → 136.0
Desmethyl-pirimicarb	5.8	225.2 → 72.0, 225.2 → 168.1
Diafenthiuron	17.4	385.2 → 329.2, 385.2 → 278.2
Diazinon	14.2	305.1 → 169.1, 305.1 → 97.0
Dichlofluanid	12.8	333.0 → 223.9, 333.0 → 122.9
Diclobutrazol A	13.7	328.0 → 70.0, 330.0 → 70.0
Dicrotofos	2.1	238.1 → 112.1, 238.1 → 193.1
Diethofencarb	11.1	268.1 → 226.1, 268.1 → 124.0
Difenoconazole	14.8	406.1 → 251.1, 408.2 → 253.1
Diflubenzuron	13.5	311.0 → 158.2, 311.0 → 141.1
Diflufenican	15.4	395.0 → 266.0, 395.0 → 246.0
Dimethachlor	10.2	256.2 → 224.0, 256.2 → 148.1
Dimethenamid	11.3	276.1 → 244.0, 278.1 → 246.0
Dimethoate	3.6	230.1 → 198.8, 230.1 →124.9
Dimethomorph	11.7	388.1 → 301.0, 388.1 → 165.1
Dimoxystrobin	13.7	327.1 → 205.0, 327.1 → 116.0
Diniconazole	14.8	326.0 → 70.0, 328.0 → 70.0
Disulfoton	15.0	275.1 → 89.0, 275.1 → 61.0
Disulfoton sulfone	9.6	307.1 → 153.0, 307.1 → 171.0
Disulfoton sulfoxide	9.2	291.1 → 212.9, 291.1 → 185.0
Ditalimfos	13.1	300.1 → 148.0, 300.1 → 130.0
Diuron	10.0	233.1 → 71.9, 235.1 → 72.0
DMST	8.0	215.2 → 106.0, 215.2 → 78.9
Dodine	13.6	228.3 → 57.0, 228.3 → 60.1
Epoxiconazole	12.9	330.1 → 120.9, 330.1 → 75.2
Ethion	16.5	385.0 → 199.0, 385.0 → 143.0

300 Pesticide Screen by LC-MS/MS

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



300 Pesticide Screen by LC-MS/MS

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
Mevinfos A	4.9	225.0 → 193.0, 225.0 → 127.0
Mevinfos B	3.4	225.0 → 193.0, 225.0 → 127.0
Molinate	12.0	188.2 → 126.2, 188.2 → 55.1
Monocrotofos	1.8	224.2 → 192.9, 224.2 → 126.9
Monolinuron	8.7	215.1 → 126.1, 215.1 → 148.1
Myclobutanil	12.2	289.2 → 70.0, 289.2 → 125.0
Napropamide	12.9	272.2 → 129.1, 272.2 → 171.1
Nitenpyram	1.3	271.1 → 189.2, 271.1 → 126.0
Novaluron	15.6	493.0 → 158.1, 493.0 → 141.1
Nuarimol	11.2	315.0 → 252.0, 315.0 → 81.0
Ofurace	7.6	282.0 → 160.1, 282.0 → 236.3
Omethoate	1.0	214.0 → 183.0, 214.0 → 125.0
Oxadiazon	16.2	345.0 → 220.0, 345.0 → 303.0
Oxadixyl	6.4	279.0 → 219.0, 279.0 → 133.0
Oxamyl NH4+	1.2	237.1 → 72.0, 220.2 → 72.0
Oxycarboxin	4.5	268.1 → 174.9, 268.1 → 147.0
Oxydemeton-methyl	1.4	247.0 → 108.9, 247.0 → 168.9
Paclobutrazol	11.8	294.0 → 70.0, 294.0 → 125.0
Paraoxon	9.4	275.9 → 219.9, 275.9 → 248.0
Paraoxon-methyl	6.1	248.1 → 202.1, 248.1 → 90.0
Parathion	13.8	292.0 → 236.0, 292.0 → 264.1
Penconazole	13.7	248.1 → 70.0, 284.1 → 159.0
Pencycuron	14.8	329.3 → 125.1, 331.3 → 127.0
Pendimethalin	16.9	282.2 → 212.1, 282.2 → 194.1
Pethoxamid	12.7	296.2 → 131.0, 296.2 → 250.0
Phenmedipham	10.8	301.2 → 168.0, 301.2 → 136.0
Phenthoate	13.9	321.0 → 247.0, 321.0 → 275.1
Phorate sulfone	9.6	293.0 → 170.8, 293.0 → 96.7
Phorate sulfoxide	9.2	277.0 → 199.0, 277.0 → 171.0
Phosalone	14.6	368.0 → 182.0, 369.9 → 183.9
Phosphamidon	6.4	300.2 → 127.1, 300.2 → 226.8
Phoxim	14.7	299.2 → 129.2, 299.2 → 77.1
Picloram	1.2	243.0 → 224.9, 241.0 → 222.9
Picolinafen	16.2	377.1 → 238.0, 377.1 → 359.0
Picoxystrobin	13.6	368.0 → 205.0, 368.0 → 145.0
Piperonyl butoxide	16.2	356.2 → 177.2, 356.2 → 119.0
Pirimicarb	9.0	239.2 → 72.0, 239.2 → 182.3
Pirimiphos-ethyl	16.3	334.1 → 198.0, 334.1 → 182.3
Pirimiphos-methyl	14.8	306.2 → 108.0, 306.2 → 164.3
Prochloraz	14.4	376.0 → 308.0, 376.0 → 70.0
Profenofos	15.6	375.0 → 304.9, 373.0 → 302.9
Prometryn	12.6	242.2 → 158.1, 242.2 → 200.0
Propachlor	9.6	212.0 → 170.0, 212.0 → 94.1
Propamocarb	1.1	189.0 → 102.0, 189.0 → 144.0
Propaquizafop	16.0	444.2 → 100.0, 444.2 → 371.0
Propargite NH4+	17.0	368.2 → 231.1, 368.2 → 175.0

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
Propazine	11.0	230.2 → 188.1, 230.2→ 146.1
Propetamfos	12.4	282.1 → 138.0, 282.1→ 156.1
Propham	9.4	180.1 → 138.1, 180.1 → 120.1
Propiconazole	14.0	342.1 → 159.0, 342.1 → 69.0
Propisochlor	14.0	284.2 → 224.0, 284.2 → 148.0
Propoxur	7.2	210.1 → 111.1, 210.1 → 168.0
Propyzamide	11.9	256.1 → 190.0, 256.1 → 173.0
Proquinazid	17.7	373.2 → 330.9, 373.2 → 289.0
Prosulfocarb	15.5	252.2 → 91.0, 252.2 → 128.1
Prosulfuron	9.0	420.1 → 141.0, 420.1 → 167.1
Prothioconazole	14.1	344.1 → 326.0, 346.1 → 328.1
Prothioconazole-desthio	13.0	312.0 → 70.0, 312.0 → 125.0
Pymetrozine	1.5	218.0 → 105.0, 218.0 → 78.0
Pyraclostrobin	14.5	388.1 → 194.0, 388.1 → 163.0
Pyrazophos	14.8	374.0 → 222.0, 374.0 → 194.0
Pyridaben	18.0	365.0 → 309.0, 365.0 → 147.0
Pyridapenthion	12.4	341.0 → 189.0, 341.0 → 205.0
Pyridate	19.1	379.1 → 206.9, 379.1 → 350.9
Pyrifenox	13.0	295.1 → 93.0, 297.1 → 93.0
Pyrimethanil	11.3	200.0 → 82.0, 200.0 → 107.0
Pyriproxyfen	16.7	322.0 → 96.0, 322.0 → 185.0
Pyroxsulam	5.6	435.0 → 195.1, 435.0 → 194.0
Quinalfos	13.9	299.0 → 271.0, 299.0 → 243.0
Quinoclamine	6.8	208.0 → 105.0, 208.0 → 77.0
Quinoxyfen	16.4	308.0 → 197.0, 308.0 → 162.0
Rotenone	13.4	395.1 → 213.1, 395.1 → 192.0
Secbumeton	10.6	226.2 → 170.1, 226.2 → 100.0
Silthiofam	13.5	268.0 → 252.0, 268.0 → 73.0
Simazine	7.2	202.2 → 132.1,202.2→ 104.0
Simetryn	9.4	214.1 → 124.1, 214.1 → 144.0
Spinosyn A	17.3	732.5 → 142.0, 732.5 → 98.0
Spinosyn D	18.3	746.5 → 142.0, 746.5 → 98.0
Spirodiclofen	17.4	313.1 → 295.0, 313.1 → 213.0
Spiromesifen	16.8	371.2 → 273.1, 371.2 → 255.2
Spirotetramat	12.8	374.2 → 302.2, 374.2 → 330.2
Spiroxamine	13.3	298.3 → 100.1, 298.3 → 144.1
Sulfotep	14.0	323.0 → 97.0, 323.0 → 115.0
Tau-fluvalinate	18.9	503.0 → 208.0, 503.0 → 181.0
Tebuconazole	13.9	308.1 → 70.0, 308.1 → 125.0
Tebufenozide	13.5	353.2 → 297.2, 353.2 → 133.0
Tebufenpyrad	15.9	334.0 → 145.0, 334.0 → 117.0
Teflubenzuron	16.3	381.1 → 158.2, 381.1 → 141.2
Tembotrione (NH4 adduct)	5.9	458.0 → 340.9, 458.0 → 441.0
Terbufos	16.1	289.1 → 103.1, 289.1 → 232.9
Terbufos sulfone	11.1	321.1 → 171.0, 321.1 → 115.0
Terbufos sulfoxide	11.0	305.1 → 187.2, 305.1 → 131.1

300 Pesticide Screen by LC-MS/MS

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
Terbumeton	11.3	226.2 → 170.1, 226.2 → 142.0
Terbuthylazine	11.4	230.2 → 174.0, 232.2 → 176.0
Terbutryn	12.9	242.1 → 186.1, 242.1 → 96.0
Tetrachlorvinfos	13.5	367.0 → 127.0, 365.0 → 127.0
Tetraconazole	12.9	372.0 → 159.0, 374.0 → 161.2
Thiabendazole	6.2	202.1 → 174.9, 202.1 → 131.0
Thiacloprid	4.7	253.1 → 126.1, 253.1 → 99.1
Thiencarbazone-methyl	2.3	391.0 → 130.0, 391.0 → 230.0
Thiodicarb	9.2	355.0 → 88.0, 355.0 → 108.0
Thiophanate-methyl	7.6	343.0 → 151.1, 343.0 → 311.0
Thiamethoxam	1.7	292.0 → 211.0, 292.0 → 181.0
Tolclophos-methyl	14.9	301.2 → 268.9, 303.1 → 270.9
Tolylfluanid	13.9	347.0 → 237.8, 347.0 → 137.1
Topramezone	1.6	364.1 → 334.1, 364.1 → 125.0

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
Triadimefon	12.1	294.2 → 197.2, 294.2 → 225.0
Triadimenol	12.4	296.2 → 70.0, 298.2 → 70.0
Triallate	16.7	304.1 → 142.9, 304.1 → 86.2
Triazofos	12.6	314.0 → 162.0, 314.2 → 119.0
Trichlorfon	3.4	257.0 → 108.9, 257.0 → 220.8
Tricyclazole	5.2	190.1 → 136.1, 190.1 → 163.0
Trifloxystrobin	15.3	409.0 → 186.0, 409.0 → 206.0
Triflumizole	15.3	346.0 → 278.0, 346.0 → 73.0
Triflumuron	14.6	359.1 → 156.2, 359.1 → 139.0
Triforin	10.6	435.0 → 390.0, 437.0 → 392.0
Triticonazole A	12.7	318.0 → 70.0, 318.0 → 125.0
Triticonazole B	10.9	318.0 → 70.0, 318.0 → 125.0
Vamidothion	3.4	288.1 → 146.0, 288.1 → 118.0
Zoxamide	14.2	336.0 → 187.0, 338.0 → 189.0



Pesticides by LC-MS/MS

Application #AN1290

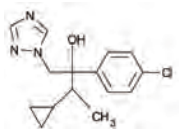
Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 0.1% formic acid + 5 mM ammonium formate in H_2O/MeOH (90:10 v/v)
B: 0.1% formic acid + 5 mM ammonium formate in H_2O/MeOH (10:90 v/v)

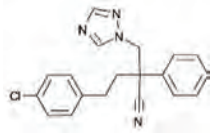
Gradient:

Time (mins)	%B
0.00	0
1.00	0
15.00	100
18.00	100
18.05	0
20.00	0

Flow Rate: 0.4 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: Agilent 6420 Triple Quadrupole MS, +ve mode ESI Dynamic MRM



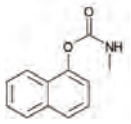
Cyproconazoles



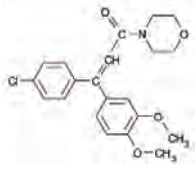
Fenbuconazole

Analytes

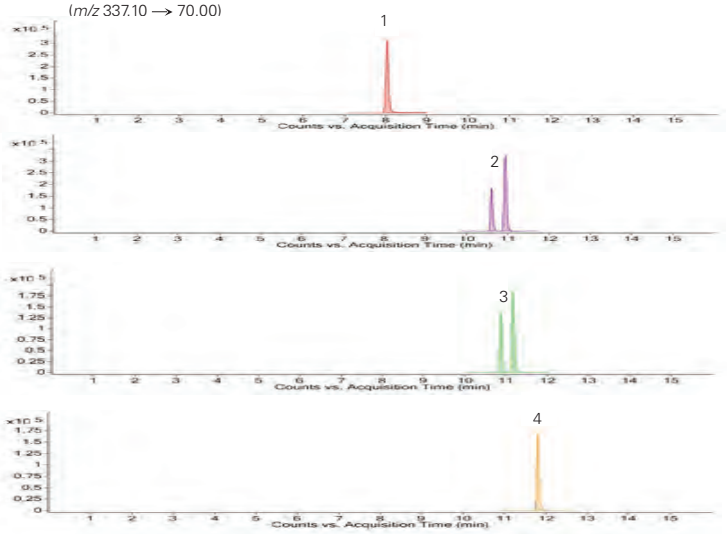
1. Carbaryl
   (*m/z* 202.10 → 145.10)
2. Dimethomorphs
   (*m/z* 388.10 → 301.10)
3. Cyproconazoles
   (*m/z* 292.10 → 70.00)
4. Fenbuconazole
   (*m/z* 337.10 → 70.00)



Carbaryl



Dimethomorphs



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

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Pesticides in Water

Application #AN3020

Conditions

Column: ACE 3 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-111-1502
Mobile Phase: A: 0.1 M ammonium acetate in H_2O
B: MeCN

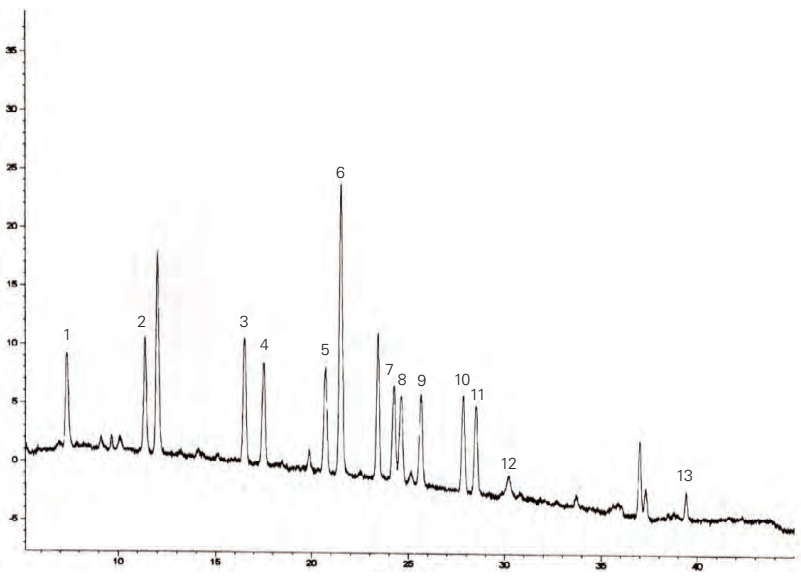
Gradient:

Time (mins)	%B
0	10
40	80
47	90
49	10

Flow Rate: 0.3 mL/min
Injection: 25 µL
Temperature: 40 °C
Detection: UV, 220 nm (Pendimethalin at 245 nm)
Sample: 0.05 µg/L standards in MeCN/H_2O (10:90 v/v)

Analytes

1. Deisopropylatrazine
2. Desethylatrazine
3. Simazine
4. Cyanazine
5. Atrazine
6. Internal standard
7. Sebuthylazine
8. Propazine
9. Terbuthylazine
10. Prometryn
11. Terbutryn
12. Alachlor
13. Pendimethalin



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Pharmaceutically Relevant Compounds (II)

Application #AN1630

Conditions

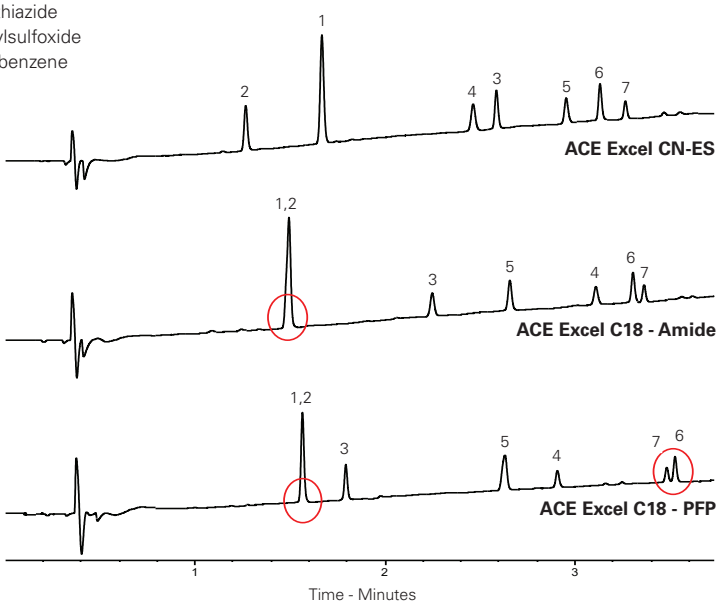
Column: ACE Excel 3 CN-ES
ACE Excel 3 C18-Amide
ACE Excel 3 C18-PFP
Dimensions: 100 x 3.0 mm
Part Numbers: EXL-1113-1003U, EXL-1112-1003U, EXL-1110-1003U
Mobile Phase: A: 20 mM ammonium formate in H_2O
B: 20 mM ammonium formate in MeOH
Gradient:

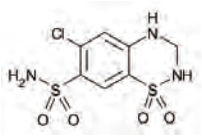
Time (mins)	%B
0.0	3
5.0	100
6.0	100
6.5	3

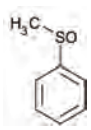
Flow Rate: 0.6 mL/min
Temperature: 40 °C
Detection: UV

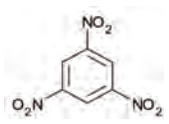
Analytes

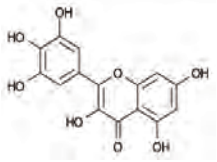
1. Hydrochlorothiazide
2. Methylphenylsulfoxide
3. 1,3,5-Trinitrobenzene
4. Myricetin
5. p-Cresol
6. Sulindac
7. Toluene

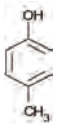


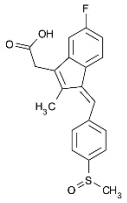

Hydrochlorothiazide

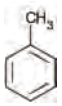

Methylphenylsulfoxide


1,3,5-Trinitrobenzene


Myricetin


p-Cresol


Sulindac


Toluene

Pharmaceutically Relevant Compounds (III)

Application #AN2400

Conditions

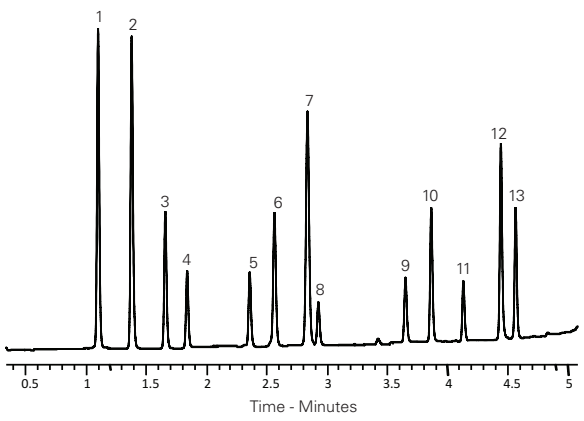
Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: A: 5 mM formic acid in H_2O
B: 5 mM formic acid in MeOH
Gradient:

Time (mins)	%B
0.0	3
5.0	100
5.5	100
6.0	3
8.5	3

Flow Rate: 1.5 mL/min
Injection: 5 µL
Temperature: 40 °C
Detection: UV, 254 nm

Analytes

1. Paracetamol
2. Hydrochlorothiazide
3. Methylphenylsulfoxide
4. Methylphenylsulfone
5. Aspirin
6. Phenacetin
7. 1,3-Dinitrobenzene
8. 1,2,4-Trimethoxybenzene
9. Ethylbenzoate
10. Nimesulide
11. Ibuprofen
12. Indomethacin
13. Mefenamic acid



Pharmaceutically Relevant Compounds (IV)

Application #AN2460

Conditions

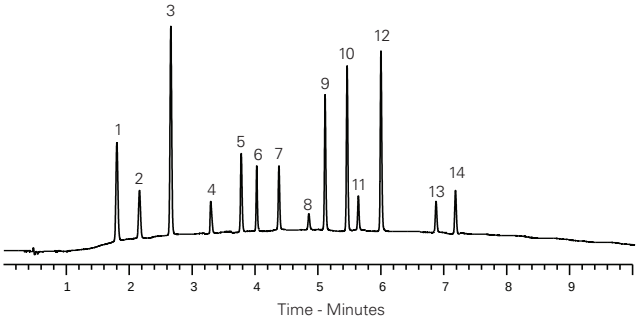
Column: ACE Excel 3 CN-ES
Dimensions: 100 x 2.1 mm
Part Number: EXL-1113-1002U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Gradient:

Time (mins)	%B
0	3
10	100

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

Analytes

1. 1,3-Dihydroxybenzene
2. Catechol
3. Hydrochlorothiazide
4. Oxprenolol
5. Salicylic acid
6. Myricetin
7. Piroxicam
8. 1,2-Dinitrobenzene
9. Tolmetin
10. 1-Naphthol
11. Piperine
12. Diflunisal
13. Propylbenzene
14. 1,2,3-Trichlorobenzene



Pharmaceutically Relevant Compounds (V)

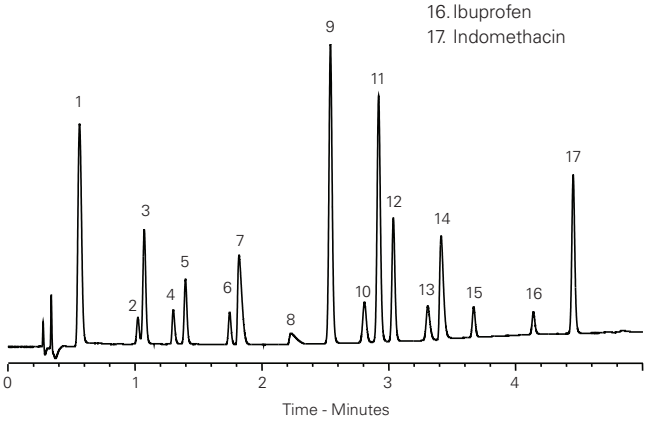
Application #AN2500

Conditions

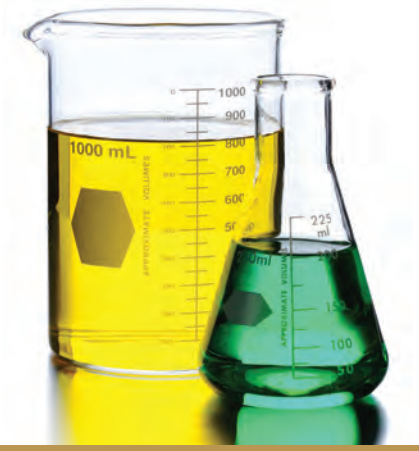
Column:	ACE 3 C18-PFP
Dimensions:	50 x 2.1 mm
Part Number:	ACE-1110-0502
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH
Gradient:	**Time (mins) %B**
	0 3
	5 100
Flow Rate:	0.6 mL/min
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Sulphanilamide
2. Nizatidine
3. Metronidazole
4. Amiloride
5. Hydrochlorothiazide
6. Caffeine
7. Pindolol
8. Metoprolol
9. Phenacetin
10. 1,3-Dinitrobenzene
11. Hexobarbital
12. Furosemide
13. Piroxicam
14. Carvedilol
15. Ketoprofen
16. Ibuprofen
17. Indomethacin



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



Pharmaceutically Relevant Mixture (I) – Different Selectivity Using pH

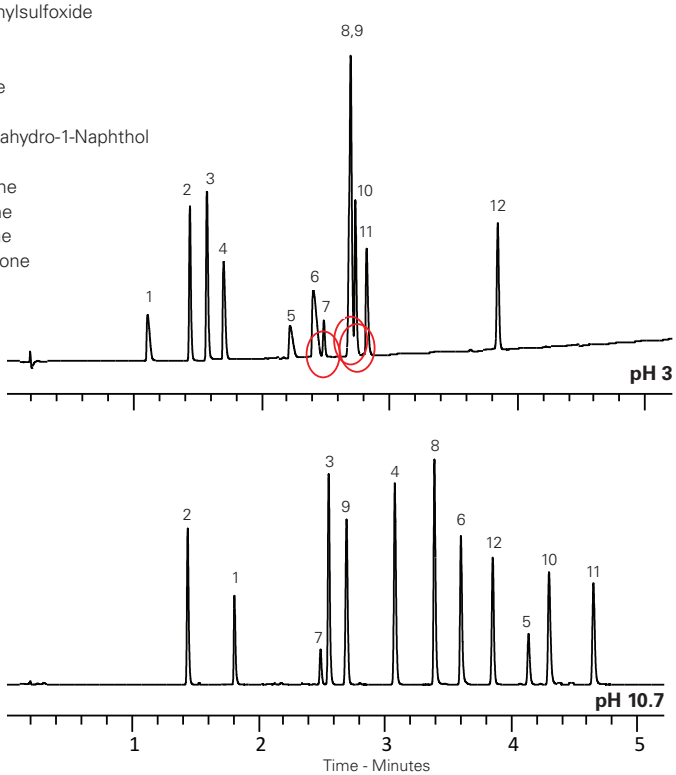
Application #AN1310

Conditions

Column:	ACE Ultracore 2.5 SuperC18
Dimensions:	50 x 2.1 mm
Part Number:	CORE-25A-0502U
Mobile Phase:	A1: 10 mM ammonium formate pH 3 in H_2O
	A2: 0.1% ammonia pH 10.7 in H_2O
	B1: 10 mM ammonium formate pH 3 in MeCN/H_2O (90:10 v/v)
	B2: 0.1% ammonia pH 10.7 in MeCN/H_2O (90:10 v/v)
Gradient:	**Time (mins) %B**
	0 3
	5 100
	6 100
Flow Rate:	0.6 mL/min
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Atenolol
2. Methylphenylsulfoxide
3. Eserine
4. Prilocaine
5. Bupivacaine
6. Tetracaine
7. 1,2,3,4-Tetrahydro-1-Naphthol
8. Carvedilol
9. Nitrobenzene
10. Methdilazine
11. Amitriptyline
12. Valerophenone



Pharmaceutically Relevant Mixture (II) – Different Selectivity Using pH

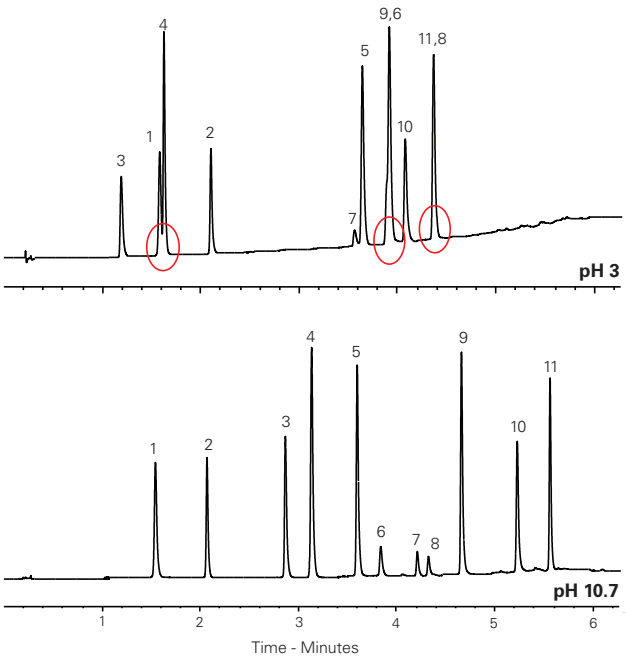
Application #AN1300

Conditions

Column:	ACE Ultracore 2.5 SuperPhenylHexyl
Dimensions:	50 x 2.1 mm
Part Number:	CORE-25B-0502U
Mobile Phase:	A1: 10 mM ammonium formate pH 3 in H_2O A2: 0.1% ammonia pH 10.7 in H_2O B1: 10 mM ammonium formate pH 3 in MeCN/H_2O (90:10 v/v) B2: 0.1% ammonia pH 10.7 in MeCN/H_2O (90:10 v/v)
Gradient:	**Time (mins) %B** 0 3 5 100 6 100
Flow Rate:	0.6 mL/min
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Benzamide
2. Caffeine
3. Procainamide
4. N-Acetylprocainamide
5. Propiophenone
6. Toluene
7. Remacemide
8. Ethylbenzene
9. Carvedilol
10. Nortriptyline
11. Clomipramine



Phenelzine in Human Plasma by LC-MS/MS

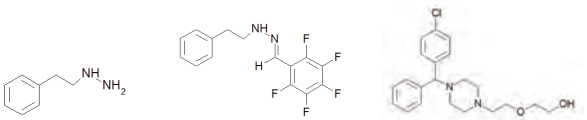
Application #AN4200

Conditions

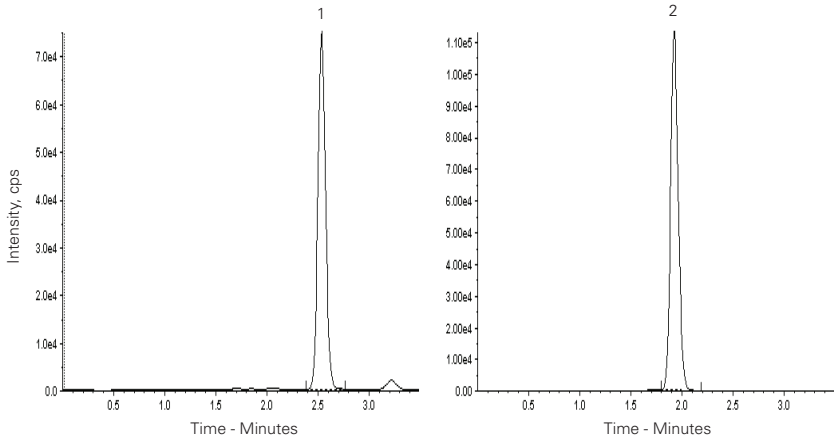
Column:	ACE 5 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-121-1046
Mobile Phase:	10 mM ammonium acetate in H_2O, pH 4.0/MeOH (20:80 v/v)
Flow Rate:	1 mL/min with 70% split flow into MS
Injection:	10 µL
Temperature:	45 °C
Detection:	AB Sciex API-4000 MS MRM using ESI in positive ion mode TurboIonSpray Interface Temperature: 600 °C IonSpray Voltage: 5500 V
Sample:	Phenelzine derivatised with pentafluorobenzaldehyde, followed by SPE extraction of derivative and hydroxyzine (I.S.) from 200 µL human plasma.

Analytes

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



Spiked human plasma



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Phenol and Phenoxy Acid Herbicides

Application #AN2290

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeOH

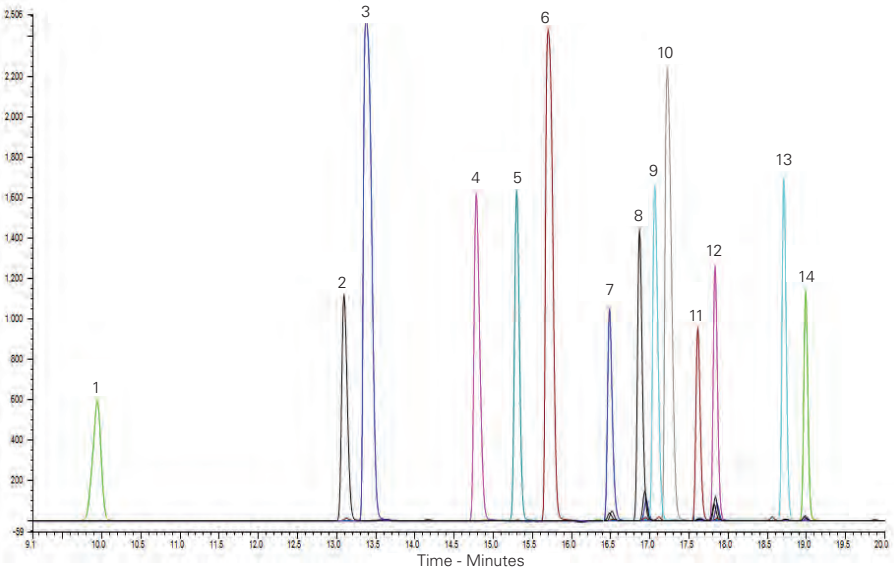
Gradient:

Time (mins)	%B
0.0	10
20.0	100

Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 35 °C
Detection: UV, 280 nm

Analytes

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



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Phenolic Acids

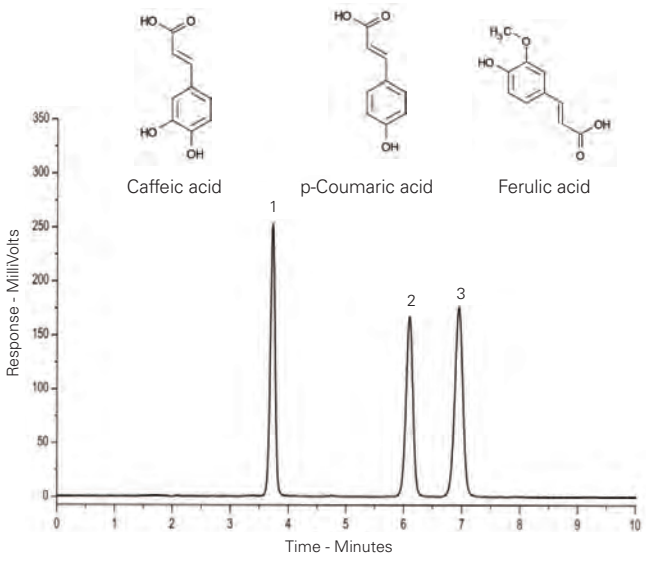
Application #AN3030

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/0.1% formic acid in H_2O (20:80 v/v)
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: Ambient
Detection: UV, 254 nm

Analytes

1. Caffeic acid
2. p-Coumaric acid
3. Ferulic acid



Phenolic Compounds in Ground Water & Landfill Leachates

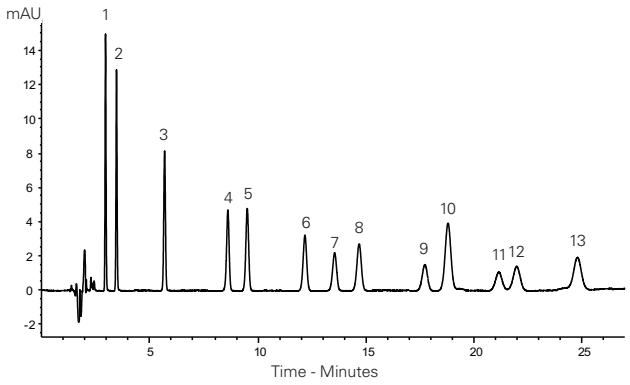
Application #AN3070

Conditions

Column: ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: EXL-1112-1546U
Mobile Phase: 0.1% formic acid v/v in H_2O
MeCN (65:35 v/v)
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 30 °C
Detection: UV, 274 nm

Analytes

1. Pyrocatechol
2. Resorcinol
3. Phenol
4. m-Cresol
5. o-Cresol
6. 2,4-Dimethylphenol
7. 3,4-Dimethylphenol
8. 3,5-Dimethylphenol
9. 1-Naphthol
10. 3,4,5-Trimethylphenol
11. 2,3,6-Trimethylphenol
12. 2,4,6-Trimethylphenol
13. 2-Naphthol



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Phenolic Compounds from Red Grape Seed Extract

Application #AN3790

Conditions

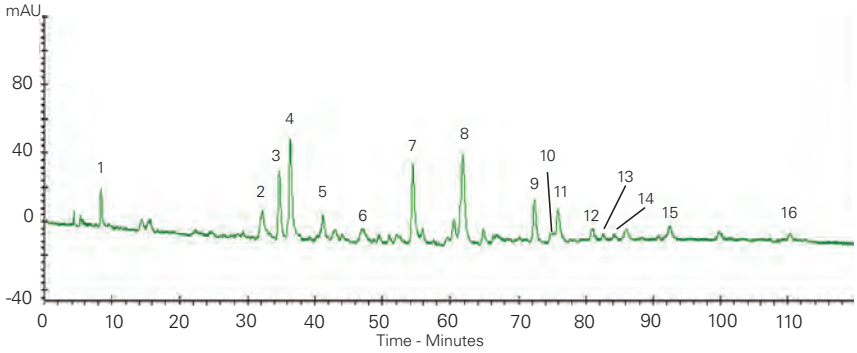
Column: ACE 3 C18-AR
Dimensions: 200 x 4.6 mm
Part Number: ACE-119-2046
Mobile Phase: A: 2% acetic acid in H_2O
B: 2% acetic acid in MeCN
Gradient:

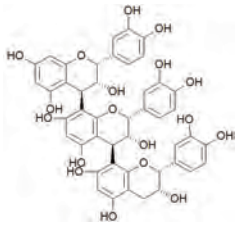
Times (mins)	%B
0	0
80	20
115	28
120	100
130	100

Flow Rate: 0.6 mL/min
Detection: UV, 280 nm
Peak identities established by combination of retention times, UV, fluorescence, NMR and ESI-MS (negative ion mode)

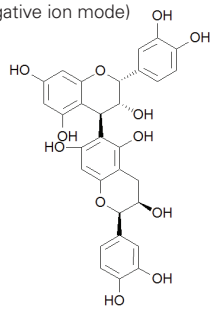
Analytes

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

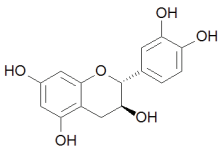




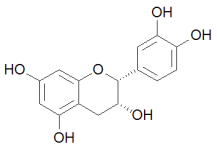
Procyanidin C1



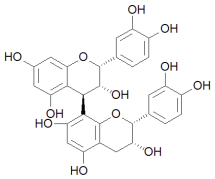
Procyanidin B5



(+)-Catechin



(-)-Epicatechin



Procyanidin B2

Grases F, Prieto R, Fernandez-Cabot R, Costa-Bauza A, Sanchez A, Prodanov M (2015) Effect of consuming a grape seed supplement with abundant phenolic compounds on the oxidative status of healthy human volunteers. Nutrition Journal 14:94 (2015) doi: 10.1186/s12937-015-0083-3

Phenols in Purple Coneflower *(Echinacea Purpurea)*

Application #AN2920

Conditions

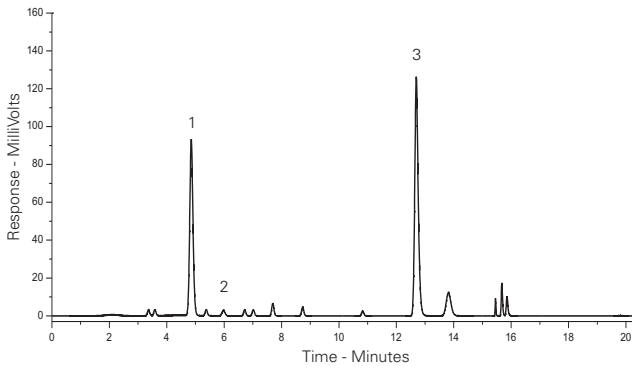
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% H_3PO_4 in H_2O
B: MeCN
Gradient:

Time (mins)	%B
0	10
13	22
14	40

Flow Rate: 1.5 mL/min
Injection: 10 µL
Temperature: 35 °C
Detection: UV, 330 nm

Analytes

1. Caftaric acid
2. Chlorogenic acid
3. Cichoric acid



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Echinacea Purpurea

Phosphatidylethanol Biomarker Analysis by UHPLC-MS/MS

Application #AN3400

Conditions

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

Gradient:

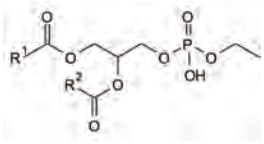
Time (mins)	%B
0.00	10
1.00	10
3.00	60
3.01	100
5.00	100
5.10	10

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

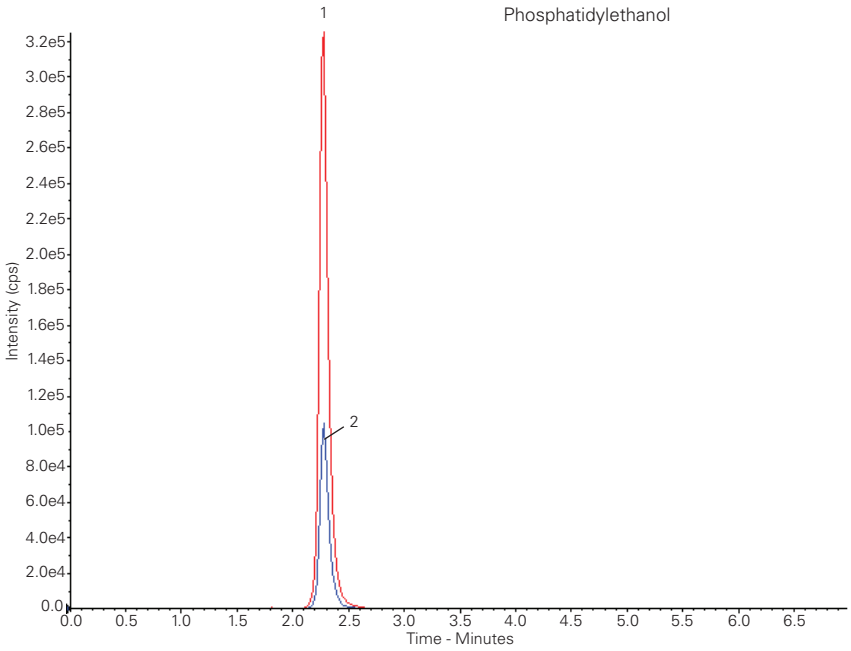
Phosphatidylethanol (PEth) measurement in blood is used as a biomarker of chronic alcohol use/abuse.

Analytes

1. R1/R2 = 18:1/18:1
(*m/z* 701.4 → 281.2)
2. R1/R2 = 16:1/16:1
(*m/z* 701.4 → 255.1)



Phosphatidylethanol



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Phytoestrogens from Hop Extract by LC-MS/MS

Application #AN1160

Conditions

Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: A: 1% formic acid in MeCN
B: 1% formic acid in MeOH
C: 1% formic acid in H_2O
D: MeOH

Gradient:

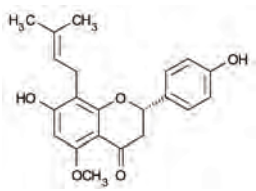
Time (mins)	%A	%B	%C	%D
0	56	0	44	0
8	51	5	44	0
10	51	5	44	0
17	95	5	0	0
22	95	0	0	5

Flow Rate: 0.6 mL/min
Detection: TSQ-Quantum triple quad ESI
Spray voltage: -4500 V
Precursor ion: 355.4 $[M+H]^+$
MRM transition ions: 179 and 299
Collision energy: 28 and 16 V

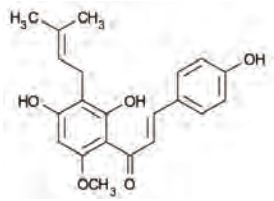


Analytes

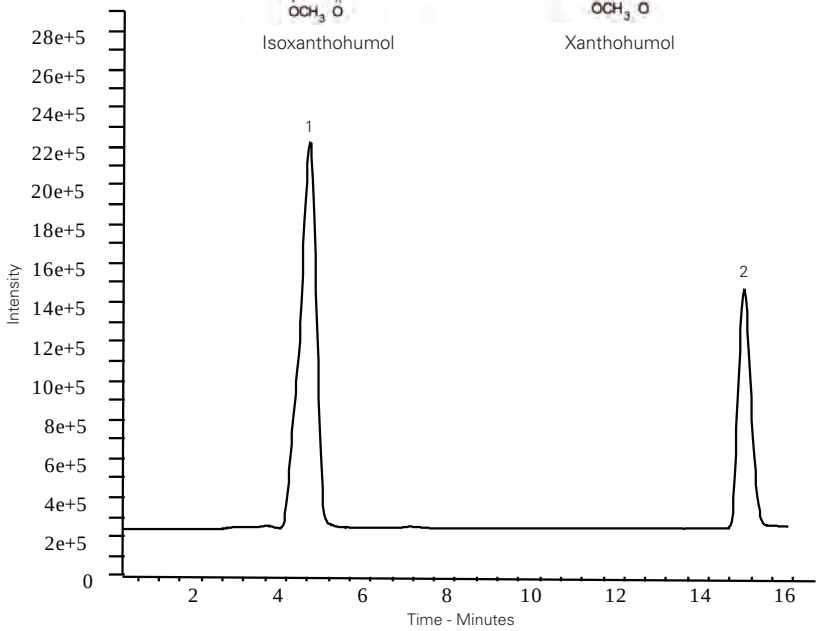
1. Isoxanthohumol
LOQ 0.07 µg/mL
2. Xanthohumol
LOQ 0.01 µg/mL



Isoxanthohumol



Xanthohumol



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Pilocarpine

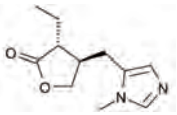
Application #AN3720

Conditions

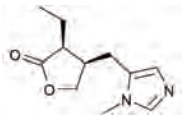
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 2 mM tetrabutylammonium dihydrogen phosphate/MeCN (85:15 v/v)
Flow Rate: 1 mL/min
Detection: UV, 254 nm

Analytes

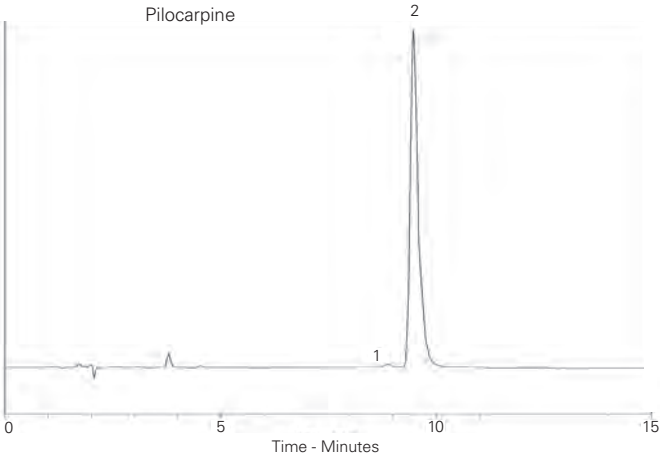
1. Isopilocarpine
2. Pilocarpine



Isopilocarpine



Pilocarpine



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Plant Hormones Involved in Abiotic Stresses

Application #AN4010

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: CORE-25A-1546U
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeCN
Gradient:

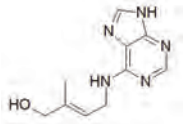
Time (mins)	%B
0	0
2	40
5	60
13	100
15	20

Flow Rate: 0.5 mL/min
Temperature: 40 °C
Detection: Shimadzu LCMS-8040 triple quad MS ESI positive and negative mode
Sample: Crude extract of *Arabidopsis thaliana* rosette leaves

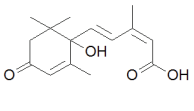
Plant hormones are involved in the regulation of response to exposure of abiotic stresses such as drought or salt

Analytes

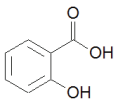
1. Zeatin (+ ESI)
   (*m/z* 220 → 119)
2. (±)-Abscisic acid (+ ESI)
   (*m/z* 247 → 91)
3. Salicylic acid (- ESI)
   (*m/z* 137 → 93)
4. (±)-Jasmonic acid (- ESI)
   (*m/z* 209 → 59)
5. Brassinolide (+ ESI)
   (*m/z* 481 → 95)



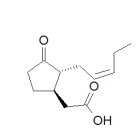
Zeatin



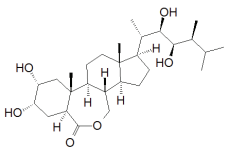
(±)-Abscisic acid



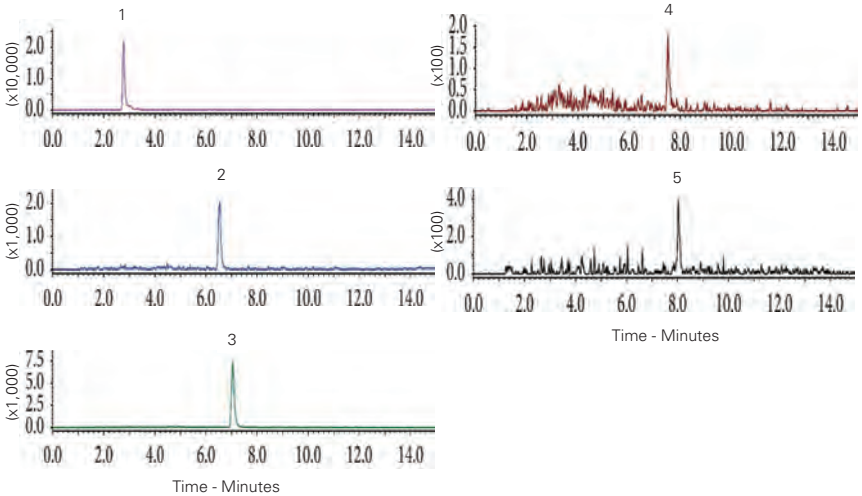
Salicylic acid



(±)-Jasmonic acid



Brassinolide



Kasote DM, Ghosh R, Chung JY, Kim J, Bae I, Bae H. Multiple Reaction Monitoring Mode Based Liquid Chromatography-Mass Spectrometry Method for Simultaneous Quantification of Brassinolide and other Plant Hormones Involved in Abiotic Stresses. International Journal of Analytical Chemistry (2016). http://dx.doi.org/10.1155/2016/7214087

Polar Compounds Separation

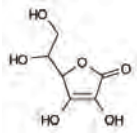
Application #AN1590

Conditions

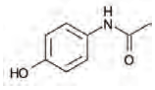
Column: ACE Excel 5 CN-ES
Dimensions: 150 x 4.6 mm
Part Number: EXL-1213-1546U
Mobile Phase: MeOH/H_2O (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 20 °C
Detection: UV, 254 nm

Analytes

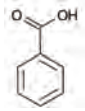
1. Ascorbic acid
2. Paracetamol
3. Benzoic acid
4. Salicylic acid



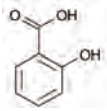
Ascorbic acid



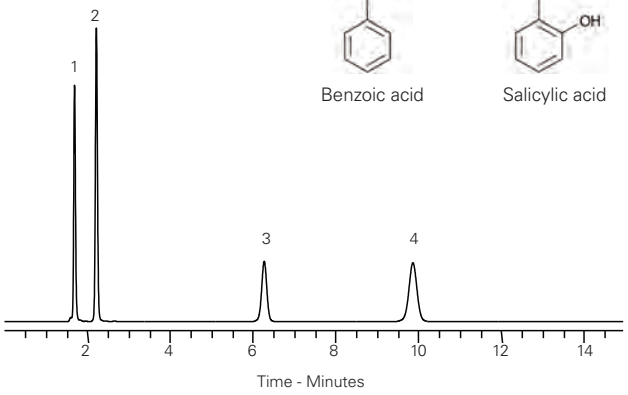
Paracetamol



Benzoic acid



Salicylic acid



Polyamines

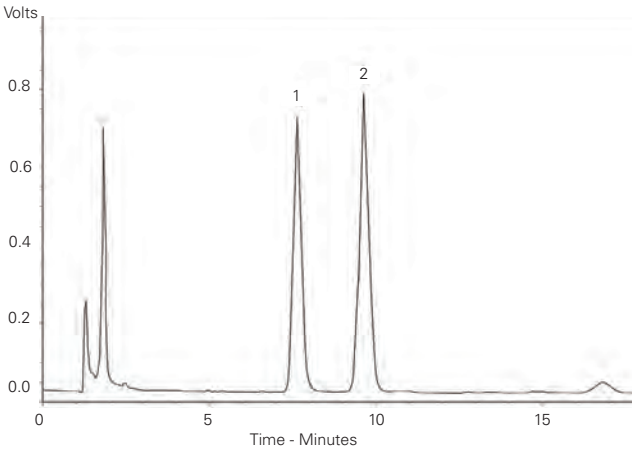
Application #AN3740

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: TRIS buffer pH 7.0/MeOH (10:90 v/v)
Flow Rate: 1.2 mL/min
Detection: Fluorescence – λ_{ex} 340 nm, λ_{em} 450 nm

Analytes

1. Putrescine
2. Cadaverine
(as OPA derivatives)



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Polycyclic Tetracarboxylic Acids

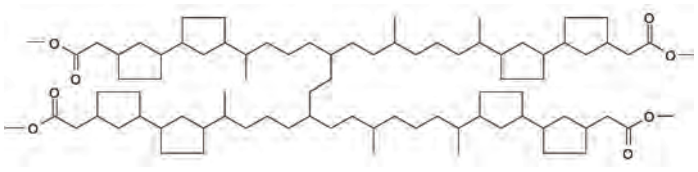
Application #AN1340

Conditions

Column: ACE UltraCore 2.5 SuperPhenylHexyl
Dimensions: 100 x 2.1 mm
Part Number: CORE-25B-1002U
Mobile Phase: A: 10 mM ammonium acetate in MeOH/H_2O (98:2 v/v)
B: 10 mM ammonium acetate in IPA/H_2O (98:2 v/v)
Gradient:

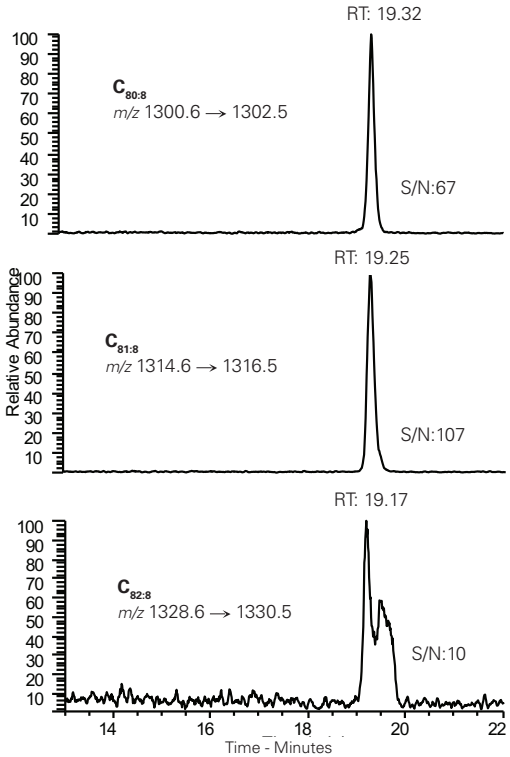
Time (mins)	%B
0.0	0
1.0	0
15.0	100
25.0	100

Flow Rate: 0.15 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: LCQ Ion trap MS
LC-ESI-MS extracted ion chromatograms
Compounds detected as ammoniated quasimolecular ions $[M+NH_4]^+$
Detection limit ~ 0.1 ppm



Tetramethyl ester of $C_{80:8}$ ring acid

C_{80-82} polycyclic tetracarboxylic acids isolated from oilfield deposits



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Polyethylene Glycol 1000

Application #AN3900

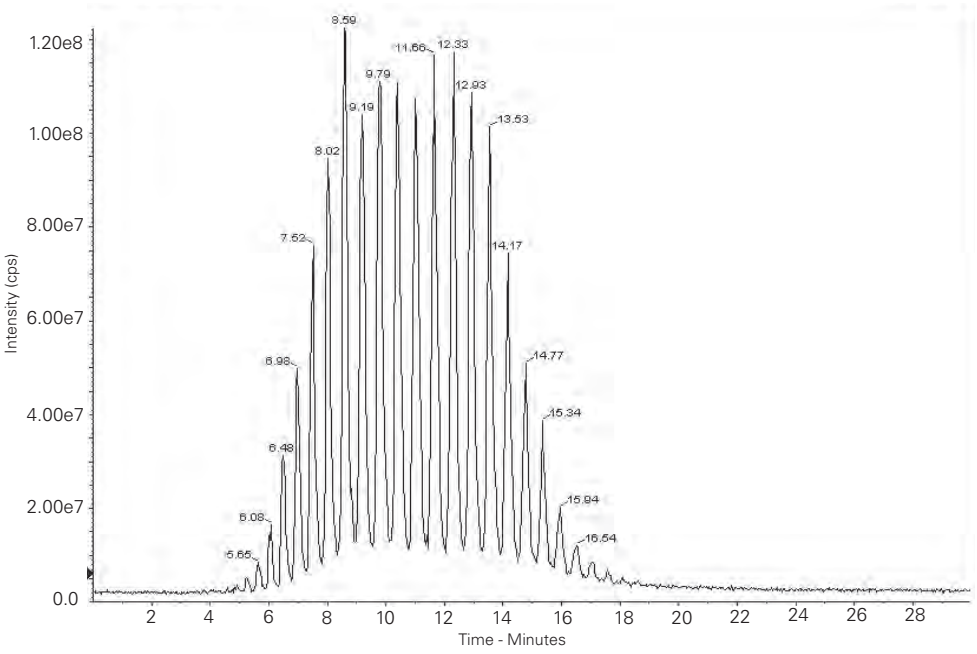
Conditions

Column: ACE 3 C8
Dimensions: 150 x 4.6 mm
Part Number: ACE-112-1546
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeOH

Gradient:

Time (mins)	%B
0	50
45	85
50	50
60	50

Flow Rate: 1 mL/min
Detection: APCI (negative ion)



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[^{14}C]Pomalidomide and Metabolites in Human Plasma and Urine

Application #AN4240

Conditions

Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: A: 25 mM ammonium acetate pH 5.5 in H_2O
B: MeOH

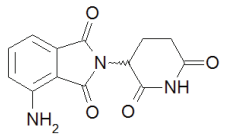
Gradient:

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

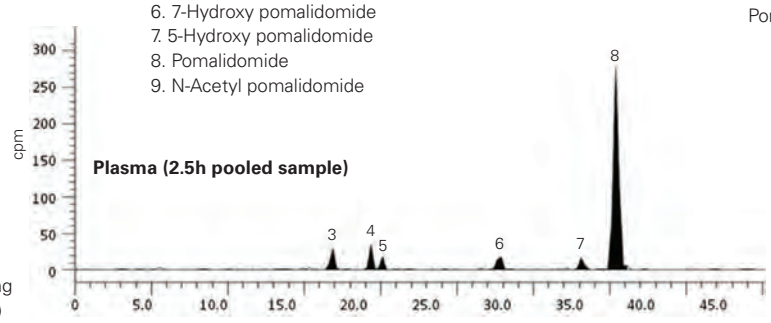
Flow Rate: 0.7 mL/min
Temperature: 30 °C
Detection: Radiometric
Metabolites characterised using LC-MS/MS (positive ion mode)

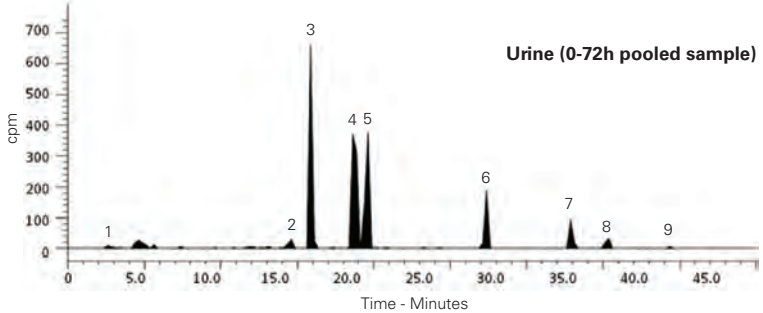
Analytes

1. 3-Aminophthalic acid
2. Hydrolysis product of pomalidomide
3. Hydrolysis product of pomalidomide
4. Glucuronide conjugate of 5-hydroxy pomalidomide
5. Glucuronide conjugate of 5-hydroxy pomalidomide
6. 7-Hydroxy pomalidomide
7. 5-Hydroxy pomalidomide
8. Pomalidomide
9. N-Acetyl pomalidomide



Pomalidomide





Hoffmann M, Kasserra C, Reyes J, Schafer P, Kosek J, Capone L, Parton A, Kim-Kang H, Surapaneni S, Kumar G. Absorption, Metabolism and Excretion of [^{14}C] Pomalidomide in Humans following Oral Administration. Cancer Chemotherapy and Pharmacology 71, 489-501 (2013) doi 10.1007/s00280-012-2040-6

Porphyrins in Oral Bacteria by LC-MS/MS

Application #AN3080

Conditions

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

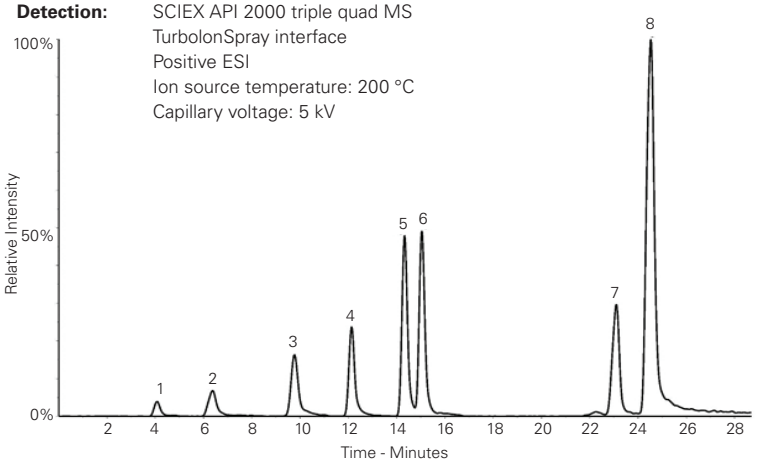
Gradient:

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

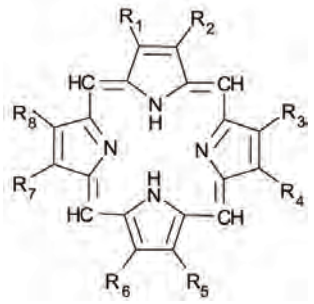
Flow Rate: 0.1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: SCIEX API 2000 triple quad MS
TurbolonSpray interface
Positive ESI
Ion source temperature: 200 °C
Capillary voltage: 5 kV

Analytes

1. Uroporphyrin I
(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)



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



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Pravastatin and Isomers by LC-MS/MS

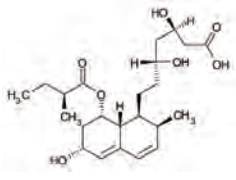
Application #AN1350

Conditions

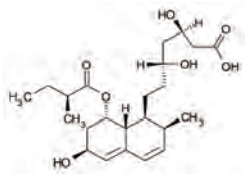
Column: ACE 3 C18
Dimensions: 50 x 3.0 mm
Part Number: ACE-111-0503
Mobile Phase: MeCN/MeOH/THF/H_2O/Acetic Acid
(15:20:5:60:0.1 v/v/v/v/v)
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: API 3000 triple quad MS
TurbolonSpray – negative mode
Extracted ion chromatogram
of MRM *m/z*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

Analytes

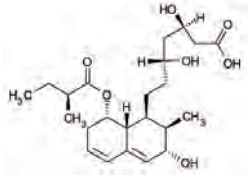
1. 6-epi-Pravastatin
(MW 424)
2. Pravastatin
(MW 424)
3. 3α-iso-Pravastatin
(MW 424)



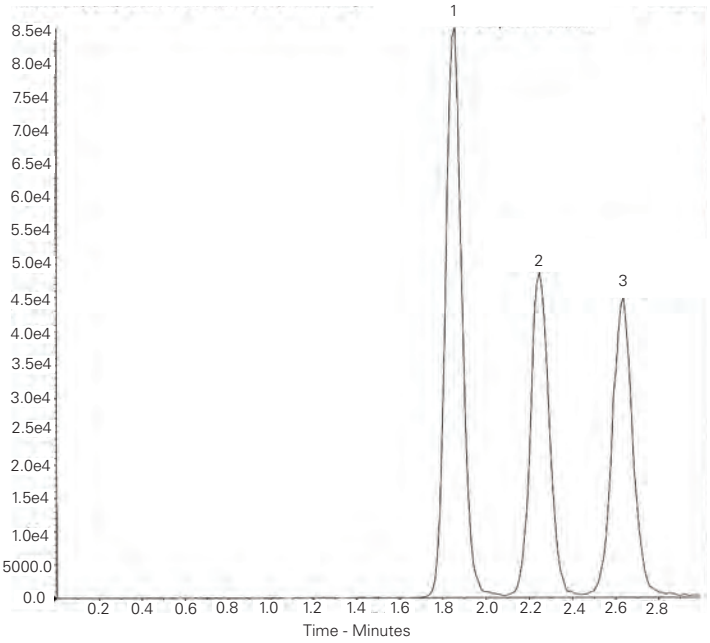
6-epi-Pravastatin



Pravastatin



3α-iso-Pravastatin



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Pravastatin in Cell Lysate Samples by LC-MS/MS

Application #AN4350

Conditions

Column: ACE Excel 3 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1111-1003U
Mobile Phase: A: 5 mM ammonium acetate pH 4.5 in H_2O
B: MeCN

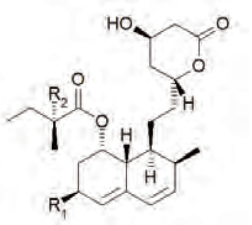
Gradient:

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

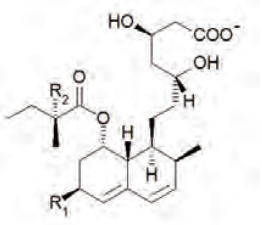
Flow Rate: 0.3 mL/min
Temperature: 40 °C
Detection: Quattro Ultima triple quad MS
ESI MRM mode: +ve (lactones)
–ve (hydroxy acids)
Source temperature: 125 °C
Desolvation temperature: 350 °C

Analytes

1. Lactone form (pharmacologically inactive)
2. Hydroxy acid form (pharmacologically active)



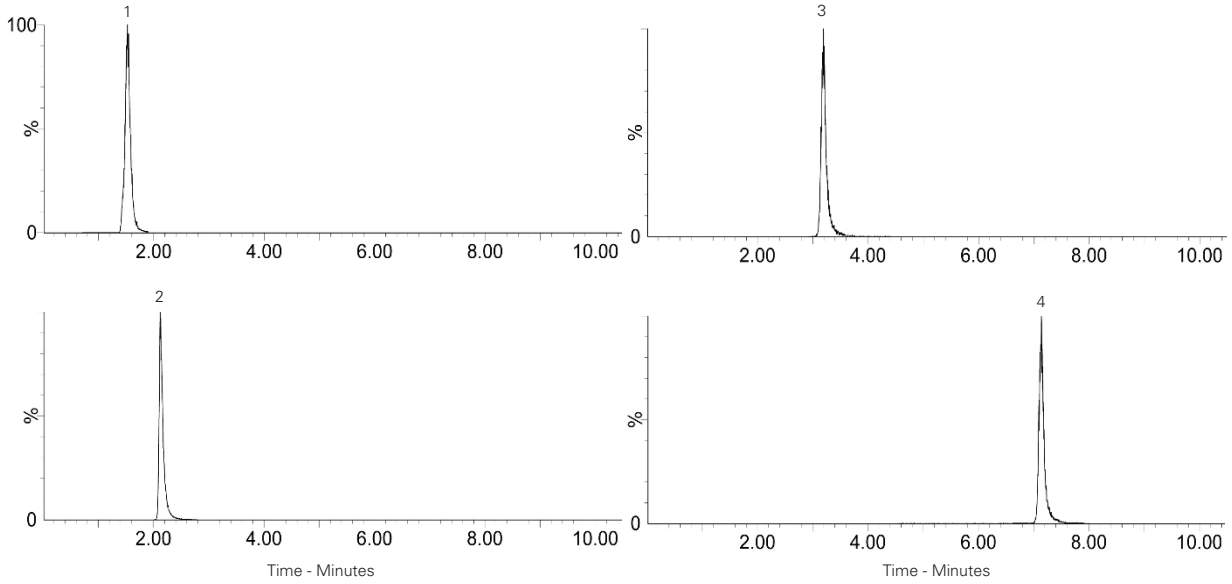
Lactone form
(pharmacologically inactive)



Hydroxy acid form
(pharmacologically active)

Peak	Analyte	Precursor ion	MRM transition *(m/z)*	LLOQ (ng/mL)
1	Pravastatin hydroxy acid	$[M-H]^-$	423.23 → 321.37	2.23
2	Pravastatin lactone	$[M+H]^+$	407.46 → 183.22	2.03
3	Lovastatin hydroxy acid (IS)	$[M-H]^-$	421.08 → 319.54	n/a
4	Lovastatin lactone (IS)	$[M+Na]^+$	427.15 → 325.36	n/a

Pravastatin: R_1 = OH, R_2 = H
Lovastatin (IS): R_1 = CH_3, R_2 = H



Taha DA, de Moor CH, Barrett DA, Lee JB, Gandhi RD, Hoo CW, Gershkovich P, (2016) The role of acid-base imbalance in statin-induced myotoxicity. Translational Research, The Journal of Laboratory and Clinical Medicine. http://dx.doi.org/10.1016/j.trsl.2016.03.015

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

Application #AN2690

Conditions

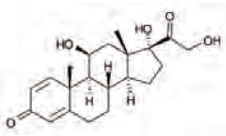
Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 4 mM ammonium acetate in H_2O
B: 0.2% (v/v) formic acid in MeOH
Gradient:

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

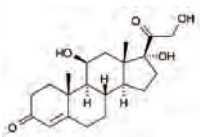
Flow Rate: 0.2 mL/min
Injection: 50 µL
Temperature: 50 °C
Detection: Applied Biosystems 5000 MS/MS
APCI in positive ion mode

Analytes

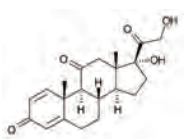
1. Prednisolone
(*m/z* 361.5 → 147.1)
2. Cortisol
(*m/z* 363.5 → 121.3)
3. Prednisone
(*m/z* 359.4 → 147.1)
4. Cortisone
(*m/z* 361.5 → 163.3)
5. Prednisolone-d6 (IS)
(*m/z* 367.4 → 150.3)
6. Cortisol-d4 (IS)
(*m/z* 367.3 → 331.3)



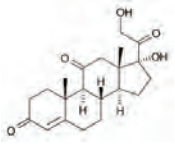
Prednisolone



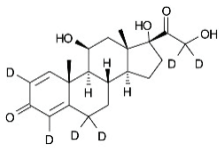
Cortisol



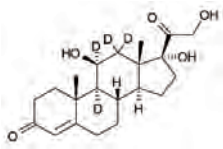
Prednisone



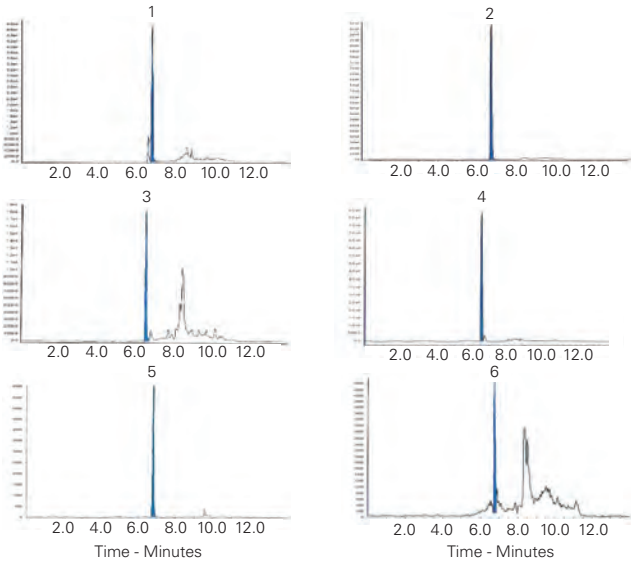
Cortisone



Prednisolone-d6 (IS)



Cortisol-d4 (IS)



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Preservatives (I)

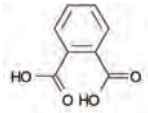
Application #AN2230

Conditions

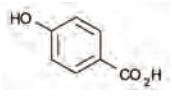
Column: ACE Excel 1.7 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-171-0503U
Mobile Phase: 20 mM potassium phosphate
pH 2.5 in MeCN/H_2O (30:70 v/v)
Flow Rate: 0.43 mL/min
Injection: 0.7 µL
Temperature: 20 °C
Detection: UV, 230 nm

Analytes

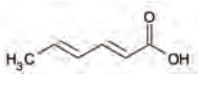
1. Phthalic acid
2. 4-Hydroxybenzoic acid
3. Sorbic acid
4. Methyl paraben
5. Ethyl paraben
6. Propyl paraben



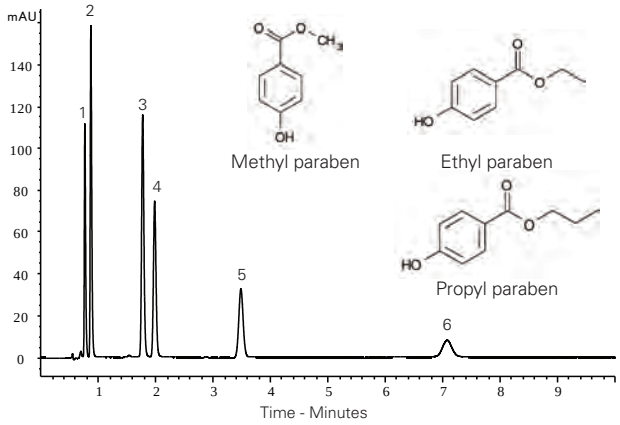
Phthalic acid



4-Hydroxybenzoic acid



Sorbic acid



Methyl paraben

Ethyl paraben

Propyl paraben

Preservatives (II)

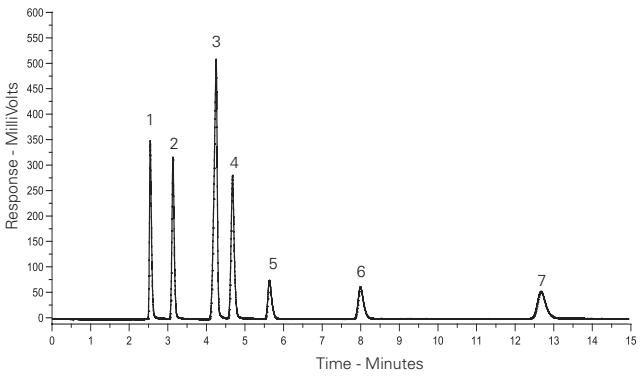
Application #AN3040

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/50 mM KH_2PO_4
pH 4.4 in H_2O (40:60 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 230 nm

Analytes

1. Phthalic acid
2. p-Hydroxybenzoic acid
3. Benzoic acid
4. Sorbic acid
5. Methyl paraben
6. Ethyl paraben
7. Propyl paraben



Pristinamycin Components in Plasma by LC-MS/MS

Application #AN1360

Conditions

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

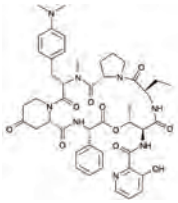
Gradient:

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

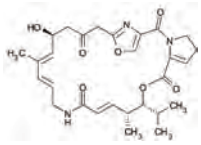
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 25 °C
Detection: MDS Sciex API 4000 TurbolonSpray positive mode

Analytes

1. Pristinamycin IA
   (*m/z* 867.5 → 134.2)
2. Pristinamycin IIA
   (*m/z* 526.3 → 355.1)
3. Virginiamycin (IS)
   (*m/z* 824.6 → 134.0)



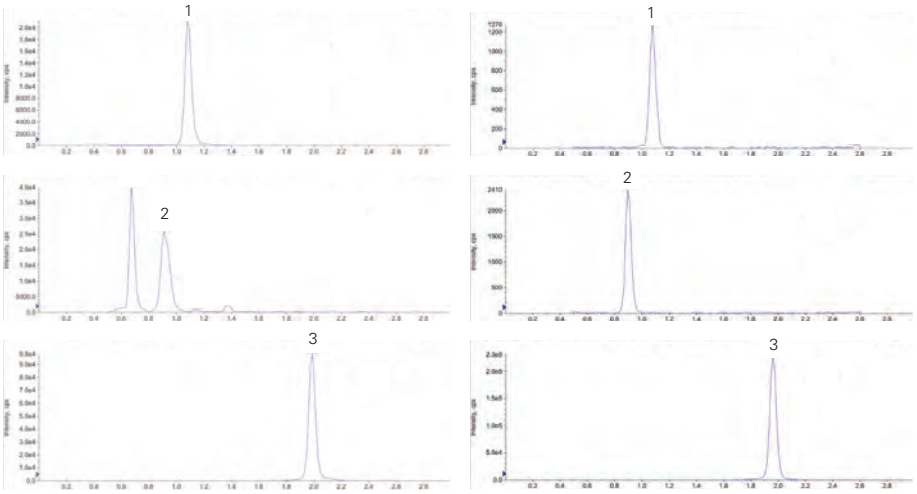
Pristinamycin IA



Pristinamycin IIA

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



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Proanthocyanidins from Cinnamon Bark Extract

Application #AN3510

Conditions

Column: ACE 3 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-111-2546
Mobile Phase: A: 1% acetic acid in H_2O
B: MeCN

Gradient:

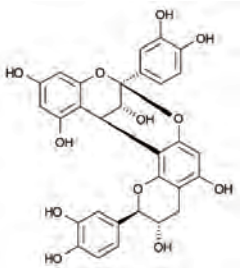
Time (mins)	%B
0	36
35	36
40	50
45	100
55	0
60	0

Flow Rate: 0.75 mL/min
Temperature: Ambient
Detection: UV, 280 nm
Sample: Cinnamon bark extract thiolysed with benzyl mercaptan

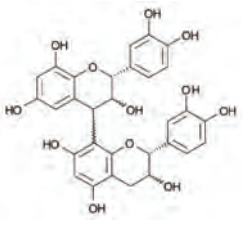
Analytes

1. Catechin
2. A-type PC dimer
3. A-type PC trimer
4. Epicatechin
5. A-type PC trimer
6. IS
7. cis-Cinnamic acid
8. A-type PC-BM trimer
9. trans-Cinnamic acid
10. cis-Catechin-BM
11. Epicatechin-BM
12. A-type PC-BM dimer

PC = Procyanidin
BM = Benzyl mercaptan adduct

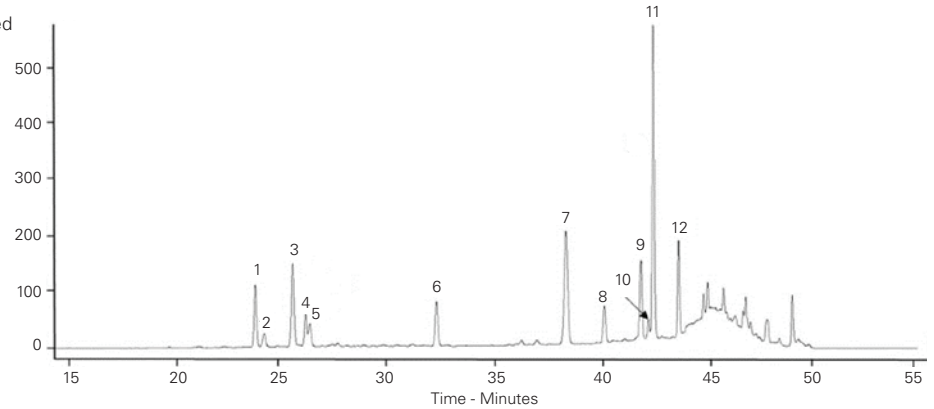


Example of A type procyanidin dimer



Example of B type procyanidin dimer





Williams, A. R. et al. Anthelmintic activity of trans-cinnamaldehyde and A and B-type proanthocyanidins derived from cinnamon (*Cinnamomum verum*). Sci. Rep. 5, 14791; doi:10.1038/srep14791 (2015).

Procaine and p-Aminobenzoic Acid Separation

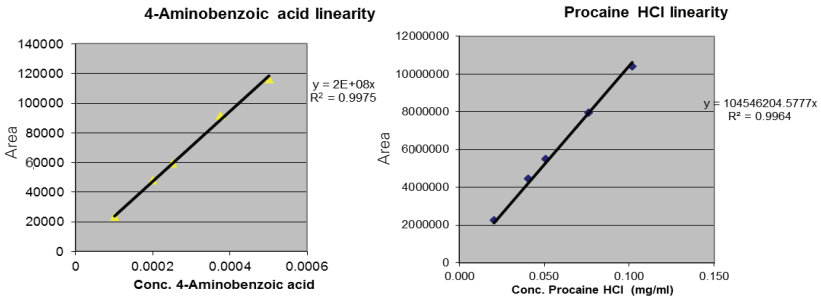
Application #AN1660

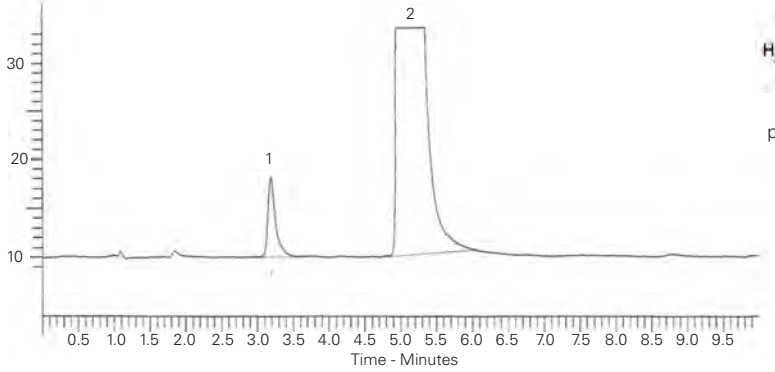
Conditions

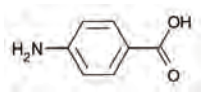
Column: ACE 3 C18-PFP
Dimensions: 100 x 4.6 mm
Part Number: ACE-1110-1046
Mobile Phase: 0.6% acetic acid in H_2O/MeOH (81:19 v/v), adjusted to pH 4.7 with 20% NaOH
Flow Rate: 1 mL/min
Detection: UV, 279 nm
S/N limit: 10
Sample: Procaine 0.0002 mg/mL, p-Aminobenzoic acid 0.00005 mg/mL

Analytes

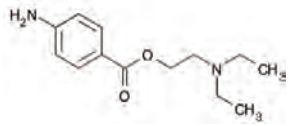
1. p-Aminobenzoic acid (4-Aminobenzoic acid)
2. Procaine







p-Aminobenzoic Acid



Procaine

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Propolis Phenolic Acids Applied to Human Skin

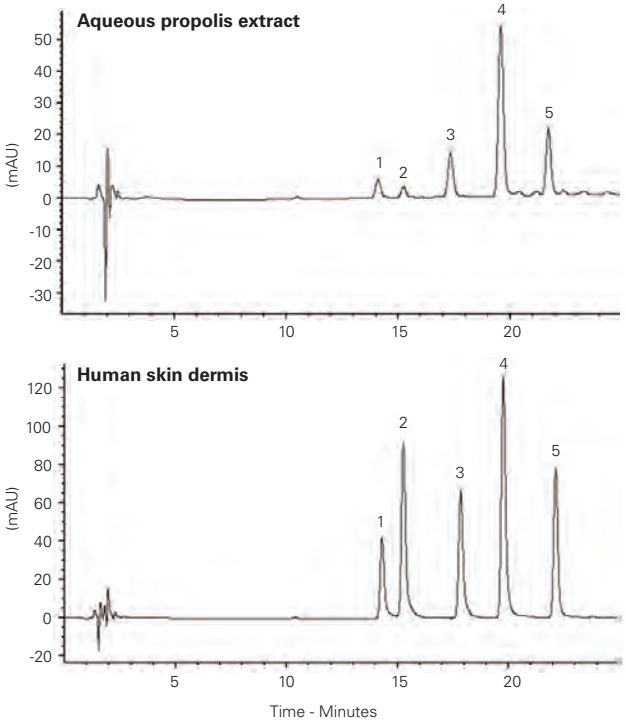
Application #AN4230

Conditions

Column: ACE 5 C18
Dimensions: 150 x 0.5 mm
Part Number: ACE-121-15005
Mobile Phase: A: 0.5% acetic acid in H_2O
B: MeCN
Gradient:

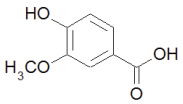
Time (mins)	%B
0	1
25	21

Flow Rate: 20 µL/min
Injection: 0.2 µL
Temperature: 25 °C
Detection: UV, 290 nm

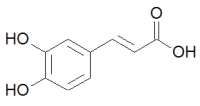


Analytes

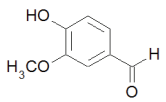
1. Vanillic acid
2. Caffeic acid
3. Vanillin
4. Coumaric acid
5. Ferulic acid



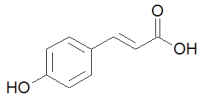
Vanillic acid



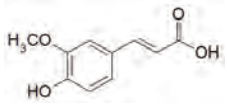
Caffeic acid



Vanillin



Coumaric acid



Ferulic acid

Zilius M, Ramanauskiene K, Briedis V. Release of Propolis Phenolic Acids from Semisolid Formulations and their Penetration into the Human Skin in vitro. Evidence-based Complementary and Alternative Medicine (2013) http://dx.doi.org/10.1155/2013/958717

Prostaglandins using LC-MS/MS

Application #AN3260

Conditions

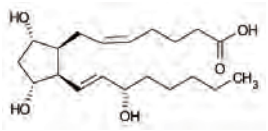
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: H_2O
B: MeOH
C: MeCN

Gradient:	**Time (mins)**	**%A**	**%B**	**%C**
	0	70.0	20.0	10.0
	9	10.0	60.0	30.0
	10	0.1	66.6	33.3

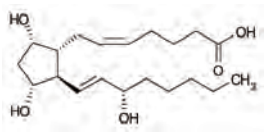
Flow Rate: 0.2 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: ESI (-) MS/MS
MRM *m/z* 353.3 → 193

Analytes

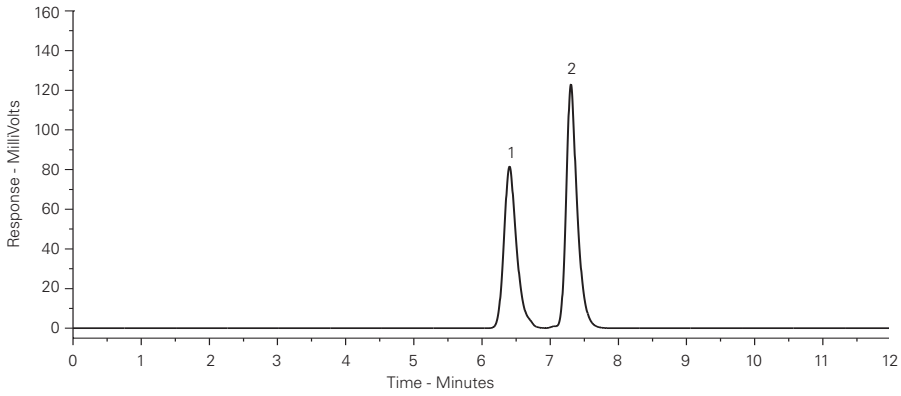
1. 8-iso-Prostaglandin $F2_\alpha$
2. Prostaglandin $F2_\alpha$



8-iso-Prostaglandin $F2_\alpha$



Prostaglandin $F2_\alpha$



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Protein Test Mix

Application #AN3730

Conditions

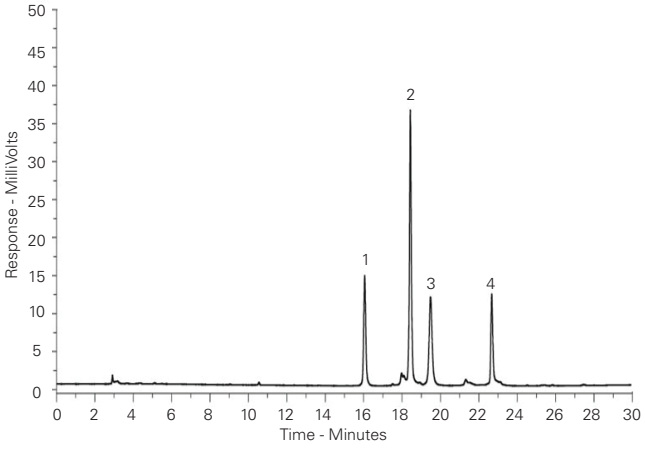
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H_2O
B: 0.1% TFA in MeCN

Gradient:	**Time (mins)**	**%B**
	0	5
	30	70

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

Analytes

1. Ribonuclease A (MW ~14 kDa)
2. Cytochrome C (MW ~12 kDa)
3. Holo-transferrin (MW ~77 kDa)
4. Apomyoglobin (MW ~17 kDa)



Proton Pump Inhibitors (PPIs)

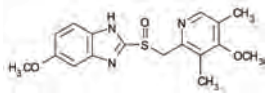
Application #AN3710

Conditions

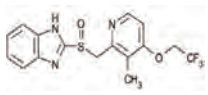
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM ammonium formate pH 3.0/MeCN (65:35 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

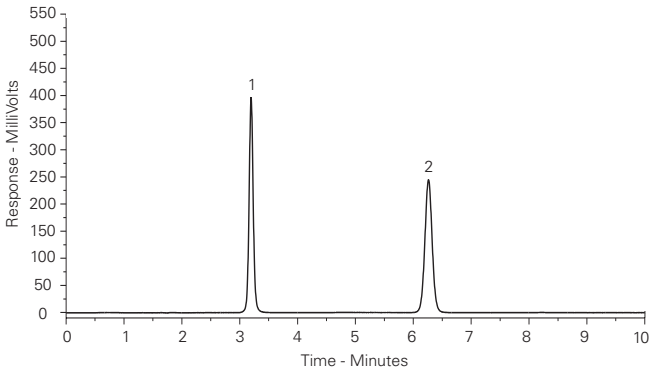
1. Omeprazole
2. Lansoprazole



Omeprazole



Lansoprazole



Psychoactive Substances in 'Synthacaine' by LC-UV

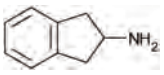
Application #AN3440

Conditions

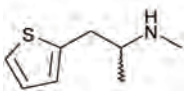
Column:	ACE 3 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-111-1546
Mobile Phase:	10 mM ammonium formate pH 3.5/MeCN (90:10 v/v)
Flow Rate:	1.2 mL/min
Temperature:	22 °C
Detection:	UV, 207 nm (2-Aminoindane) and 233 nm (Methiopropamine)
Sample:	Synthacaine 40 µg/mL

Analytes

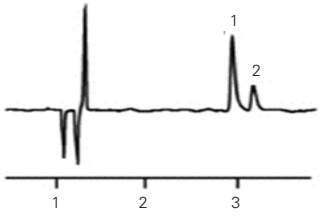
1. 2-Aminoindane
   LOD 0.83 µg/mL
2. Methiopropamine
   LOD 0.31 µg/mL



2-Aminoindane



Methiopropamine



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

Quinidine, Quinine and their Hydroderivatives Separation

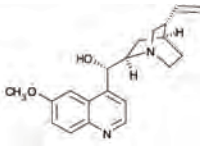
Application #AN1600

Conditions

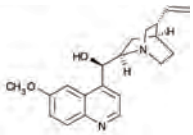
Column:	ACE 3 C18-AR
Dimensions:	50 x 4.6 mm
Part Number:	ACE-119-0546
Mobile Phase:	20 mM ammonium formate pH 3.0 in MeOH/H_2O (30:70 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	30 °C
Detection:	UV, 254 nm

Analytes

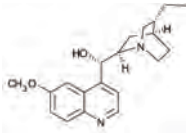
1. Quinidine
2. Quinine
3. Hydroquinidine
4. Hydroquinine



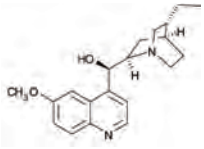
Quinidine



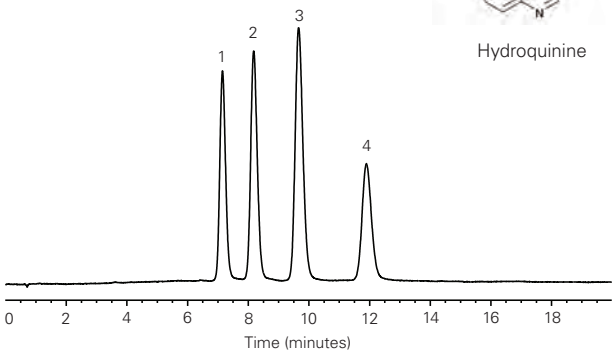
Quinine



Hydroquinidine



Hydroquinine



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Ranitidine Hydrochloride and Related Impurities

Application #AN3450

Conditions

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

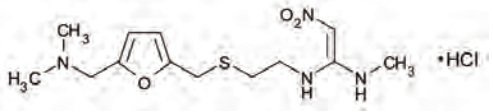
Gradient:

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

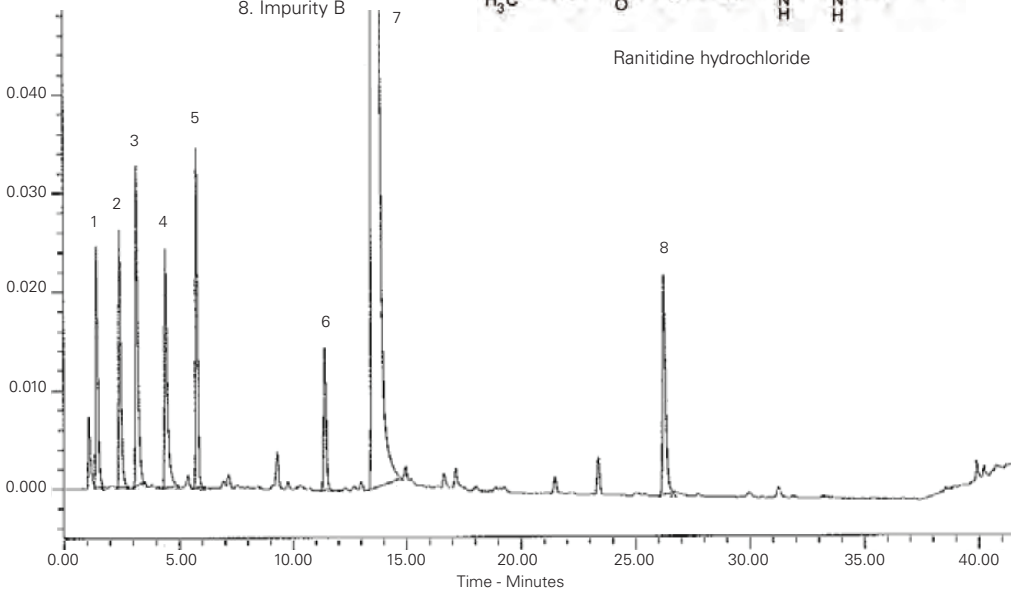
Flow Rate: 1 mL/min
Injection: 40 µL
Temperature: 40 °C
Detection: UV, 230 nm

Analytes

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



Ranitidine hydrochloride



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

Recombinant hGMCSF Purified from *Escherichia Coli*

Application #AN3840

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: A: 0.1% TFA in H_2O/MeCN (90:10 v/v)
B: 0.1% TFA in H_2O/MeCN (10:90 v/v)

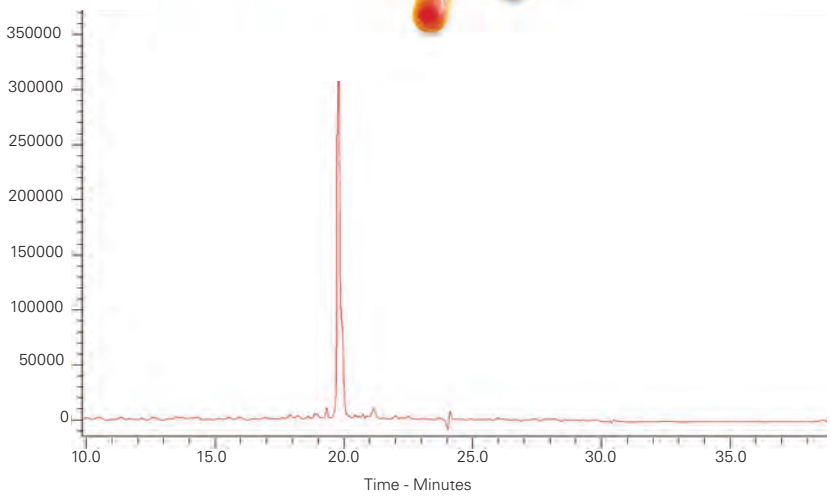
Gradient:

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

Flow Rate: 1 mL/min
Temperature: 30 °C
Detection: UV, 215 nm

hGMCSF = human Granulocyte Macrophage Colony Stimulating Factor, a 127 amino acid residue cytokine with a molecular weight of 14,477 Da





Das KMP, Banerjee S, Shekhar N, Damodaran K, Nair R, Somani S, Raiker VP, Jain S, Padmanabhan S. Cloning, Soluble Expression and Purification of High Yield Recombinant hGMCSF in *Escherichia coli*. Int. J. Mol. Sci. 2011, 12, 2064-2076; doi:10.3390/ijms12032064

Rifamycin Anti-tubercular Antibiotics in Human Plasma

Application #AN4090

Conditions

Column: ACE 3 C18
Dimensions: 100 x 3.0 mm
Part Number: ACE-111-1003
Mobile Phase: A: 15 mM ammonium formate pH 5.0 with formic acid in H_2O
B: 0.1% formic acid in MeOH

Gradient:

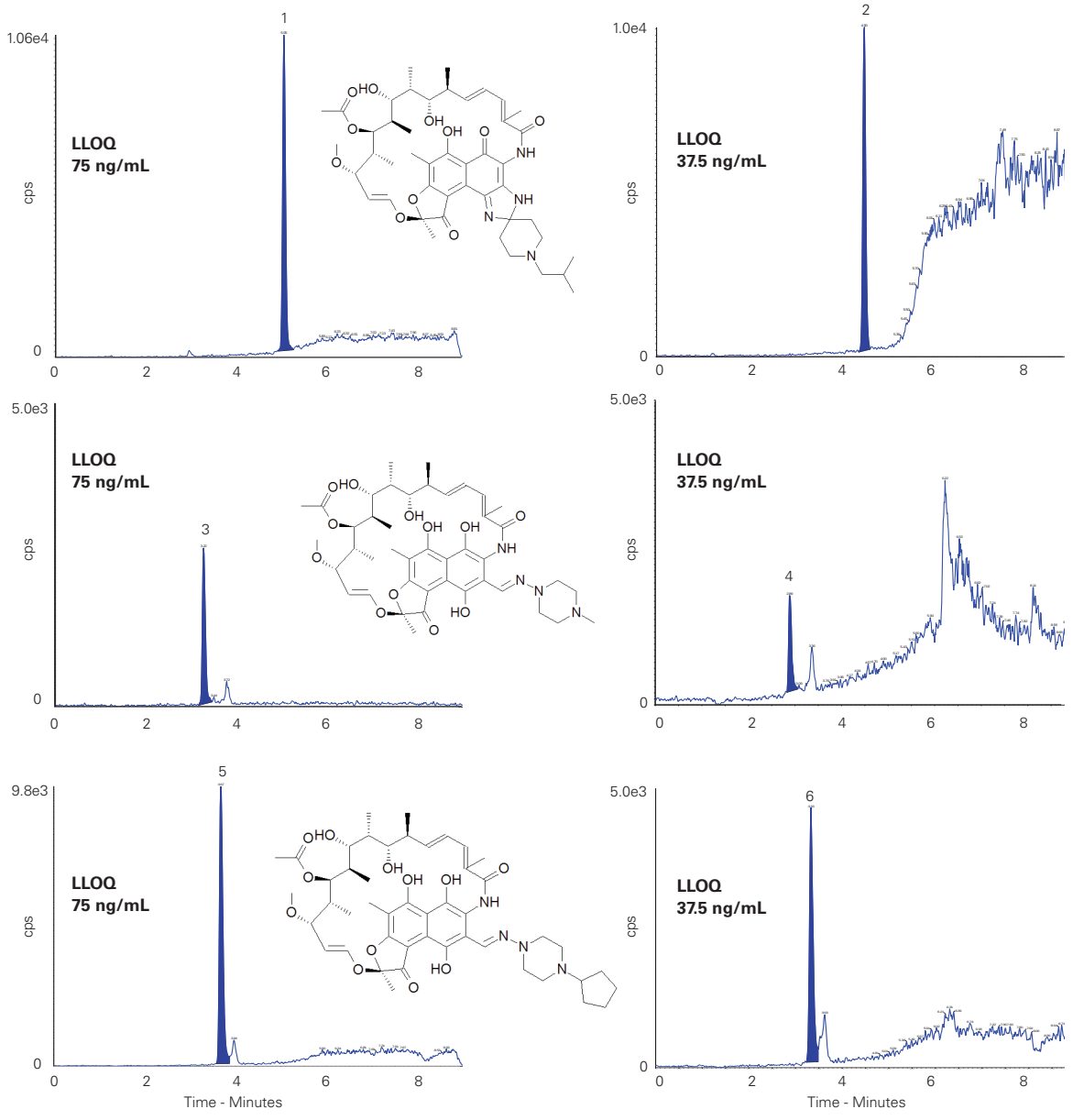
Time (mins)	%B
0.0	60
4.0	95
7.0	95
7.2	60
9.0	60

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

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

Analytes

1. Rifabutin
   (*m/z* 847.5 → 815.5)
2. Desacetyl rifabutin
   (*m/z* 805.5 → 773.4)
3. Rifampicin
   (*m/z* 823.5 → 791.4)
4. Desacetyl rifampicin
   (*m/z* 781.5 → 749.4)
5. Rifapentine
   (*m/z* 877.5 → 845.4)
6. Desacetyl rifapentine
   (*m/z* 835.5 → 803.5)



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Sennosides in Traditional Chinese Medicine

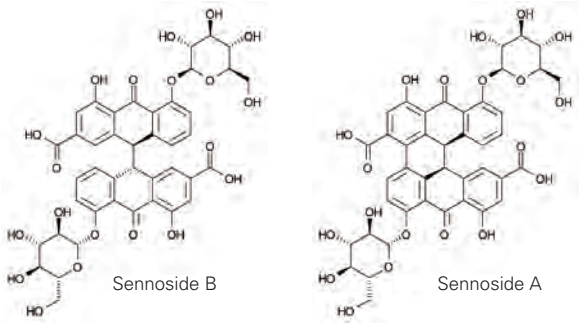
Application #AN1390

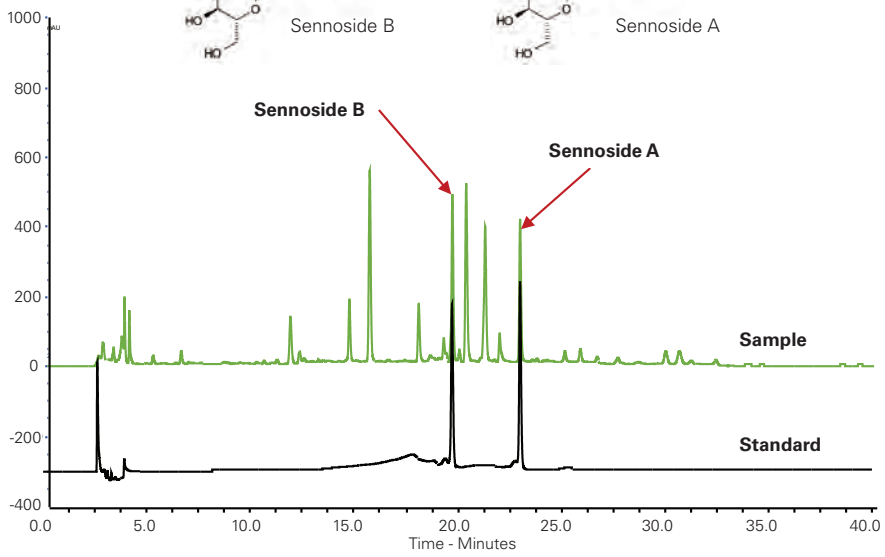
Conditions

Column:	ACE 3 C18-PFP
Dimensions:	150 x 4.6 mm
Part Number:	ACE-1110-1546
Mobile Phase:	A: 0.75% acetic acid in H_2O B: MeCN/MeOH (90:10 v/v)
Gradient:	**Time (mins) %B** 0 9 23 28 40 28
Flow Rate:	0.6 mL/min
Temperature:	35 °C
Detection:	UV, 271 nm
Sample:	Herbal tea bag containing Folium Sennae, Peppermint, Folium Mori, Folium Nelumbinis, Glycyrrhiza Uralensis and Lalang Grass Rhizome

Analytes

Sennoside A
Sennoside B





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Sotalol

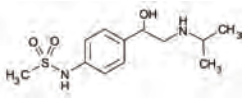
Application #AN3700

Conditions

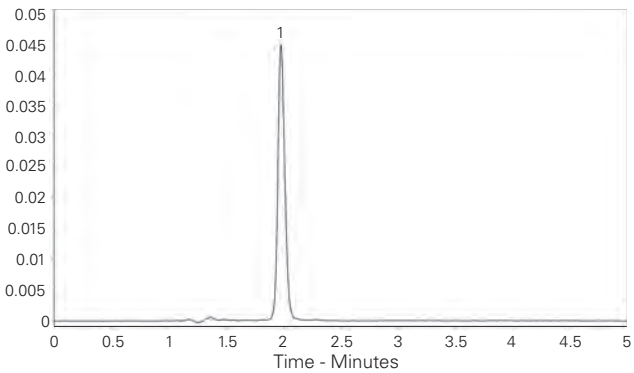
Column:	ACE 5 CN
Dimensions:	150 x 4.6 mm
Part Number:	ACE-124-1546
Mobile Phase:	20 mM ammonium formate pH 3.0/MeOH (85:15 v/v)
Flow Rate:	1 mL/min
Injection:	20µL (0.2mg/mL solution)
Temperature:	Ambient
Detection:	UV, 254 nm

Analyte

1. Sotalol



Sotalol



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Snake Venom from *Crotalus Durissus Terrificus*

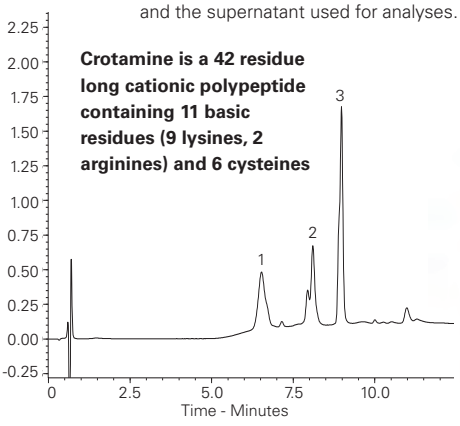
Application #AN4190

Conditions

Column:	ACE 3 C8-300
Dimensions:	50 x 4.6 mm
Part Number:	ACE-212-0546
Mobile Phase:	A: 0.1% TFA in H_2O B: 0.1% TFA in MeCN/H_2O (90:10 v/v)
Gradient:	**Time (mins) %B** 0 20 2 20 27 70
Flow Rate:	1.2 mL/min
Injection:	20 µL
Detection:	UV, 214 nm
Sample:	Lyophilised crude venom powder was solubilised (1 mg/mL) in 0.1% TFA. Resulting solutions were centrifuged and the supernatant used for analyses.

Analytes

1. Crotamine
2. Crotapotin
3. Phospholipase A2 (PLA_2)



Crotamine is a 42 residue long cationic polypeptide containing 11 basic residues (9 lysines, 2 arginines) and 6 cysteines



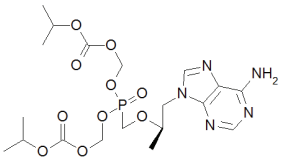
Reproduced with permission of Center for the Study of Venoms and Venomous Animals, (CEVAP), UNESP, Sao Paulo State University, Brazil

Stability Indicating Method for HIV Injection Treatment

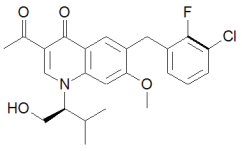
Application #AN4170

Conditions

Column:	ACE Excel 2 C18	
Dimensions:	50 x 3.0 mm	
Part Number:	EXL-101-0503U	
Mobile Phase:	A: 0.1% TFA in H_2O	
	B: 0.1% TFA in MeCN	
Gradient:	**Time (mins)**	**%B**
	0.0	10
	3.0	90
	6.0	90
	6.1	10
	8.0	10
Flow Rate:	0.4 mL/min	
Injection:	20 µL	
Temperature:	30 °C	
Detection:	UV, 240 nm	



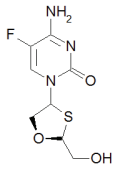
Tenofovir disoproxil



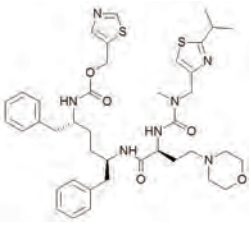
Elvitegravir

Analytes

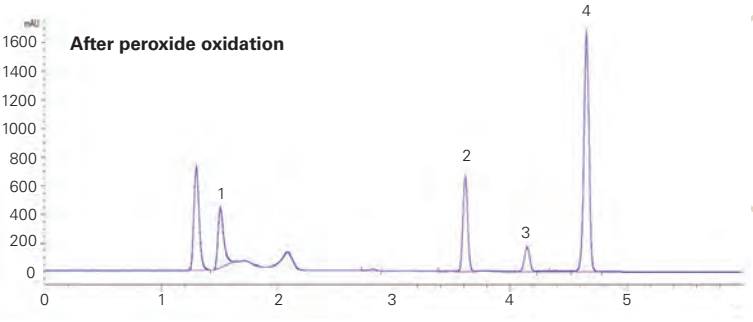
1. Emtricitabine (LLOQ 0.10 µg/mL)
2. Tenofovir disoproxil (LLOQ 0.10 µg/mL)
3. Cobicistat (LLOQ 0.20 µg/mL)
4. Elvitegravir (LLOQ 0.02 µg/mL)

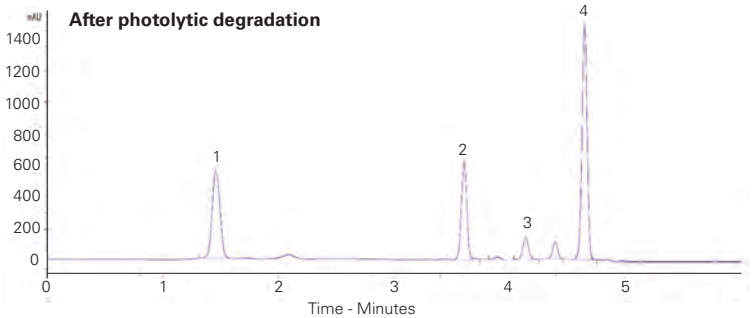


Emtricitabine



Cobicistat





Revath Naga Lakshmi P., Prahlad P., Mastananna SK., Ravindra N., Venkata Basaveswara Rao M, UPLC Separation Analysis of Emtricitabine, Tenofovir, Cobicistat and Elvitegravir from their Degradation products, Int. J. Pharm & Pharm Sci, 8(4), 362- 369 (2016)



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

Statins in Lactone and Hydroxy Acid Forms by HPLC-UV

Application #AN4360

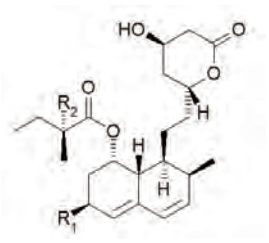
Conditions

Column: ACE Excel 3 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1111-1003U
Mobile Phase: A: MeCN
B: 5 mM ammonium acetate pH 4.5 in H_2O
A/B (I) 73:27 v/v (II) 55:45 v/v
Flow Rate: (I) 0.4 mL/min (II) 0.3 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: UV, 238 nm

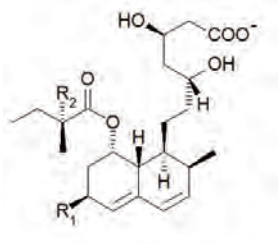
Analytes

1. Simvastatin hydroxy acid
2. 4,4-Dichlorodiphenyl trichloroethane (I.S.)
3. Simvastatin lactone
4. Pravastatin hydroxy acid
5. Griseofulvin (I.S.)
6. Pravastatin lactone

Simvastatin: R_1, R_2 = CH_3
Pravastatin: R_1 = OH, R_2 = H

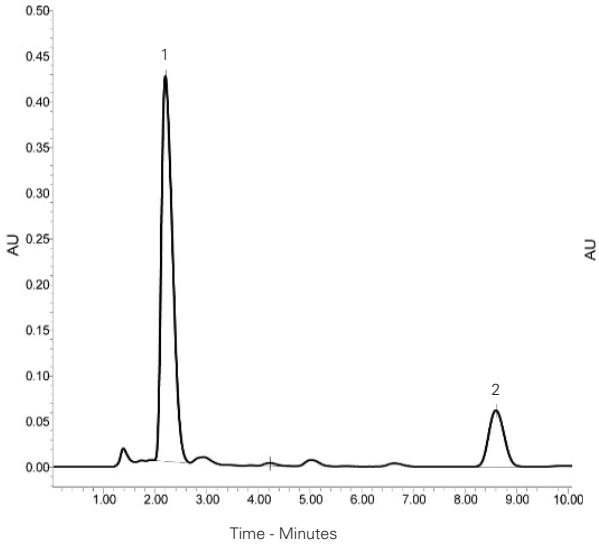


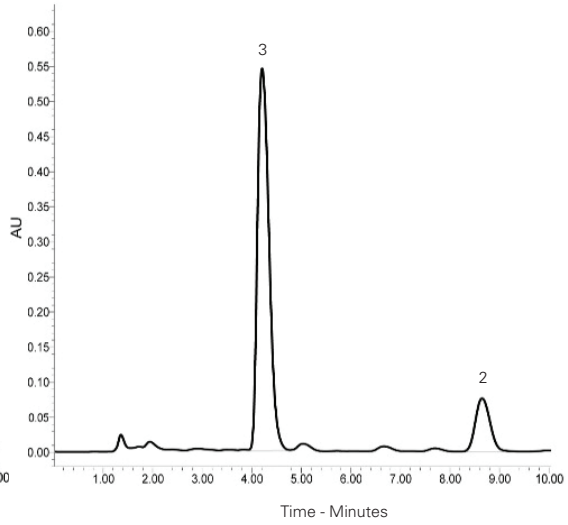
Lactone form
(pharmacologically inactive)



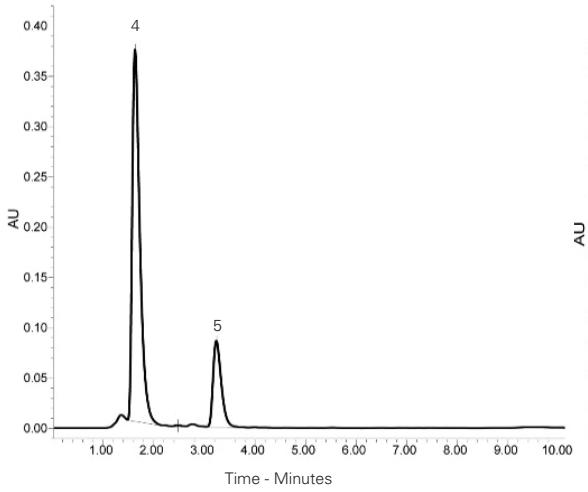
Hydroxy acid form
(pharmacologically active)

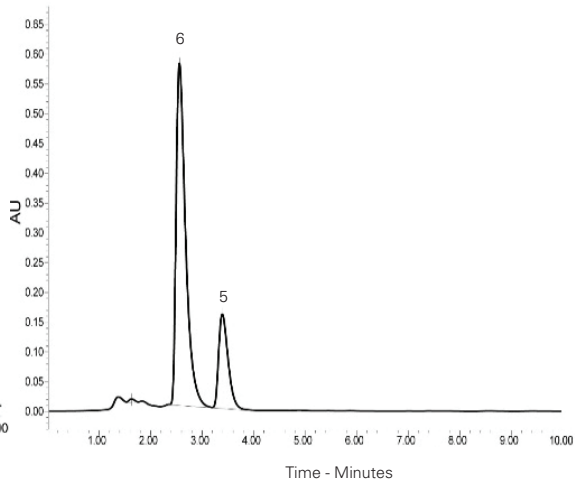
Conditions (I)





Conditions (II)





Taha DA, de Moor CH, Barrett DA, Lee JB, Gandhi RD, Hoo CW, Gershkovich P, (2016). The role of acid-base imbalance in statin-induced myotoxicity. Translational Research, The Journal of Laboratory and Clinical Medicine. http://dx.doi.org/10.1016/j.trsl.2016.03.015

Statins – Atorvastatin

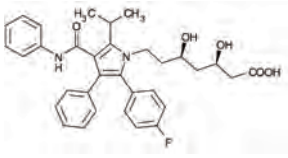
Application #AN3310

Conditions

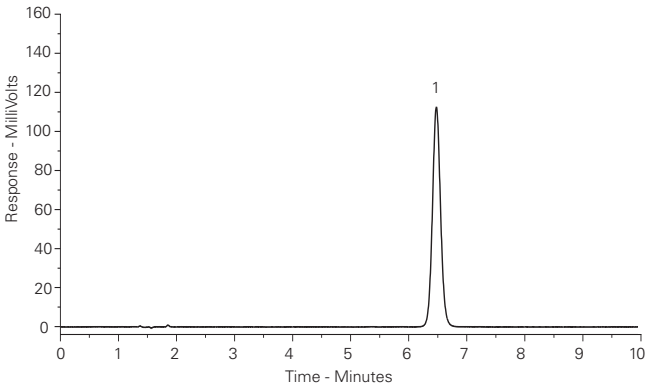
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM ammonium formate pH 3.0/MeCN (47:53 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Atorvastatin



Atorvastatin



Statins – Fluvastatin

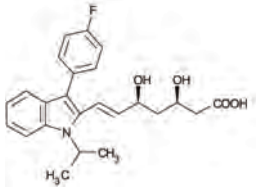
Application #AN3320

Conditions

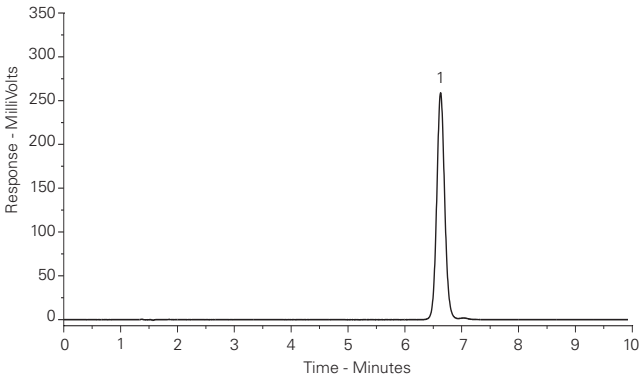
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM ammonium formate pH 3.0/MeCN (47:53 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 254 nm

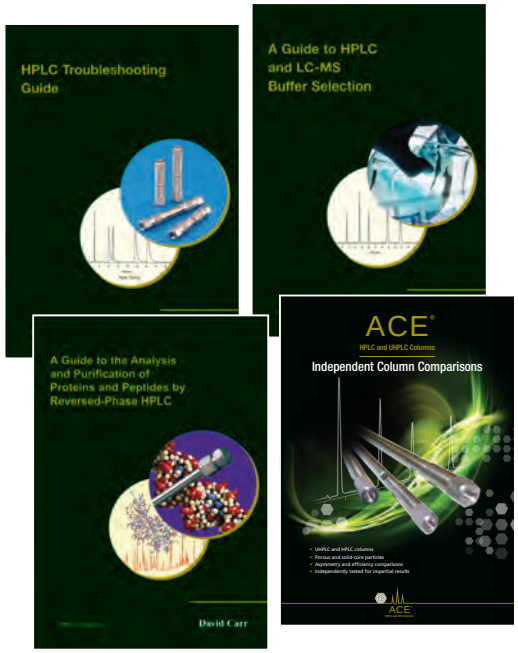
Analyte

1. Fluvastatin



Fluvastatin





FREE HPLC Technical Guides

- HPLC Column Comparison Guide
- HPLC Protein and Peptide Guide
- HPLC & LC-MS Buffer Selection Guide
- HPLC Troubleshooting Guide

To receive your FREE copies of these guides or the latest ACE HPLC Columns Catalogue contact your local distributor or

email: info@ace-hplc.com

Statins – Pravastatin

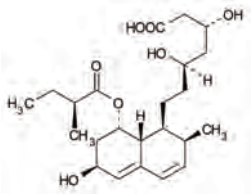
Application #AN3330

Conditions

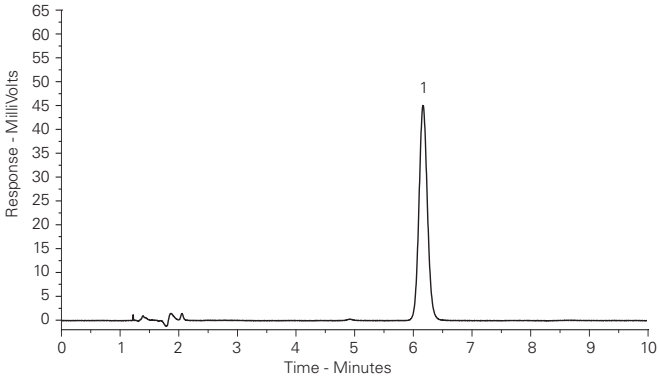
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM ammonium formate pH 3.0/MeCN (68:32 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Pravastatin



Pravastatin



Statins – Simvastatin

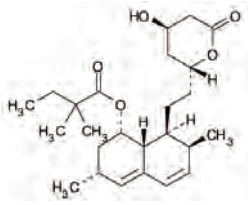
Application #AN3340

Conditions

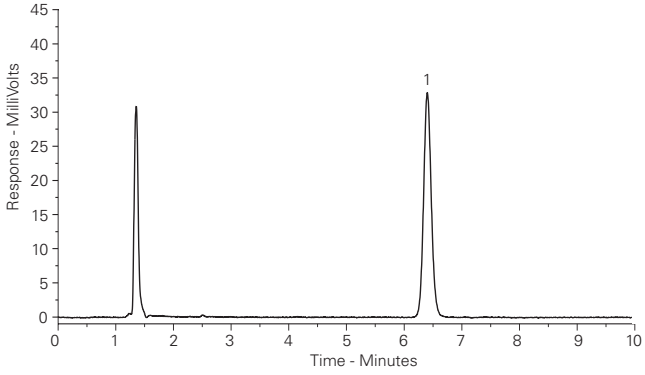
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM ammonium formate pH 3.0/MeCN (25:75 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Simvastatin



Simvastatin



Steroid Hormones (Endogenous) by LC-MS/MS

Application #AN2640

Conditions

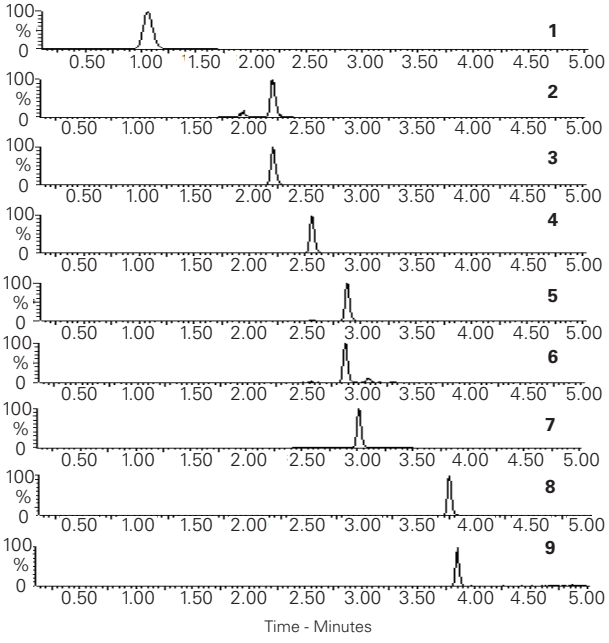
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeOH
Gradient:

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

Analytes

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. Androstenedione (*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

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

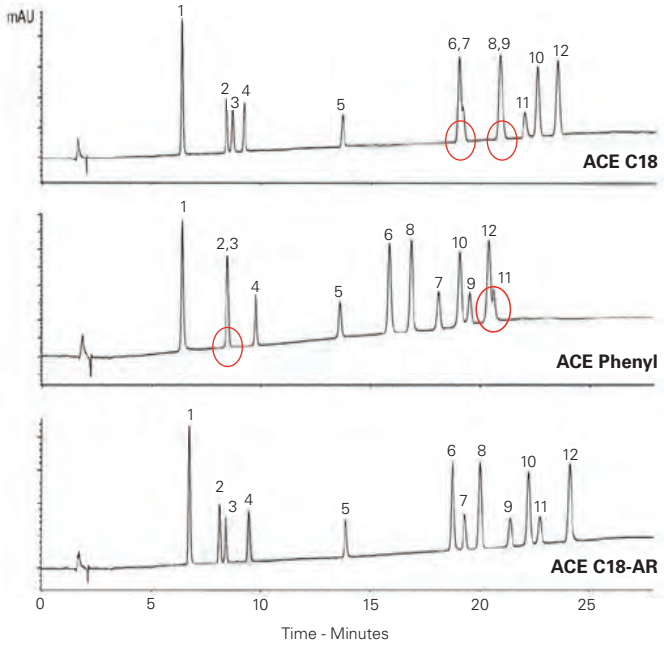
Gradient:

Time (mins)	%B
0	25
24	46
26	46
27	25

Flow Rate: 1 mL/min
Temperature: 20 °C
Detection: UV, 214 nm

Analytes

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



Steroids UHPLC-UV Analysis and Comparison

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

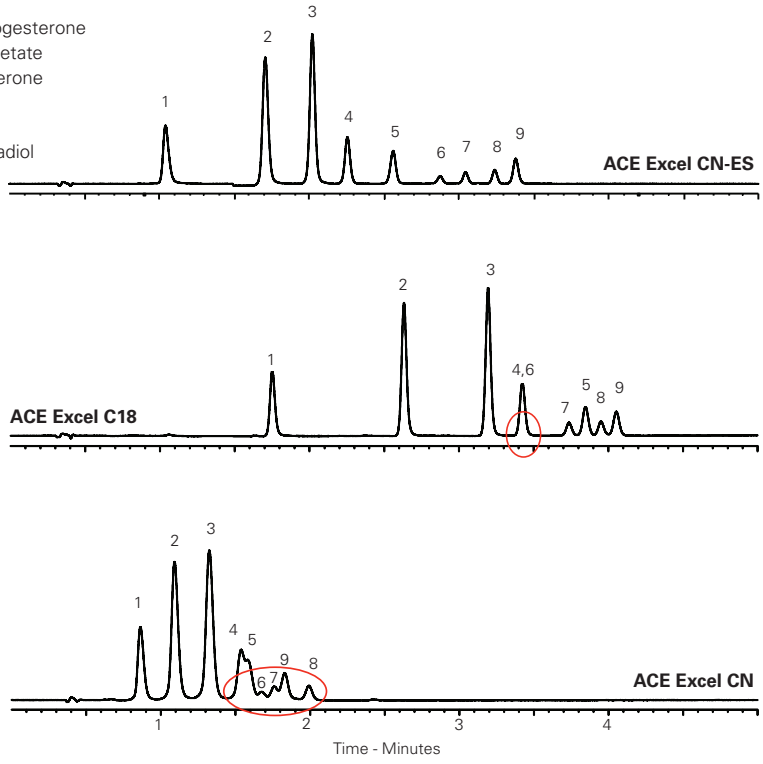
Gradient:

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

Analytes

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



Steroids Separation using Enhanced Polar Selectivity

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

Gradient:	**Time (mins)**	**%B**
	0	25
	10	80

Flow Rate:	0.4 mL/min
Temperature:	20 °C
Detection:	UV, 260 nm

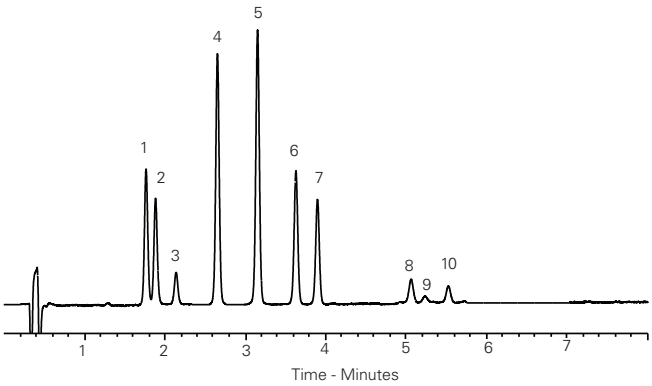
Analytes

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

Explore Selectivity

2 and 3 column kits available for the **same price** as a single column

See page 5 for details





Steroids (Veterinary) by LC-MS/MS

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

Gradient:	**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

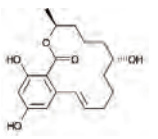
Analytes

1. α- and β-Zearalenol (*m/z* 319.17 → 275.12)
2. Diethylstilbestrol-d8 (*m/z* 275.23 → 245.09)

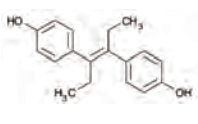
Also analysed in -ESI:
Taleranol and zeranol-d4
Taleranol and zeranol
Zearalenone
Hexestrol
Diethylstilbestrol
Dienestrol

3. α- and β-Boldenone (*m/z* 287.17 → 121.12)
4. α- and β-Nortestosterone (*m/z* 275.23 → 109.09)

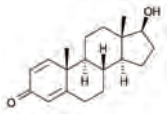
Also analysed in +ESI:
Hydroxystanozolol
Hydroxystanozolol-d3
Methyltestosterone
Methyltestosterone-d3
β-Nortestosterone-d3
β-Trenbolone
α-Trenbolone



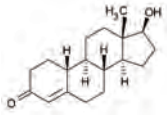
α- and β-Zearalenol



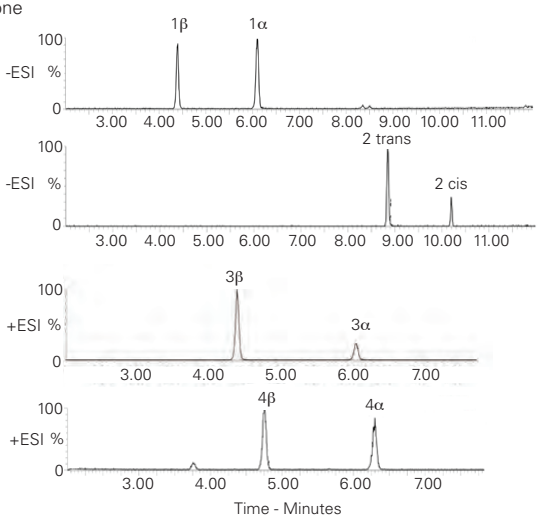
Diethylstilbestrol



α- and β-Boldenone



α- and β-Nortestosterone



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St John's Wort

Application #AN4300

Conditions

Column: ACE Excel 1.7 SuperC18
Dimensions: 100 x 3.0 mm; 2 x 100 x 3.0 mm (coupled); 3 x 100 x 3.0 mm (coupled)
Part Number: EXL-1711-1003U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

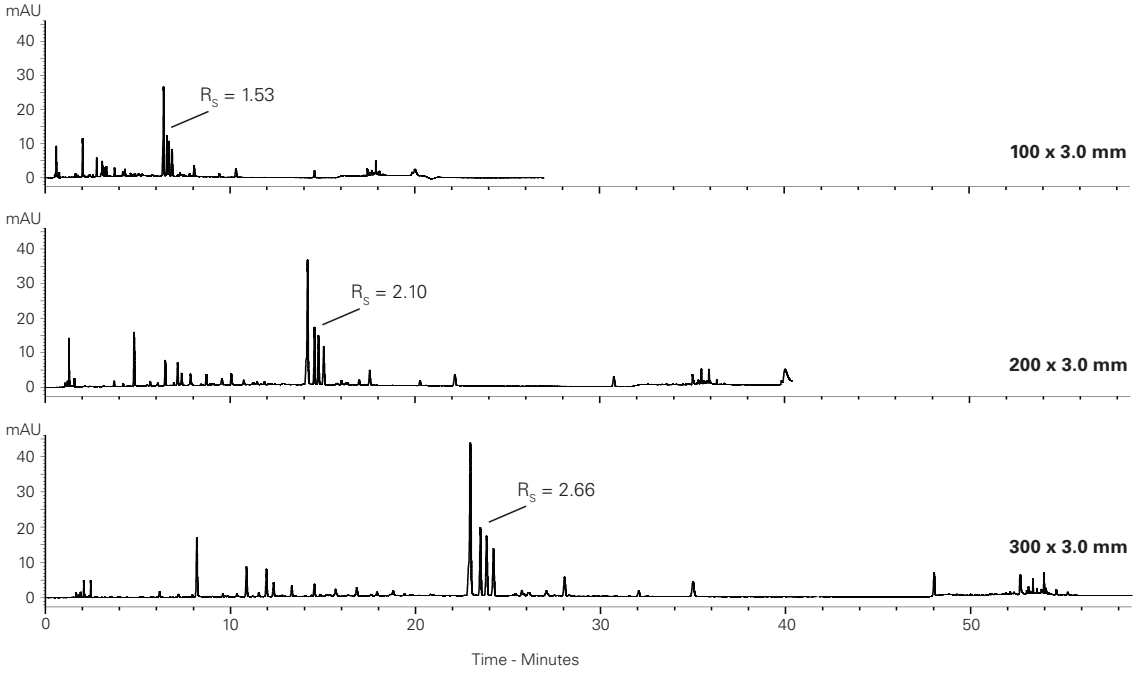
Gradient:

Time (mins)			
100 x 3.0 mm	**200 x 3.0 mm**	**300 x 3.0 mm**	**%B**
-	0.00	0.00	5
0.00	0.35	0.71	5
15.00	30.35	45.71	30
17.00	34.35	51.71	100
19.00	38.35	57.71	100
20.00	39.35	58.71	5
27.00	53.35	79.71	5

Flow Rate: 0.8 mL/min
Injection: 2 µL (100 x 3.0 mm); 4 µL (200 x 3.0 mm); 6 µL (300 x 3.0 mm)
Temperature: 80 °C
Detection: UV, 280 nm
Sample: Tablet ground to fine powder and extracted with MeCN/H_2O (1:1 v/v) with ultrasonication. Supernatant diluted with H_2O and filtered using Whatman Mini-Uniprep syringeless filter
System: Chromaster Ultra Rs



Hypericum perforatum



Substituted Methoxybenzene Isomers

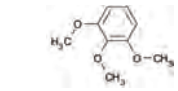
Application #AN2430

Conditions

Column:	ACE 3 C18-PFP
Dimensions:	150 x 4.6 mm
Part Number:	ACE-1110-1546
Mobile Phase:	H_2O/MeOH (50:50 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	40 °C
Detection:	UV, 214 nm

Analytes

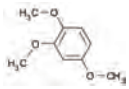
1. 1,2,3-Trimethoxybenzene
2. 1,2-Dimethoxybenzene
3. 1,2,4-Trimethoxybenzene
4. 1,4-Dimethoxybenzene
5. Methoxybenzene
6. 1,3-Dimethoxybenzene
7. 1,3,5-Trimethoxybenzene
8. Toluene



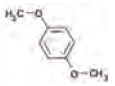
1,2,3-Trimethoxybenzene



1,2-Dimethoxybenzene



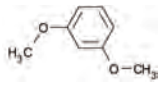
1,2,4-Trimethoxybenzene



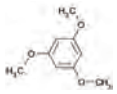
1,4-Dimethoxybenzene



Methoxybenzene



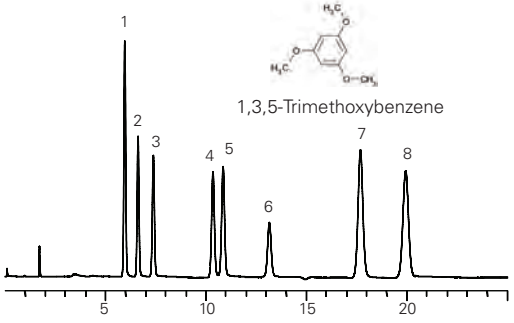
1,3-Dimethoxybenzene



1,3,5-Trimethoxybenzene



Toluene



Sugars – Cola vs Diet Cola

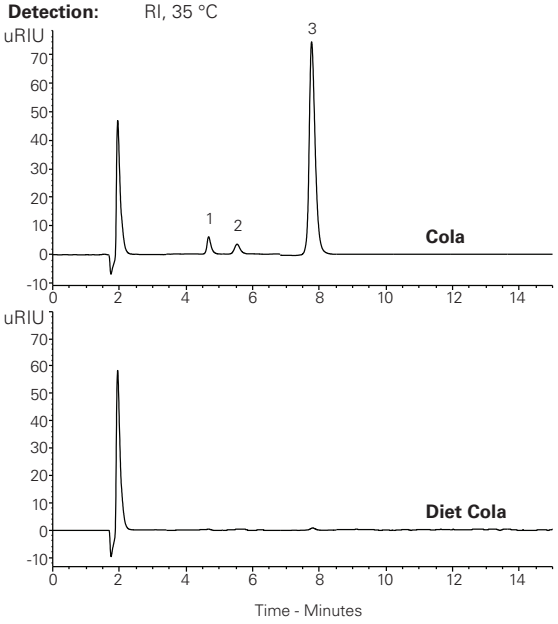
Application #AN4150

Conditions

Column:	ACE Excel 3 NH_2
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1114-1546U
Mobile Phase:	MeCN/H_2O (75:25 v/v)
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	RI, 35 °C

Analytes

1. Fructose
2. Glucose
3. Sucrose



Sugars – Disaccharides

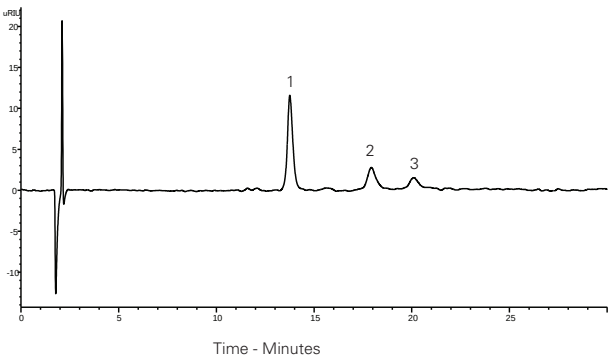
Application #AN4320

Conditions

Column:	ACE Excel 3 NH_2
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1114-1546U
Mobile Phase:	MeCN/H_2O (80:20 v/v)
Flow Rate:	1 mL/min
Injection:	20 µL
Temperature:	35 °C
Detection:	RI, 35 °C
Sample:	2 mg/mL each disaccharide in MeCN/H_2O (80:20 v/v)
System:	Chromaster 600

Analytes

1. Sucrose
2. Maltose
3. Lactose



Sugars – Lactulose

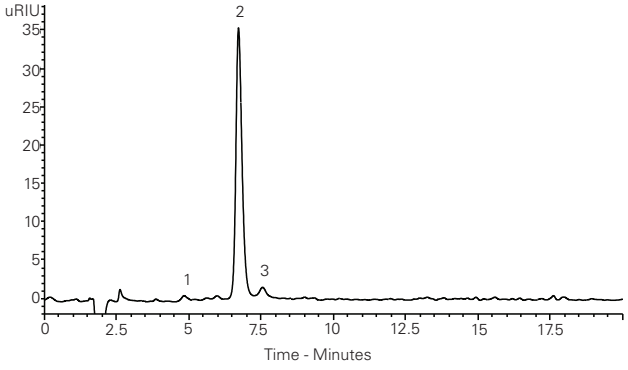
Application #AN4020

Conditions

Column:	ACE Excel 5 NH_2
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1214-1546U
Mobile Phase:	MeCN/H_2O (70:30 v/v)
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	RI, 35 °C

Analytes

1. Galactose
2. Lactulose
3. Lactose



Sugars – Maple Syrup

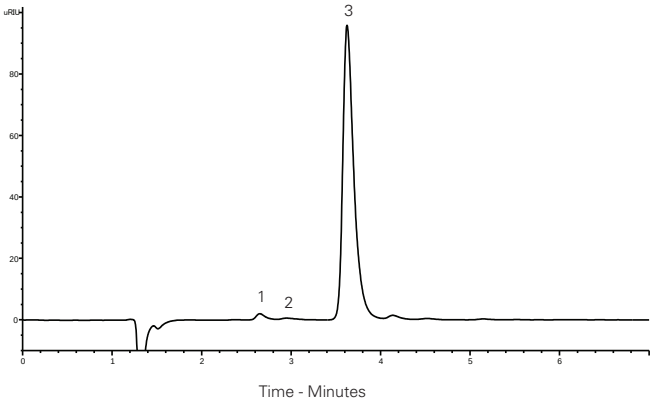
Application #AN4310

Conditions

Column:	ACE Excel 1.7 NH_2
Dimensions:	100 x 3.0 mm
Part Number:	EXL-1714-1003U
Mobile Phase:	MeCN/H_2O (70:30 v/v)
Flow Rate:	0.43 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	RI, 35 °C
Sample:	100 µL maple syrup in 9900 µL mobile phase
System:	Chromaster 600

Analytes

1. Fructose
2. Glucose
3. Sucrose



Sugars – Monosaccharides

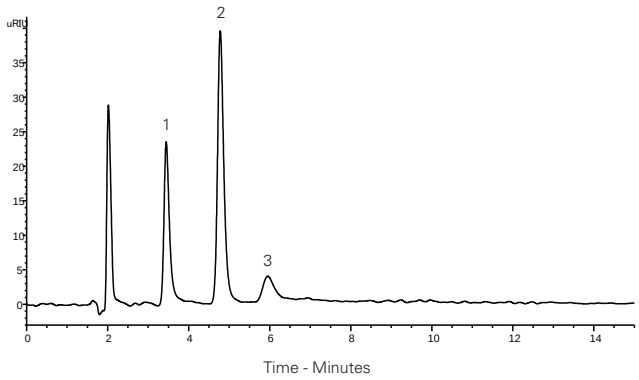
Application #AN4330

Conditions

Column:	ACE Excel 5 NH_2
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1214-1546U
Mobile Phase:	MeCN/H_2O (75:25 v/v)
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	RI, 35 °C
Sample:	5 mg/mL per monosaccharide in MeCN/H_2O (70:30 v/v)
System:	Chromaster 600

Analytes

1. Fructose
2. Galactose
3. Rhamnose





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

Sugars – Orange Juice

Application #AN4160

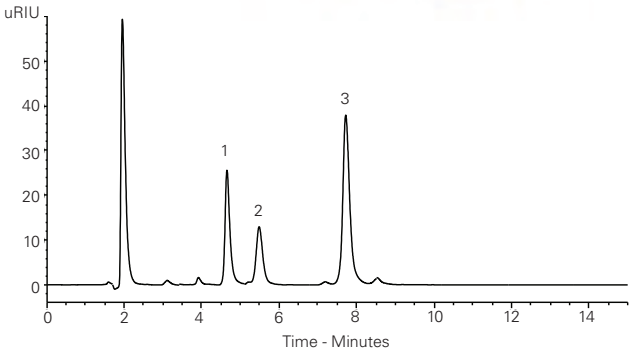
Conditions

Column:	ACE Excel 3 NH_2
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1114-1546U
Mobile Phase:	MeCN/H_2O (75:25 v/v)
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	RI, 35 °C

Analytes

1. Fructose
2. Glucose
3. Sucrose





Sugars Separation

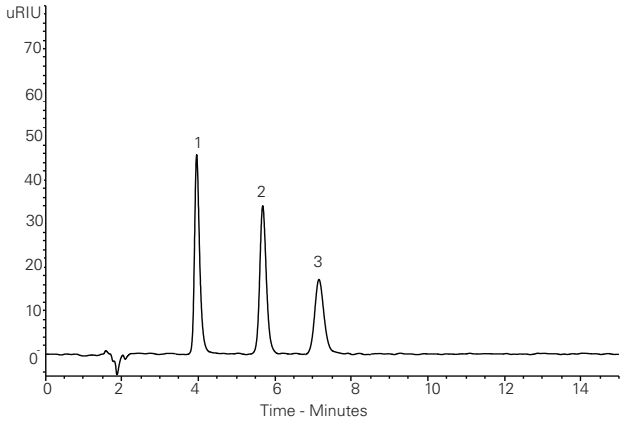
Application #AN4030

Conditions

Column:	ACE Excel 5 NH_2
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1214-1546U
Mobile Phase:	MeCN/H_2O (70:30 v/v)
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	RI, 35 °C

Analytes

1. Fructose
2. Sucrose
3. Lactose



Sulfonamides

Application #AN1610

Conditions

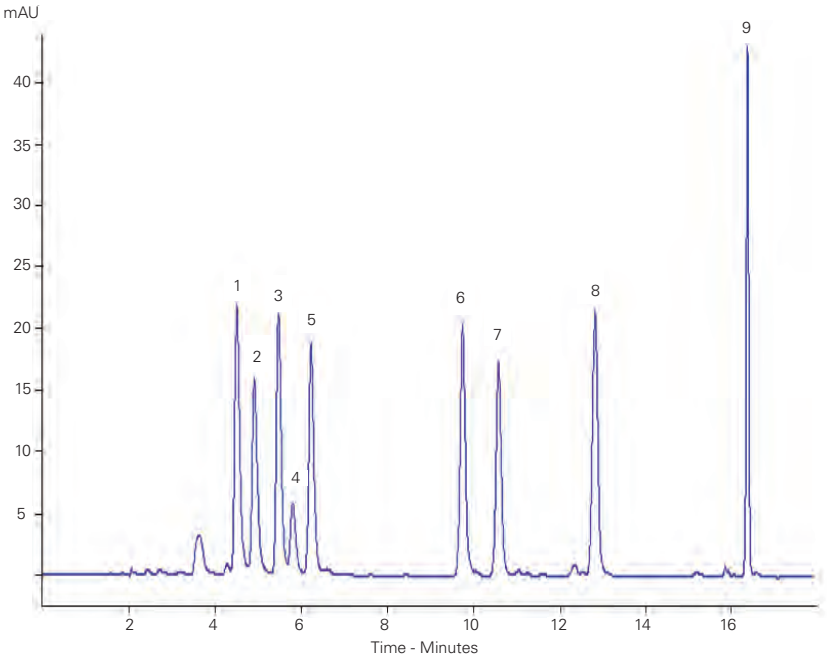
Column:	ACE Excel 3 C18-PFP
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1110-1546U
Mobile Phase:	A: H_2O
	B: MeCN
	C: 10% formic acid

Gradient:	**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

Analytes

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



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Sulfurous Analytes Separation Comparison

Application #AN1320

Conditions

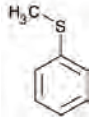
Column:	ACE 3 C18-AR, ACE 3 C18
Dimensions:	50 x 2.1 mm
Part Number:	ACE-119-0502, ACE-111-0502
Mobile Phase:	A: H_2O
	B: MeOH

Gradient:	**Time (mins)**	**%B**
	0.0	30
	5.0	30
	9.0	95
	9.5	30
	13.5	30

Flow Rate:	0.5 mL/min
Injection:	1 µL
Temperature:	22 °C
Detection:	UV, 254 nm



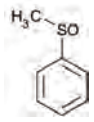
Toluene



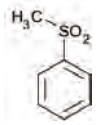
Thioanisole

Analytes

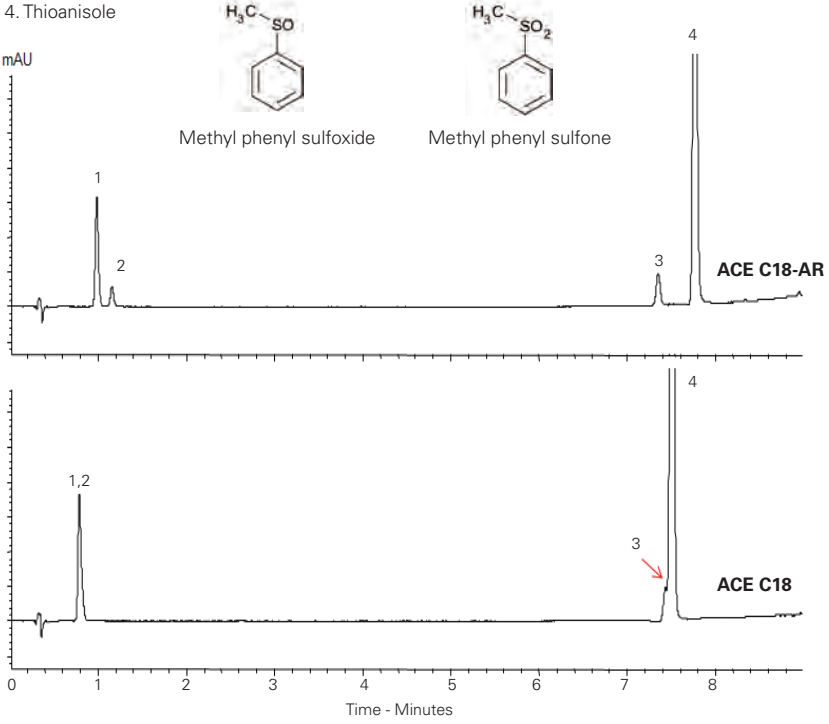
1. Methyl phenyl sulfoxide
2. Methyl phenyl sulfone
3. Toluene
4. Thioanisole



Methyl phenyl sulfoxide



Methyl phenyl sulfone



Sumatriptan and Promethazine by LC-MS/MS

Application #AN2530

Conditions

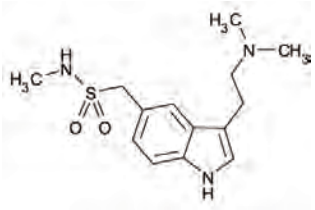
Column:	ACE Excel 2 C18-PFP
Dimensions:	100 x 2.1 mm
Part Number:	EXL-1010-1002U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH

Gradient:	**Time (mins)**	**%B**
	0.0	15
	0.5	15
	2.5	90
	3.5	90
	5.5	15

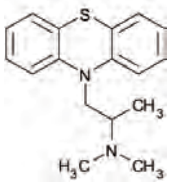
Flow Rate:	0.7 mL/min
Temperature:	50 °C
Detection:	AB Sciex QTRAP 6500
	DuoSpray Ion source (ESI/APCI)
	Positive ion MRM mode

Analytes

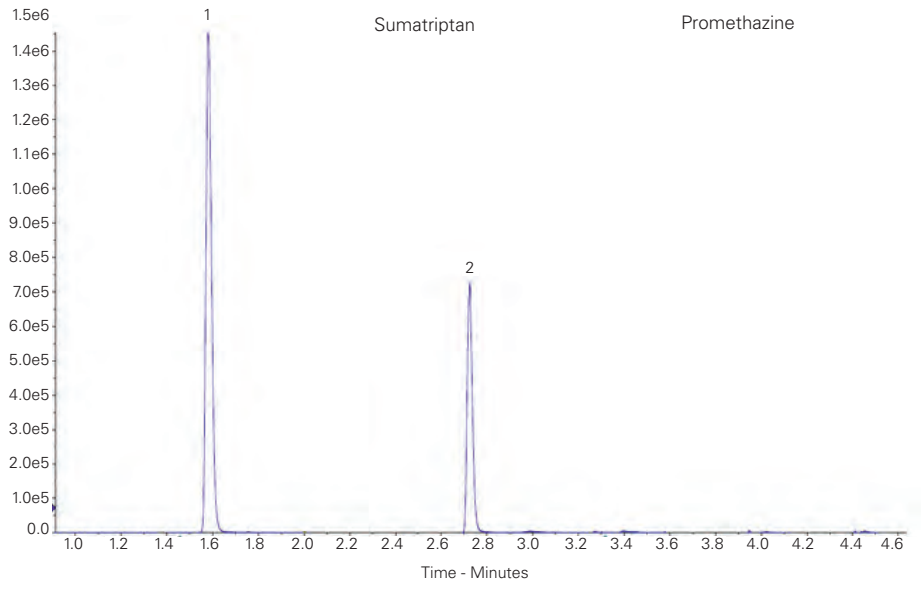
1. Sumatriptan
   (*m/z* 296 → 58)
2. Promethazine
   (*m/z* 286 → 86)



Sumatriptan



Promethazine



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Sunscreen Agents

Application #AN4370

Conditions

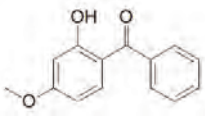
Column:	ACE 3 C18
Dimensions:	150 x 4.0 mm
Part Number:	ACE-111-1504
Mobile Phase:	A: MeOH/H_2O (85:15 v/v)
	B: THF

Gradient:	**Time (mins)**	**%B**
	0	0
	7	0
	10	50
	14	50
	16	0

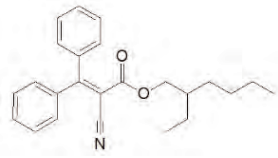
Flow Rate:	0.85 mL/min
Temperature:	30 °C
Detection:	UV, 310 nm
Sample:	40 µg/mL each standard

Analytes

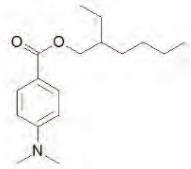
1. Benzophenone-3
2. Octocrylene
3. Octyl dimethyl PABA
4. Octyl methoxycinnamate
5. Avobenzone
6. Ethylhexyl salicylate
7. Homosalate
8. Ethylhexyl triazone
9. Tinosorb® M
10. Tinosorb® S



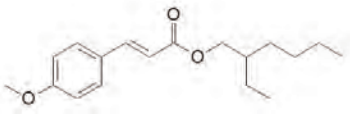
Benzophenone-3



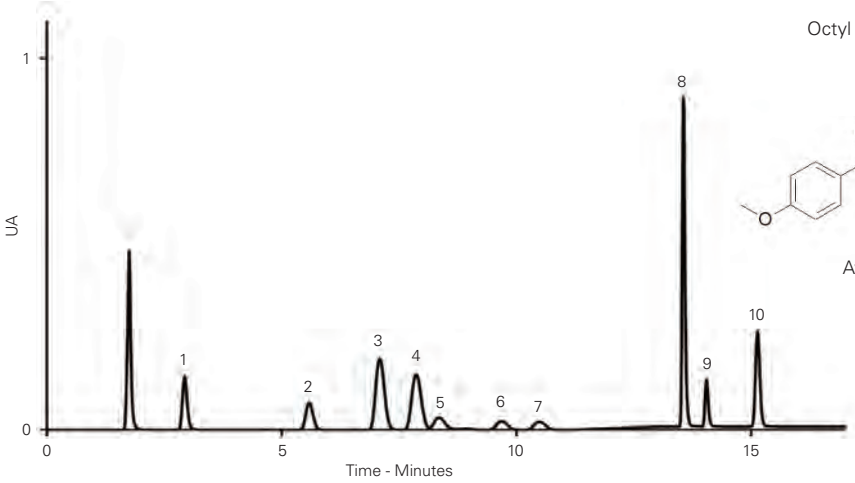
Octocrylene

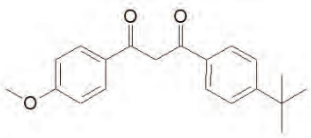


Octyl dimethyl PABA

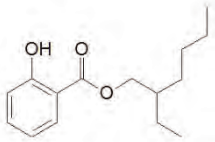


Octyl methoxycinnamate



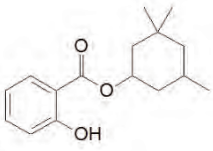


Avobenzone

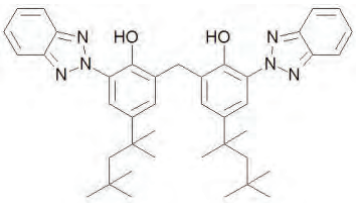


Ethylhexyl salicylate

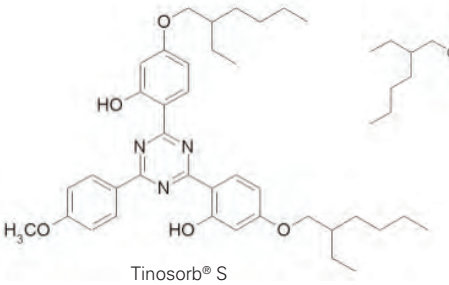
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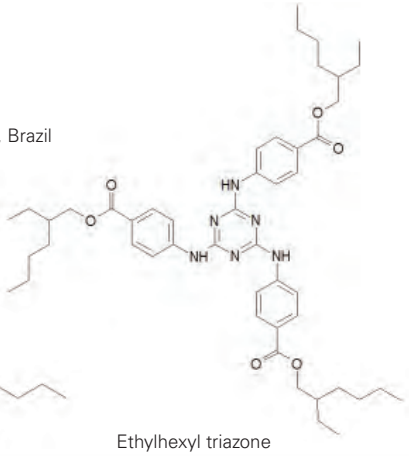
Homosalate



Tinosorb® M



Tinosorb® S



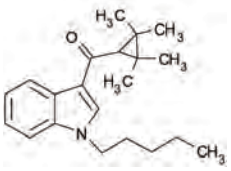
Ethylhexyl triazone

Synthetic Cannabinoids (SPICE) from Oral Fluid

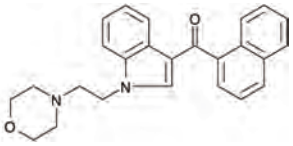
Application #AN1650

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



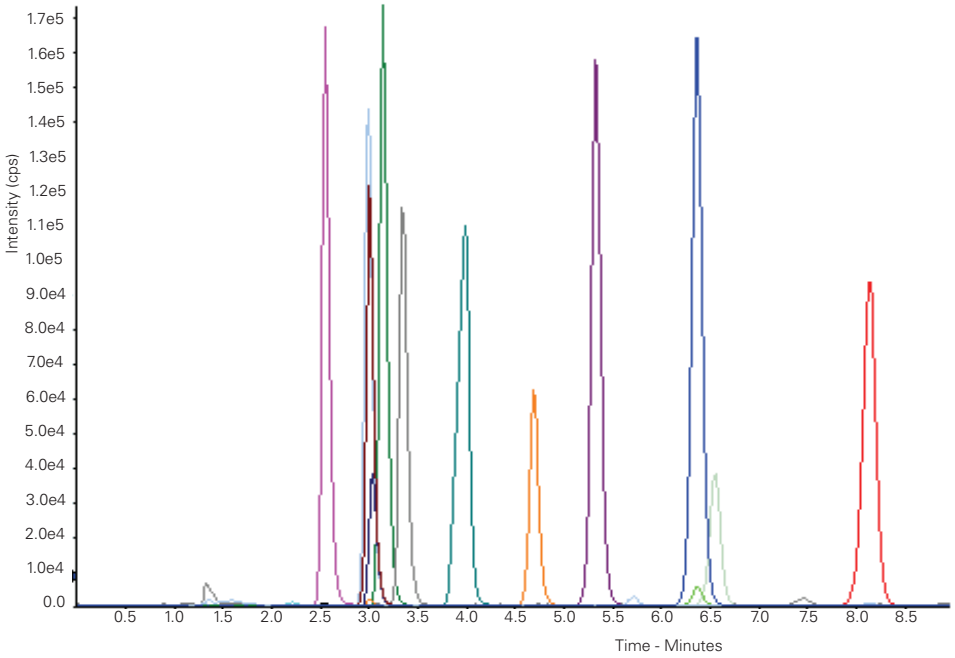
UR - 144



JWH - 200

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

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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Taxol in Fungal Extract by LC-MS/MS

Application #AN1670

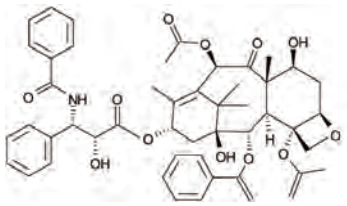
Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: CORE-25A-1502U
Mobile Phase: A: 0.5% formic acid in H_2O
B: 0.5% formic acid in MeCN

Gradient:

Time (mins)	%B
0.0	10
1.0	10
3.0	40
22.0	60
25.0	95

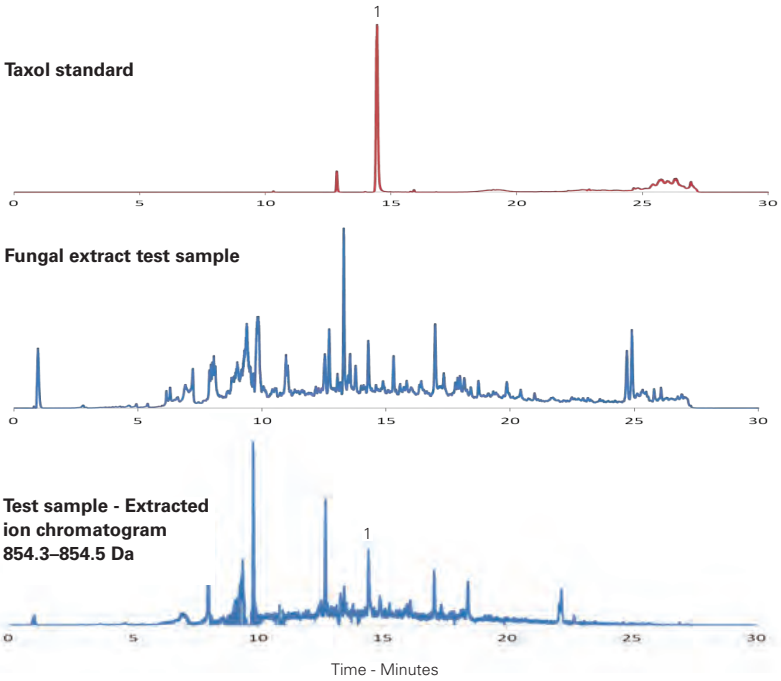
Flow Rate: 0.35 mL/min
Detection: Orbitrap Elite MS
FT positive ion mode
Collision induced dissociation isolation width 5 Da
Normalised collision energy 32 eV
Activation Q 0.25
Activation times 10 ms



Taxol (Paclitaxel)

Analyte

1. Taxol (Paclitaxel)



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Telithromycin Analysis

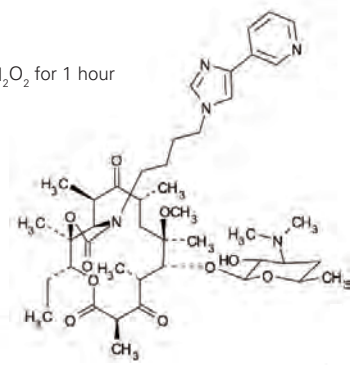
Application #AN3280

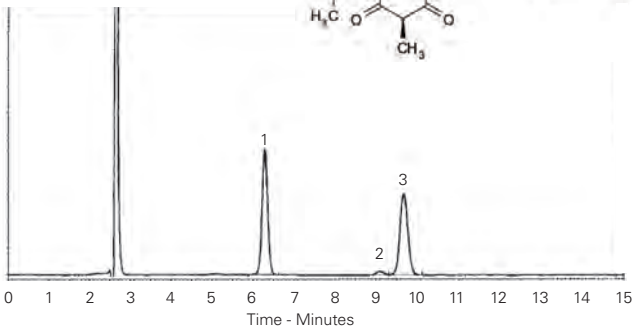
Conditions

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

Analytes

1. Telithromycin
2. Degradant 1
3. Degradant 2





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Terfenadine and Fexofenadine in Rat Plasma

Application #AN3290

Conditions

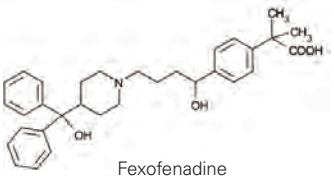
Column: ACE 5 AQ
Dimensions: 50 x 3.0 mm
Part Number: ACE-126-0503
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeOH
Gradient:

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

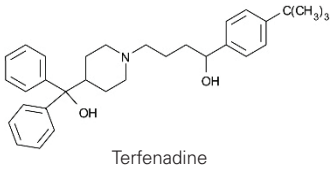
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: Ambient
Detection: TurbolonSpray MS/MS
Positive ion mode

Analytes

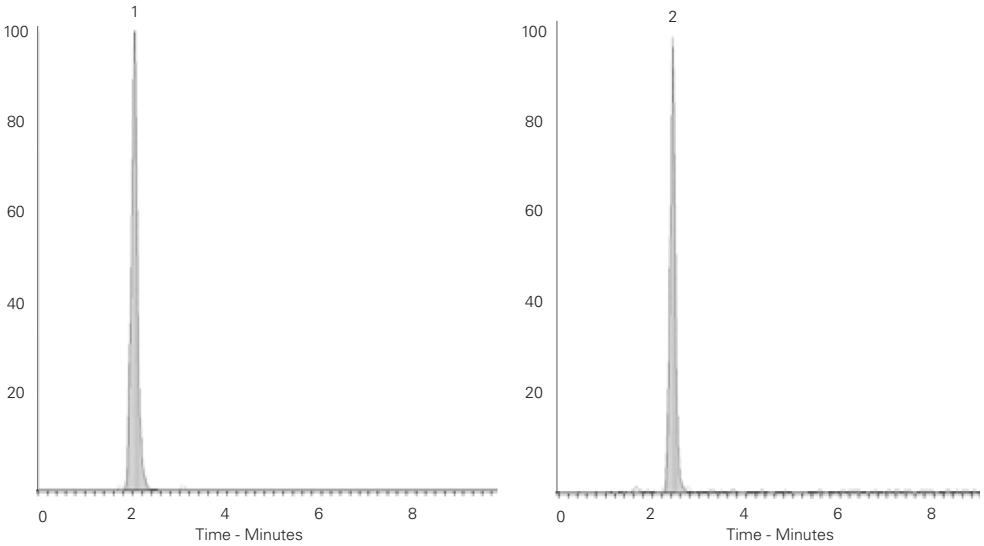
1. Fexofenadine
(*m/z* 502.3 → 466.3)
2. Terfenadine
(*m/z* 472.3 → 436.3)



Fexofenadine



Terfenadine



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Testosterone

Application #AN3300

Conditions

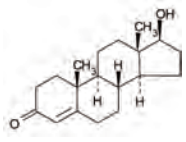
Column: ACE 5 C18
Dimensions: 150 x 0.075 mm
Part Number: ACE-121-1500075
Mobile Phase: A: 0.1% formic acid in MeCN/0.1% formic acid in H_2O (10:90 v/v)
B: 0.1% formic acid in MeCN/0.1% formic acid in H_2O (90:10 v/v)
Gradient:

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

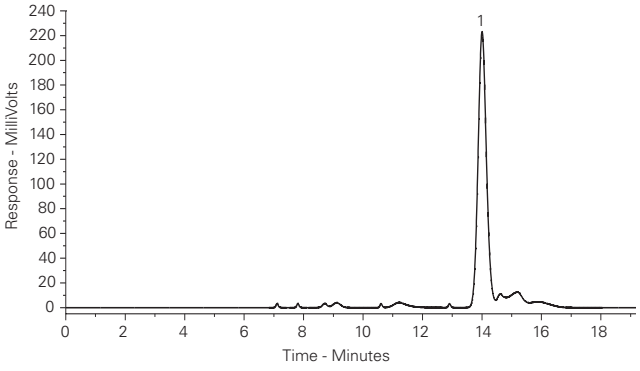
Flow Rate: 1 µL/min
Temperature: Ambient
Detection: ESI MS/MS
Positive ion mode

Analyte

1. Testosterone



Testosterone



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Tetracyclines

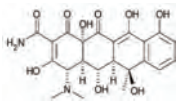
Application #AN3680

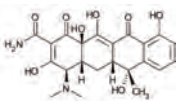
Conditions

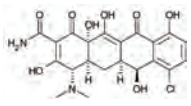
Column: ACE 5 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-121-1503
Mobile Phase: 10 mM oxalic acid pH 2.9/MeCN (80:20 v/v)
Flow Rate: 0.5 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV-Vis, 350 nm

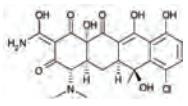
Analytes

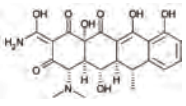
1. Oxytetracycline
2. Tetracycline
3. Demeclocycline
4. Chlortetracycline
5. Doxycycline

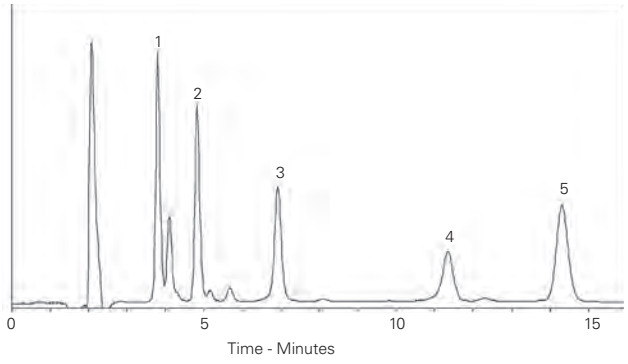

Oxytetracycline


Tetracycline


Demeclocycline


Chlortetracycline


Doxycycline



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Thyroid Hormones by LC-MS/MS (I)

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

Gradient:

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

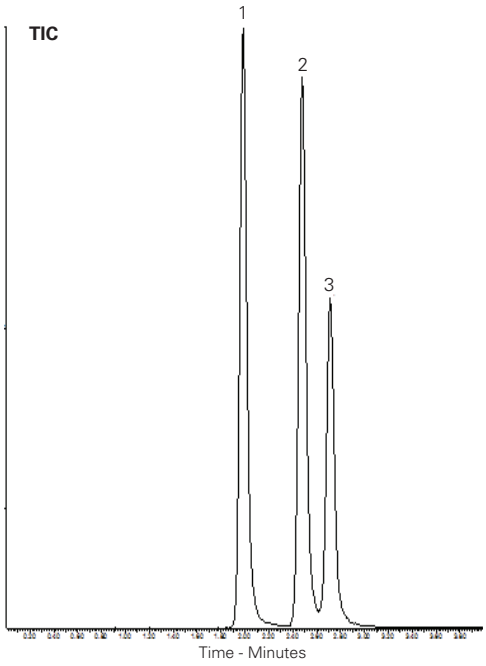
Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: XEVO TQS triple quad MS
Desolvation temperature: 500 °C
Ion source temperature: 150 °C
Positive mode ESI, MRM
Sample: Serum samples extracted using Biotage EVOLUTE EXPRESS AX methodology

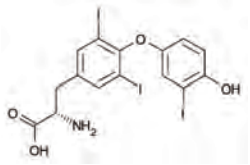
Analyte	Q1 (Da)	Q3 (Da)
T3	651.8	605.8
	(651.8)	(507.8)
	(651.8)	(478.9)
rT3	651.8	605.8
	(651.8)	(507.8)
	(651.8)	(478.9)
T3/rT3-d6 I.S.	657.8	611.8
T4	777.7	731.7
	(777.7)	(351)
	(777.7)	(633.8)

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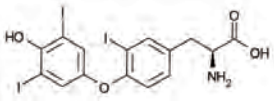
Analytes

1. T3 (Tri-iodothyronine)
2. rT3 (Reversed tri-iodothyronine)
3. T4 (Thyroxine)

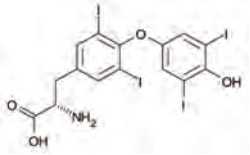




T3 (Tri-iodothyronine)



rT3 (Reversed tri-iodothyronine)



T4 (Thyroxine)

Tocopherols Mixture Separation

Application #AN3390

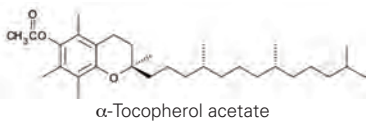
Conditions

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

Gradient:

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

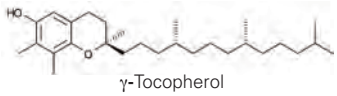
Flow Rate: 1.2 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: UV, 285 nm



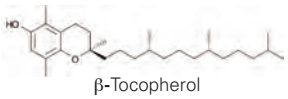
α-Tocopherol acetate

Analytes

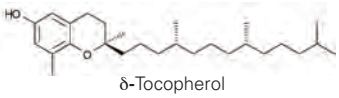
1. γ-Tocopherol
2. β-Tocopherol
3. δ-Tocopherol
4. α-Tocopherol
5. α-Tocopherol acetate



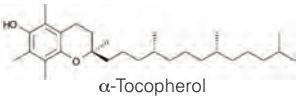
γ-Tocopherol



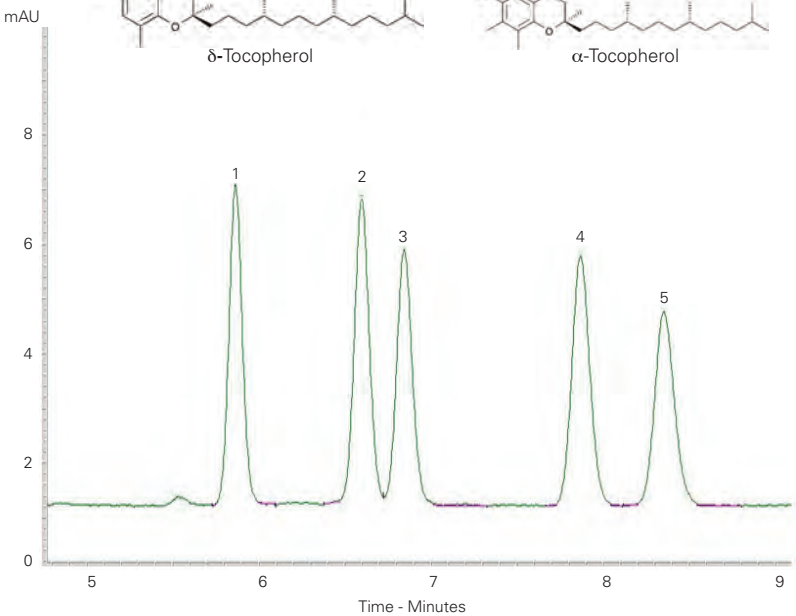
β-Tocopherol



δ-Tocopherol



α-Tocopherol



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Tocopherols

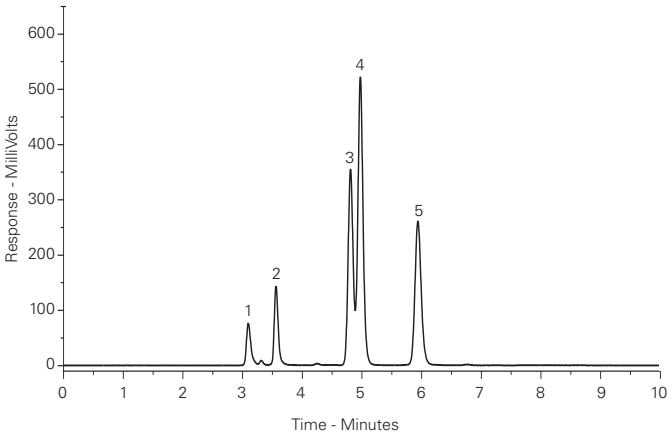
Application #AN2790

Conditions

Column:	ACE 5 SIL
Dimensions:	250 x 4.6 mm
Part Number:	ACE-127-2546
Mobile Phase:	Hexane/IPA (98:2 v/v)
Flow Rate:	1 mL/min
Injection:	1 µL
Temperature:	Ambient
Detection:	UV-Vis, 450 nm

Analytes

1. γ-Tocopherol
2. α–Tocopherol
3. β-Tocopherol
4. β-Tocopherol
5. δ-Tocopherol



Tricyclic Antidepressants

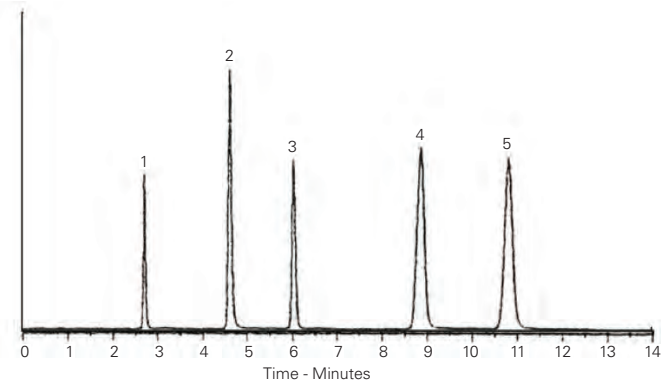
Application #AN3920

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	MeOH/25 mM KH_2PO_4 pH 6.0 in H_2O (80:20 v/v)
Flow Rate:	1 mL/min
Temperature:	22 °C
Detection:	UV, 215 nm

Analytes

1. Norephedrine
2. Nortriptyline
3. Toluene
4. Imipramine
5. Amitriptyline



Toxins from *Amanita Phalloides* Mushrooms by LC-HRMS

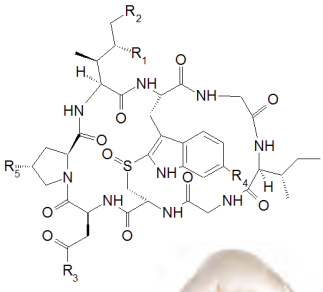
Application #AN4060

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 MeOH	
Gradient:	**Time (mins)**	**%B**
	0	15
	17	100
	22	100
	22	15
	30	15
Flow Rate:	0.4 mL/min	
Injection:	10 µL	
Temperature:	50 °C	
Detection:	Thermo Exactive MS ESI in positive ion mode	

Analyte

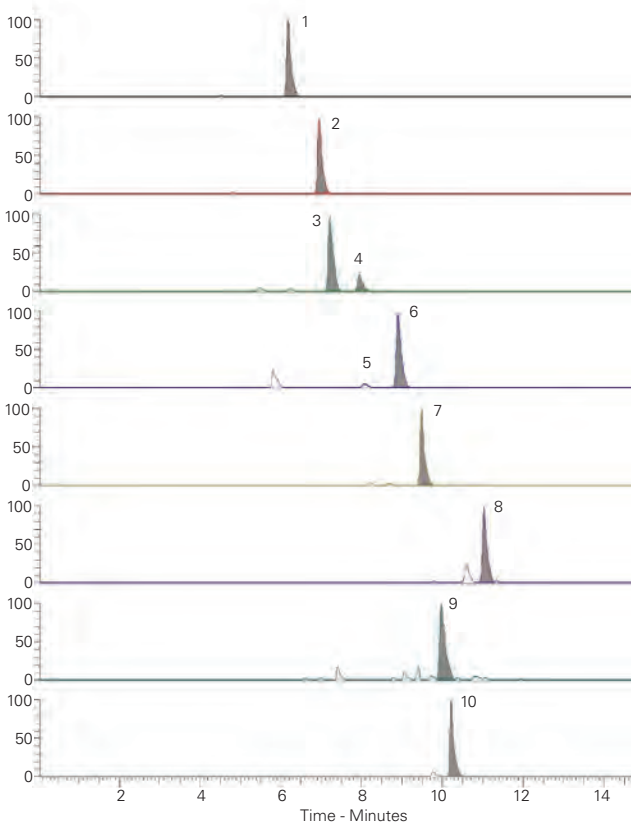
1. Amatoxins





Amanita Phalloides

Peak	Analyte	R1	R2	R3	R4	R5	Exact Mass
1	α - Amanitin	OH	OH	NH_2	OH	OH	918.35417
2	β - Amanitin	OH	OH	OH	OH	OH	919.338182
3	γ - Amanitin	H	OH	NH_2	OH	OH	902.359252
4	Amaninamide	OH	OH	NH_2	H	OH	902.359252
5	Amanin	OH	OH	OH	H	OH	903.343267
6	ε - Amanitin	H	OH	OH	OH	OH	903.343267
7	Amanullin	H	H	NH_2	OH	OH	886.364337
8	Proamanullin	H	H	NH_2	OH	H	870.369423
9	Amanullinic Acid	H	H	OH	OH	OH	887.348353
10	Bacitracin (IS)	-	-	-	-	-	1421.7489



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Tricyclic Antidepressants (Gradient)

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)

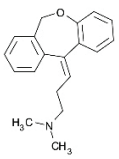
Gradient:

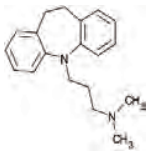
Time (mins)	%B
0.0	50
6.0	70
7.0	70
7.5	50

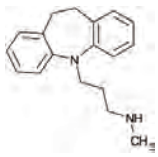
Flow Rate: 1.2 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: UV, 260 nm

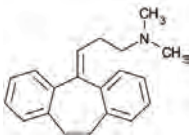
Analytes

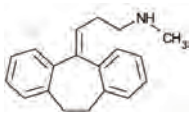
1. Doxepin + isomer
2. Imipramine
3. Desipramine
4. Amitriptyline
5. Nortriptyline
6. Clomipramine

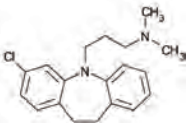

Doxepin + isomer

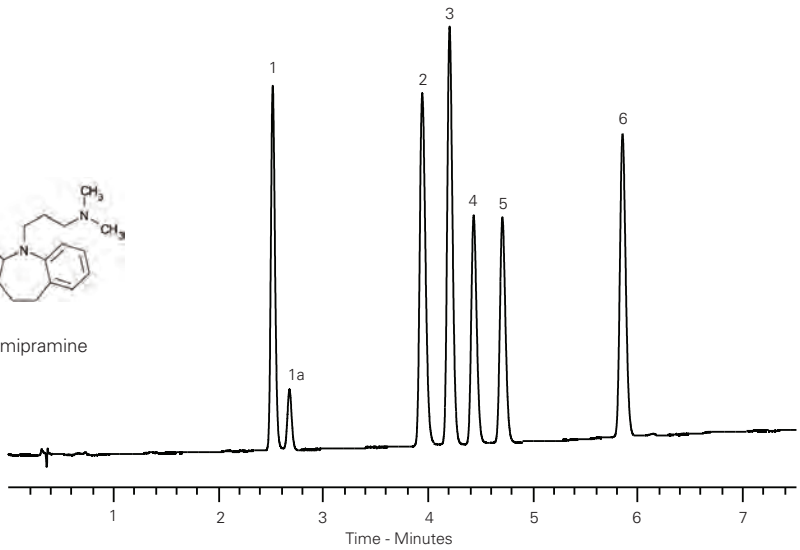

Imipramine


Desipramine


Amitriptyline


Nortriptyline


Clomipramine



Tricyclic Antidepressants (Isocratic)

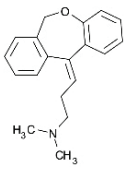
Application #AN1680

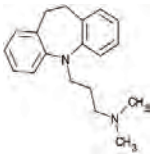
Conditions

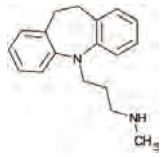
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 3.0 mm
Part Number: EXL-1010-1003U
Mobile Phase: 20 mM ammonium formate pH 3.0 in MeOH/H_2O (54:46 v/v)
Flow Rate: 1.2 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: UV, 260 nm

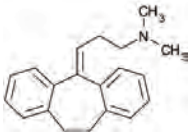
Analytes

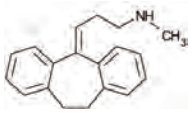
1. Doxepin
2. Imipramine
3. Desipramine
4. Amitriptyline
5. Nortriptyline
6. Clomipramine

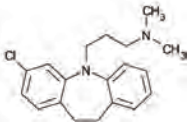

Doxepin

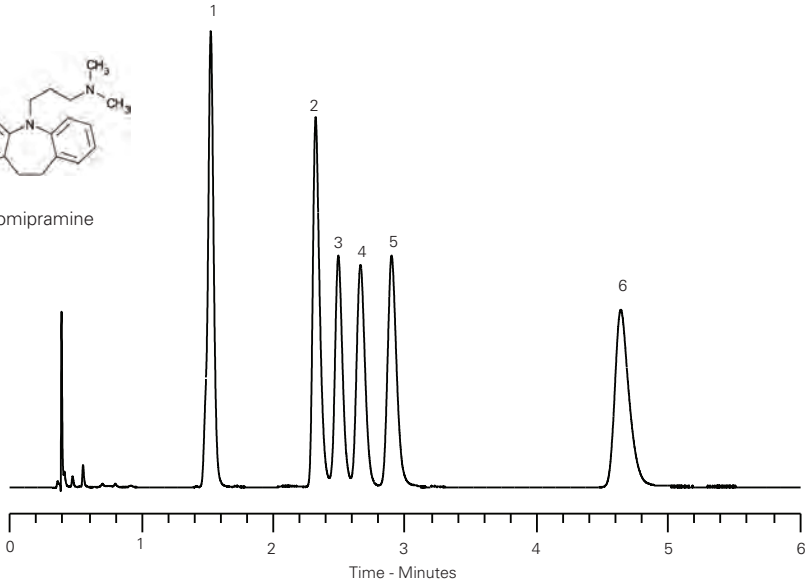

Imipramine


Desipramine


Amitriptyline


Nortriptyline


Clomipramine



Tricyclic Antidepressants (Isocratic Rapid Analysis)

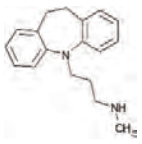
Application #AN1700

Conditions

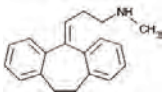
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	20 mM ammonium acetate pH 6.3 MeCN/H_2O (65:35 v/v)
Flow Rate:	1.5 mL/min
Injection:	10 µL
Temperature:	60 °C
Detection:	UV, 215 nm

Analytes

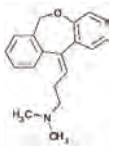
1. Desipramine
2. Nortriptyline
3. Doxepin
4. Imipramine
5. Amitriptyline



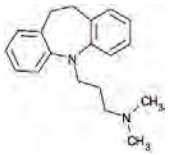
Desipramine



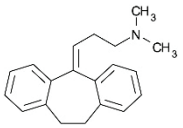
Nortriptyline



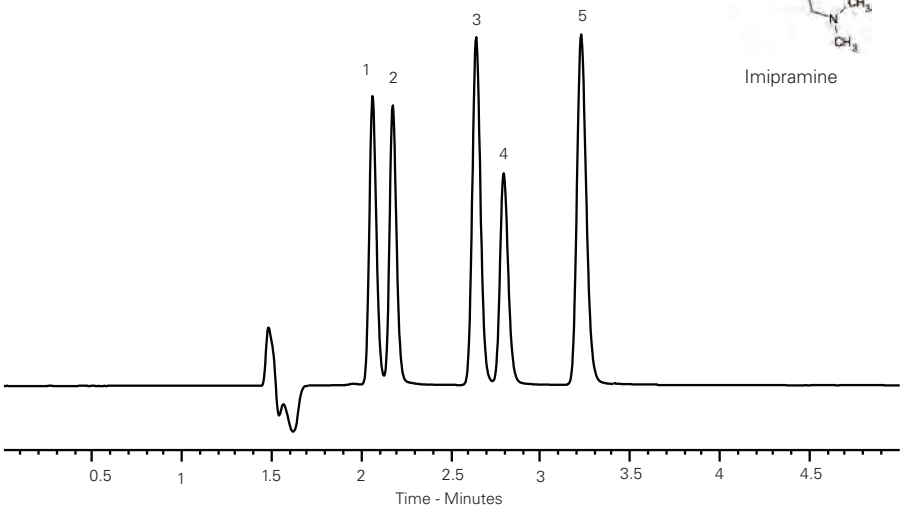
Doxepin



Imipramine



Amitriptyline



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Triple API Pharmaceutical and Related Substances using Ultra Resolution

Application #AN3560

Conditions

Column: ACE Excel 1.7 SuperC18
Dimensions: 100 x 3.0 mm; 2 x 100 x 3.0 mm (coupled); 3 x 100 x 3.0 mm (coupled)
Part Number: EXL-1711-1003U
Mobile Phase: A: H_2O
B: MeCN
C: 200 mM ammonium formate pH 3.0

Gradient:

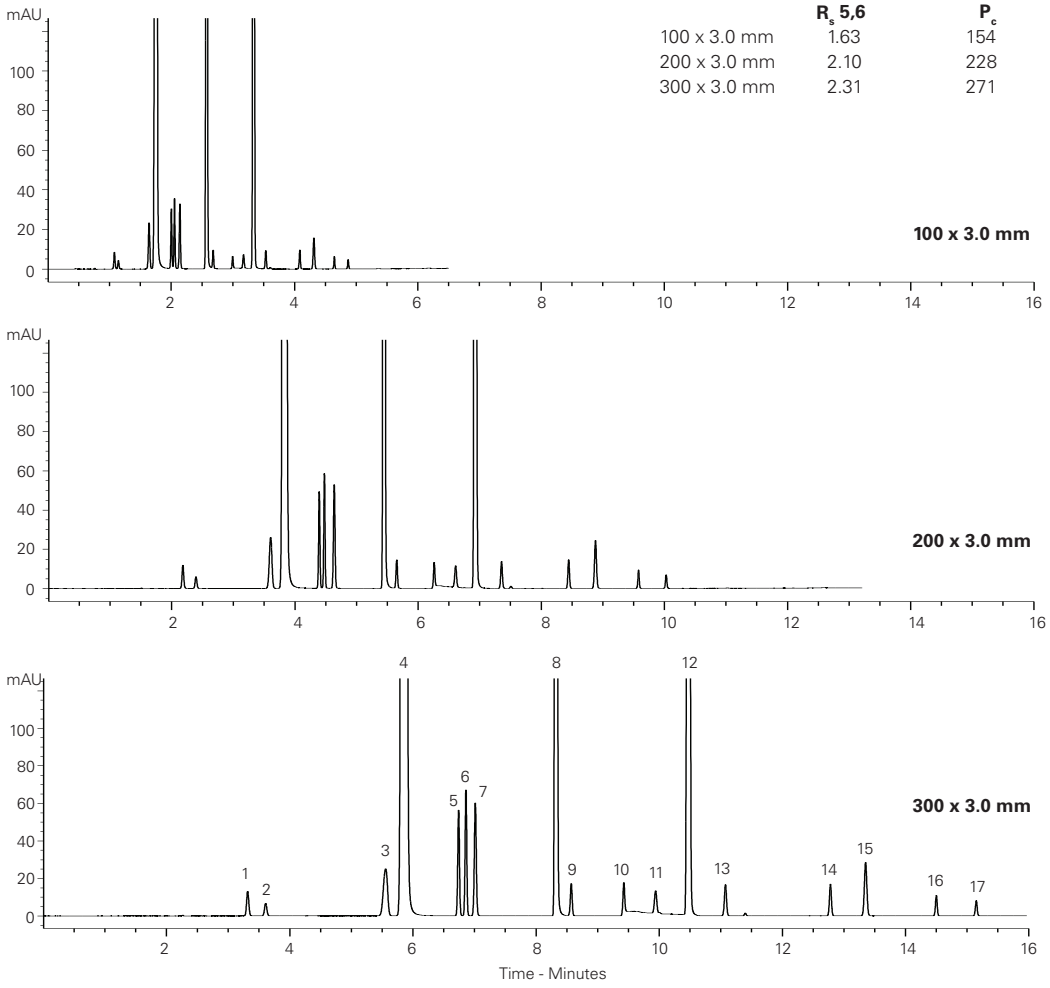
Time (mins)					
100 x 3.0 mm	**200 x 3.0 mm**	**300 x 3.0 mm**	**%A**	**%B**	**%C**
-	0.00	0.00	90	5	5
0.00	1.21	2.41	90	5	5
5.00	11.21	17.41	20	75	5
6.00	12.21	18.41	20	75	5
6.50	13.21	19.41	90	5	5

Flow Rate: 0.8 mL/min
Temperature: 80 °C
Detection: UV, 270 nm

Analytes

1. 2-Aminophenol
2. Hydroquinone
3. Theobromine
4. Paracetamol
5. Paraxanthine
6. Theophylline
7. 4-Hydroxybenzoic acid
8. Caffeine
9. 2-Acetamidophenol
10. 2-Hydroxybenzoic acid
11. Phenol
12. Aspirin
13. 4-Nitrophenol
14. 4-Chloroacetanilide
15. 2-Nitrophenol
16. Acetylsalicylsalicylic acid
17. Salsalate

Dimensions	Resolution, R_s 5,6	Peak Capacity, P_c
100 x 3.0 mm	1.63	154
200 x 3.0 mm	2.10	228
300 x 3.0 mm	2.31	271



Tyrosine, Tryptophan and Tramadol by HPLC with Fluorescence Detection

Application #AN4180

Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	A: 50 mM NaH_2PO_4 in H_2O
	B: MeCN/H_2O (60:40 v/v)

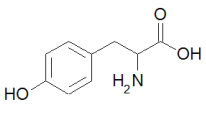
Gradient:

Time (mins)	%B
0.0	0
5.0	10
8.0	100
9.0	100
9.5	0
14.0	0

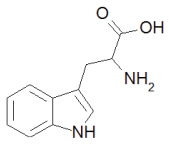
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	25 °C
Detection:	Fluorescence, λ_{Ex} 280 nm, λ_{Em} 340 nm

Analytes

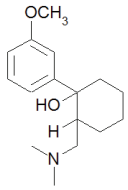
1. L-Tyrosine
2. L-Tryptophan
3. Tramadol



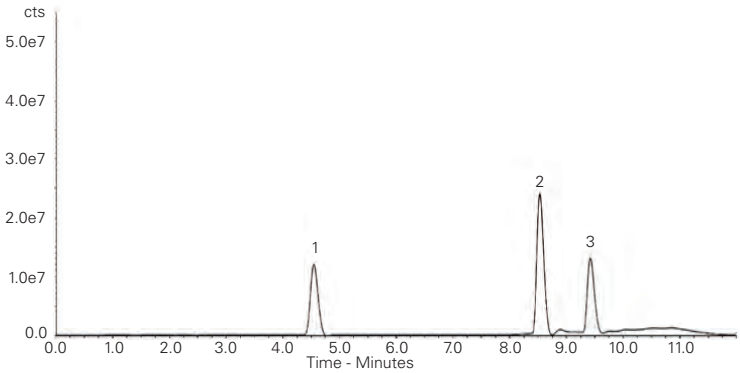
L-Tyrosine



L-Tryptophan



Tramadol



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USP Monograph – 17α-Ethinylestradiol

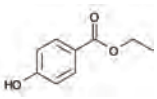
Application #AN1710

Conditions

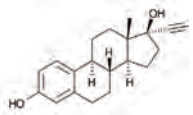
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 3.0 mm
Part Number:	CORE-25A-0503U
Mobile Phase:	H_2O/MeCN (50:50 v/v)
Flow Rate:	0.43 mL/min
Injection:	3.1 µL
Temperature:	Ambient (22 °C)
Detection:	UV, 280 nm

Analytes

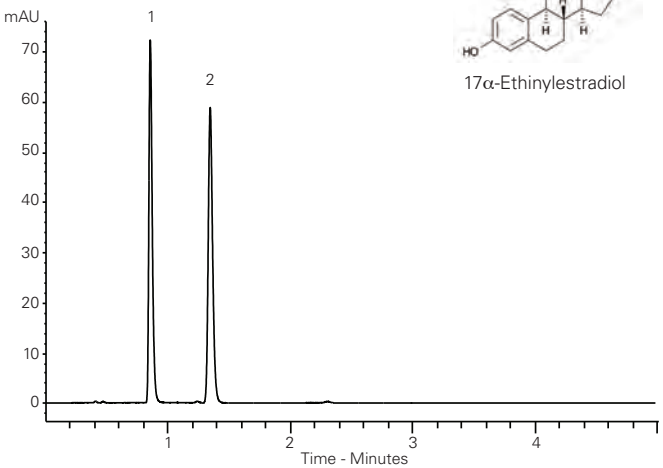
1. Ethylparaben
2. 17α-Ethinylestradiol



Ethylparaben



17α-Ethinylestradiol



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Amlodipine Besylate

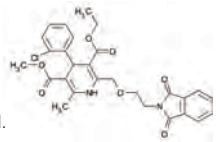
Application #AN2550

Conditions

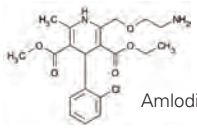
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	75 x 3.0 mm
Part Number:	CORE-25A-7503U
Mobile Phase:	MeOH/MeCN/buffer pH 3.0 (35:15:50 v/v/v)
Buffer:	7.0 mL triethylamine in 900 mL H_2O to 1000 mL volumetric flask. Adjust to pH 3.0 with phosphoric acid. Dilute to volume with H_2O
Flow Rate:	0.8 mL/min
Injection:	5 µL
Temperature:	25 °C
Detection:	UV, 237 nm

Analytes

1. Impurity A
2. Amlodipine

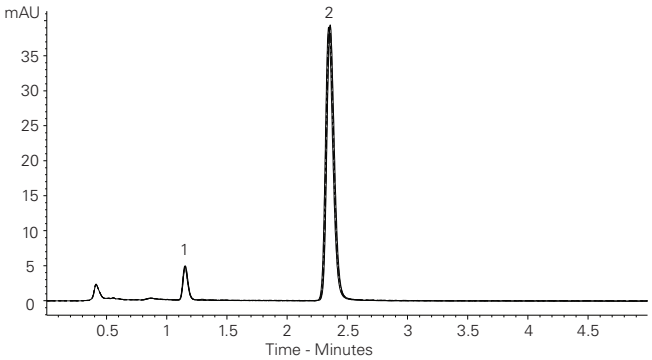


Impurity A



Amlodipine

Chromatogram shows 6 injections overlaid



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Budesonide

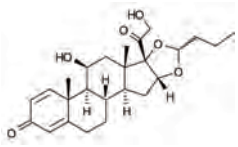
Application #AN1720

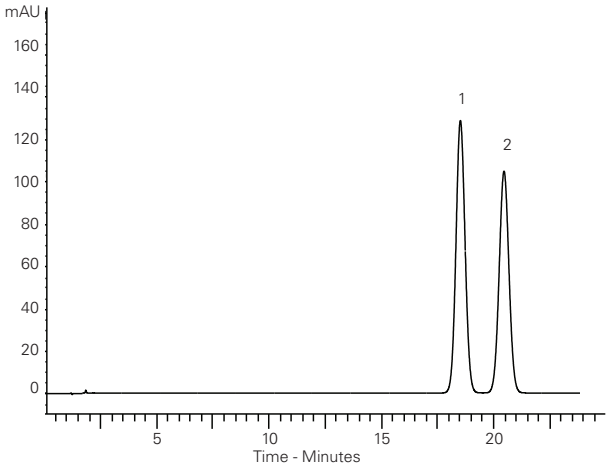
Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	18 mM monobasic sodium phosphate pH 3.2 in H_2O/MeCN (68:32 v/v)
Flow Rate:	1.5 mL/min
Injection:	20 µL
Temperature:	Ambient (22 °C)
Detection:	UV, 254 nm

Analytes

1. Budesonide B
2. Budesonide A





Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Doxepin

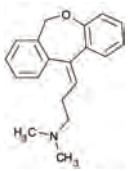
Application #AN1730

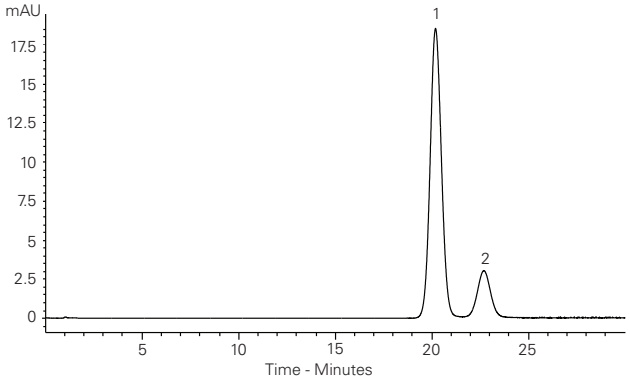
Conditions

Column:	ACE 3 C8
Dimensions:	50 x 4.6 mm
Part Number:	ACE-112-0546
Mobile Phase:	0.2 M monobasic NaH_2PO_4 pH 2.5 in H_2O/MeOH (30:70 v/v)
Flow Rate:	0.56 mL/min
Injection:	4.5 µL
Temperature:	50 °C
Detection:	UV, 254 nm

Analytes

1. Doxepin isomer
2. Doxepin isomer





Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Estradiol

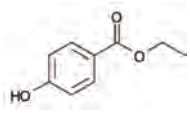
Application #AN1740

Conditions

Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	100 x 4.6 mm
Part Number:	CORE-25A-1046U
Mobile Phase:	H_2O/MeCN (45:55 v/v)
Flow Rate:	1.39 mL/min
Injection:	10.1 µL
Temperature:	Ambient (22 °C)
Detection:	UV, 205 nm

Analytes

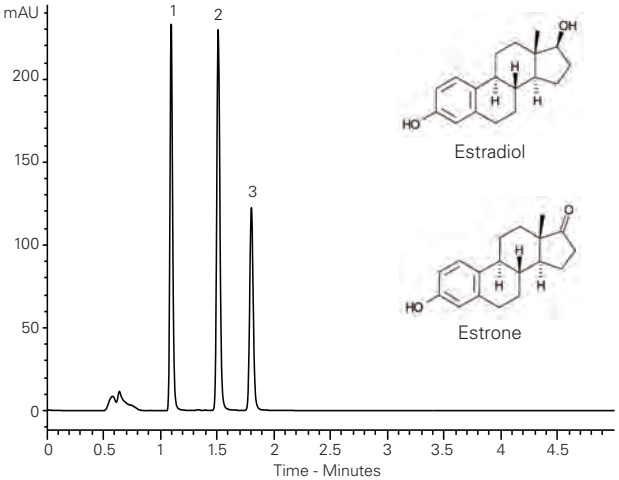
1. Ethylparaben
2. Estradiol
3. Estrone



Ethylparaben

Estradiol

Estrone



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Glimepiride

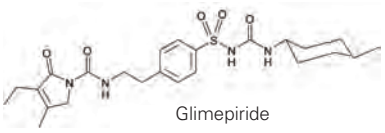
Application #AN1760

Conditions

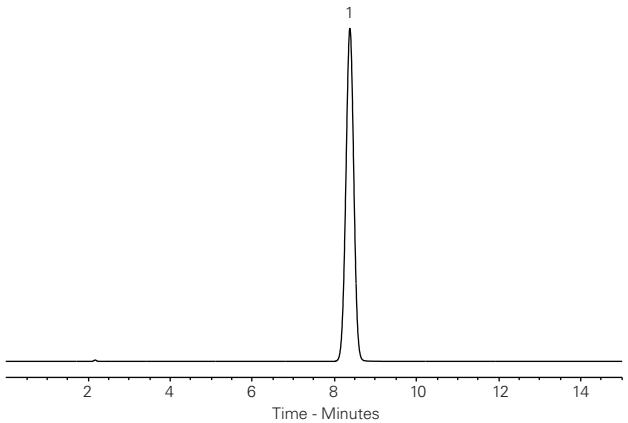
Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	8 mM monobasic sodium phosphate pH 2.4/MeCN (1:1 v/v)
Flow Rate:	1.32 mL/min
Injection:	16 µL
Temperature:	Ambient (22 °C)
Detection:	UV, 228 nm

Analyte

1. Glimepiride



Glimepiride



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Guaifenesin

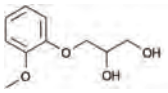
Application #AN1750

Conditions

Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 3.0 mm
Part Number:	CORE-25A-0503U
Mobile Phase:	H_2O/MeOH/Glacial acetic acid (60:40:1.5 v/v/v)
Flow Rate:	0.85 mL/min
Injection:	1.5 µL
Temperature:	Ambient (22 °C)
Detection:	UV, 276 nm

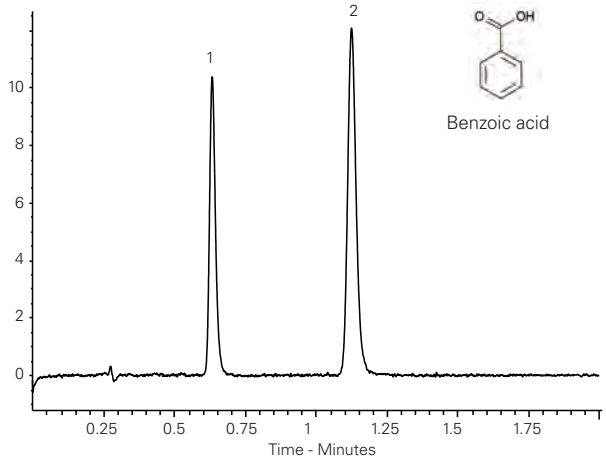
Analytes

1. Guaifenesin
2. Benzoic acid



Guaifenesin

Benzoic acid



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Hydrocortisone

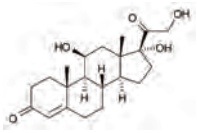
Application #AN1770

Conditions

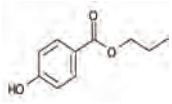
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	100 x 4.6 mm
Part Number:	CORE-25A-1046U
Mobile Phase:	H_2O/MeCN/MeOH (50:25:25 v/v/v)
Flow Rate:	1 mL/min
Injection:	5.8 µL
Temperature:	Ambient (22 °C)
Detection:	UV, 254 nm

Analytes

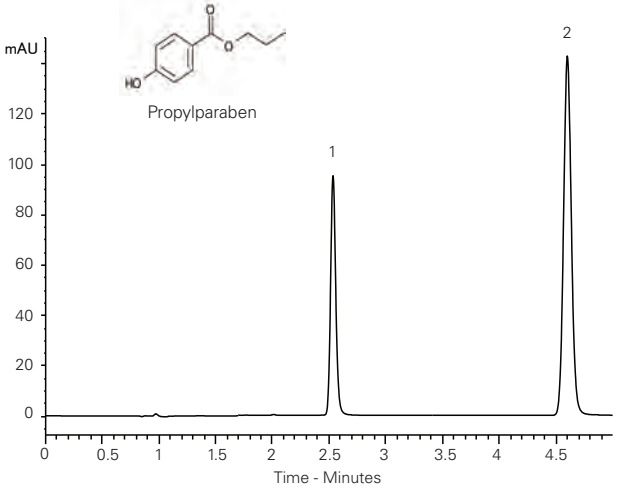
1. Hydrocortisone
2. Propylparaben



Hydrocortisone



Propylparaben



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Hydroquinone

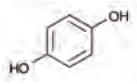
Application #AN1780

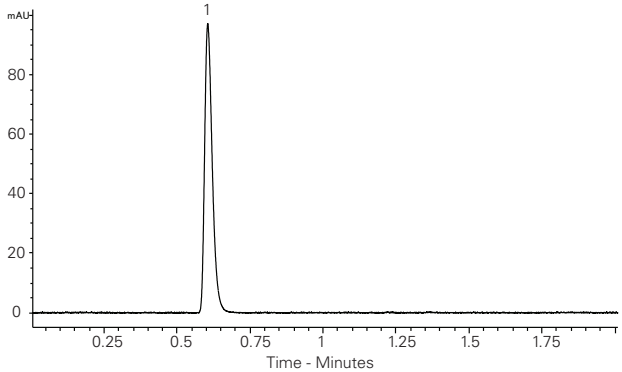
Conditions

Column:	ACE Excel 2 C18
Dimensions:	50 x 3.0 mm
Part Number:	EXL-101-0503U
Mobile Phase:	H_2O/MeOH (45:55 v/v)
Flow Rate:	0.45 mL/min
Injection:	0.9 µL
Temperature:	Ambient (22 °C)
Detection:	UV, 280 nm

Analyte

1. Hydroquinone





Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Indomethacin

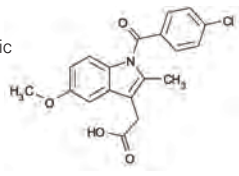
Application #AN1790

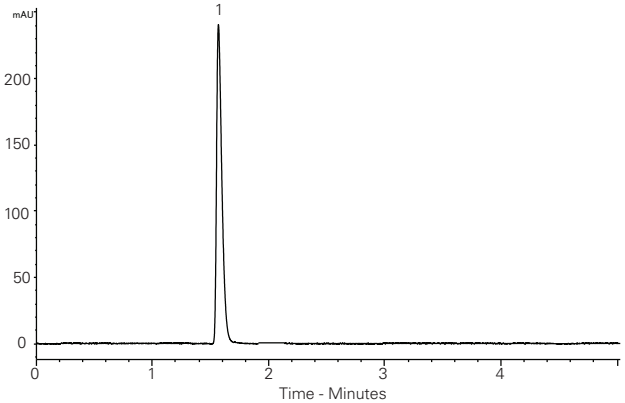
Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	0.01 M monobasic sodium phosphate and 0.01 M dibasic sodium phosphate in MeCN/H_2O (1:1 v/v)
Flow Rate:	1.32 mL/min
Injection:	13 µL
Temperature:	Ambient (22 °C)
Detection:	UV, 254 nm

Analyte

1. Indomethacin





Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Metronidazole

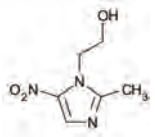
Application #AN1800

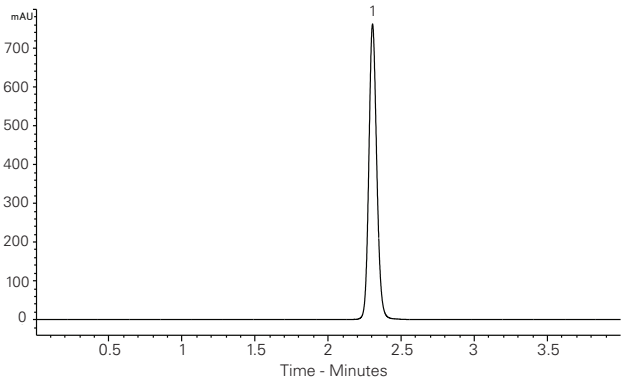
Conditions

Column: ACE 3 C8
Dimensions: 75 x 4.6 mm
Part Number: ACE-112-7546
Mobile Phase: H_2O/MeOH (4:1 v/v)
Flow Rate: 1 mL/min
Injection: 15 µL
Temperature: 30 °C
Detection: UV, 319 nm

Analyte

1. Metronidazole





Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Naproxen

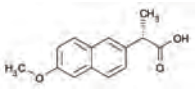
Application #AN1810

Conditions

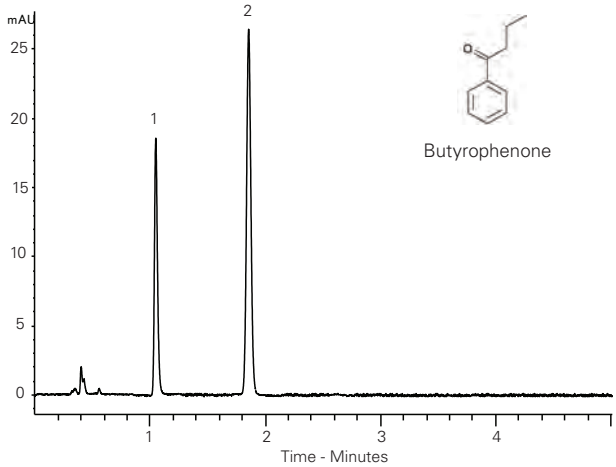
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: H_2O with glacial acetic acid (49:1)/MeCN (50:50 v/v)
Flow Rate: 0.51 mL/min
Injection: 2.8 µL
Temperature: Ambient (22 °C)
Detection: UV, 254 nm

Analytes

1. Naproxen
2. Butyrophenone



Naproxen



Butyrophenone

Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Paracetamol/Aspirin/Caffeine

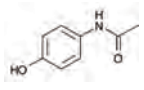
Application #AN1820

Conditions

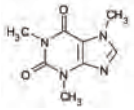
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 4.6 mm
Part Number: CORE-25A-0546
Mobile Phase: H_2O with glacial acetic acid (69:3)/MeOH (72:28 v/v)
Flow Rate: 2 mL/min
Injection: 2.5 µL
Temperature: 45 °C
Detection: UV, 275 nm

Analytes

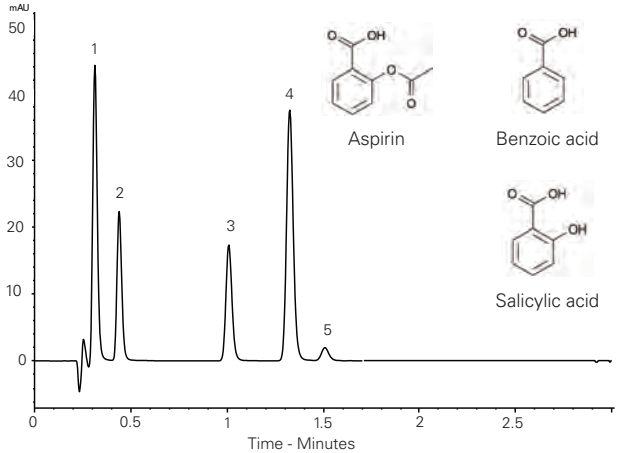
1. Paracetamol
2. Caffeine
3. Aspirin
4. Benzoic acid
5. Salicylic acid



Paracetamol



Caffeine



Aspirin

Benzoic acid

Salicylic acid

Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

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Vanilla Flavourings – Natural and Artificial

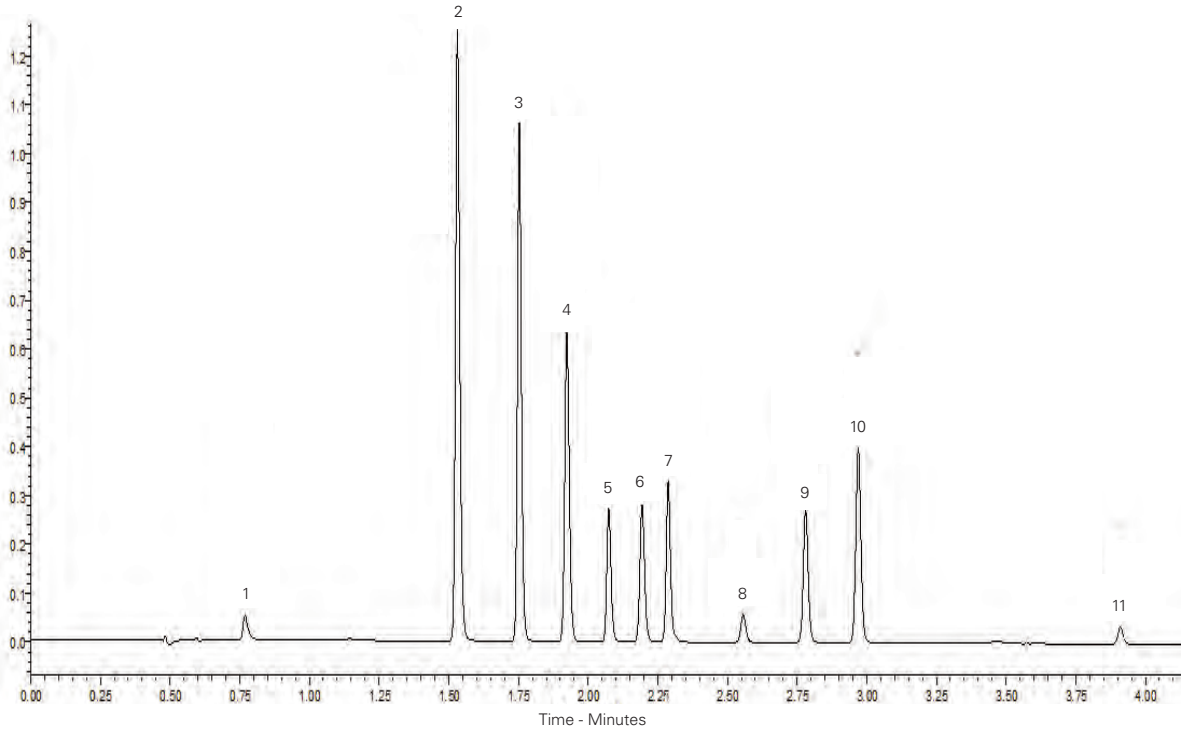
Application #AN4390

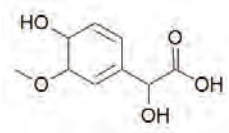
Conditions

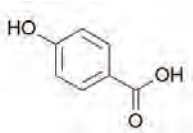
Column:	ACE UltraCore 2.5 SuperPhenylHexyl	
Dimensions:	100 x 2.1 mm	
Part Number:	CORE-25B-1002U	
Mobile Phase:	A: 10 mM ammonium formate in H_2O	
	B: MeCN	
Gradient:	**Time (mins)**	**%B**
	0.0	5
	5.5	70
Flow Rate:	0.5 mL/min	
Injection:	3 µL	
Temperature:	50 °C	
Detection:	UV, 254 nm	

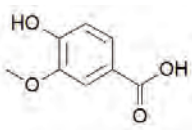
Analytes

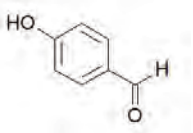
1. Vanillylmandelic acid
2. 4-Hydroxybenzoic acid
3. Vanillic acid
4. 4-Hydroxybenzaldehyde
5. p-Coumaric acid
6. Vanillin
7. Ferulic acid
8. Guaiacol
9. Ethyl vanillin
10. Coumarin
11. Eugenol

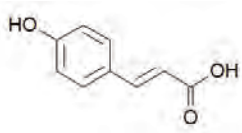


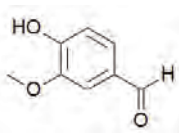

Vanillylmandelic acid

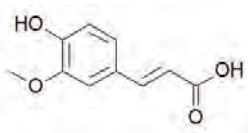

4-Hydroxybenzoic acid

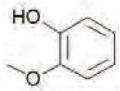

Vanillic acid

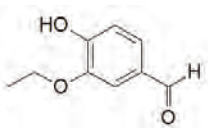

4-Hydroxybenzaldehyde

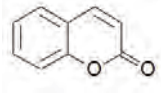

p-Coumaric acid

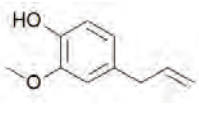

Vanillin


Ferulic acid


Guaiacol


Ethyl vanillin


Coumarin


Eugenol

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Vanillins

Application #AN1620

Conditions

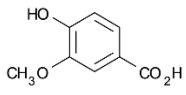
Column:	ACE Excel 3 C18-Amide
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1112-1546U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

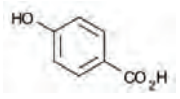
Gradient:	**Time (mins)**	**%B**
	0.0	30
	10.0	55
	10.5	55
	15.0	30
	20.0	30

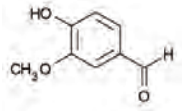
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	40 °C
Detection:	UV, 260 nm

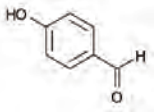
Analytes

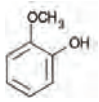
1. Vanillic acid
2. 4-Hydroxybenzoic acid
3. Vanillin
4. 4-Hydroxybenzaldehyde
5. Guaiacol
6. Ethyl Vanillin
7. Eugenol

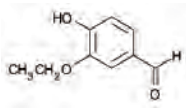

Vanillic acid


4-Hydroxybenzoic acid

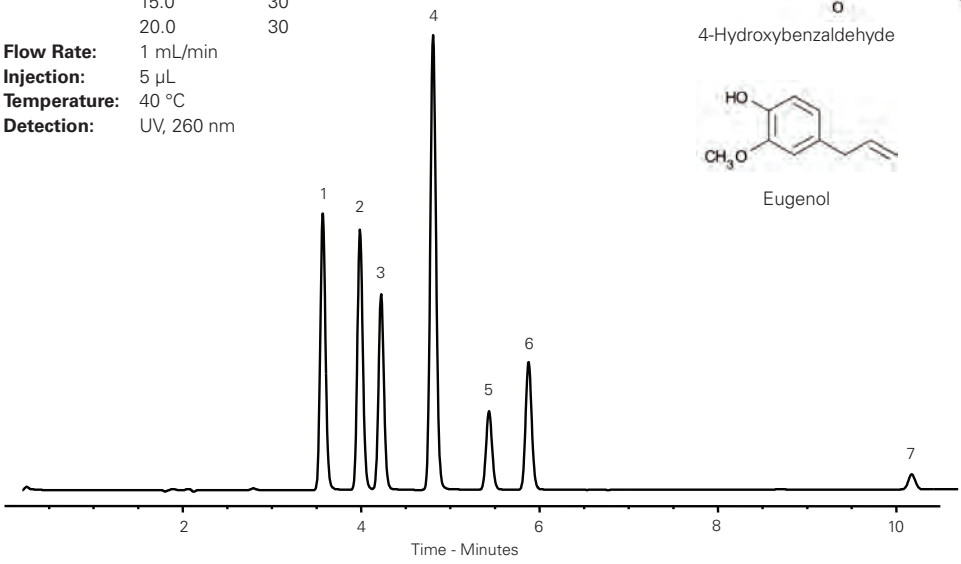

Vanillin


4-Hydroxybenzaldehyde


Guaiacol


Ethyl Vanillin

Eugenol



Vanillins – Fast Analysis

Application #AN2240

Conditions

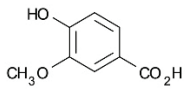
Column:	ACE Excel 1.7 C18-Amide
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1712-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

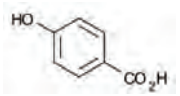
Gradient:	**Time (mins)**	**%B**
	0.0	25
	1.32	75
	1.49	75
	1.60	25

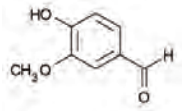
Flow Rate:	1.3 mL/min
Injection:	1 µL
Temperature:	45 °C
Detection:	UV, 260 nm

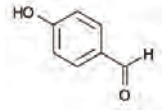
Analytes

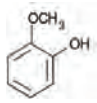
1. Vanillic acid
2. 4-Hydroxybenzoic acid
3. Vanillin
4. 4-Hydroxybenzaldehyde
5. Guaiacol
6. o-Vanillin
7. Ethyl Vanillin
8. Eugenol


Vanillic acid

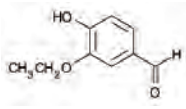

4-Hydroxybenzoic acid

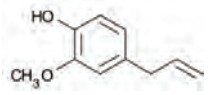

Vanillin

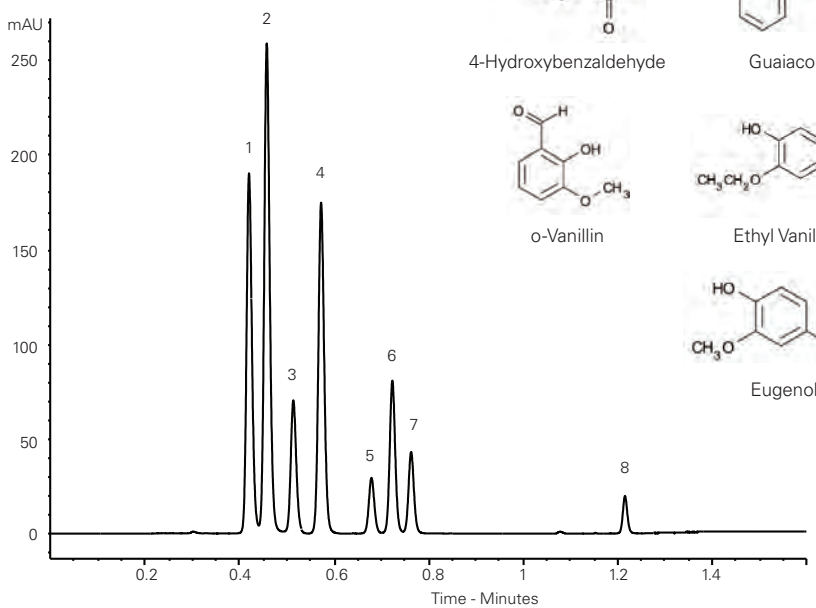

4-Hydroxybenzaldehyde


Guaiacol

o-Vanillin


Ethyl Vanillin


Eugenol



Vitamin D2/D3

Application #AN1840

Conditions

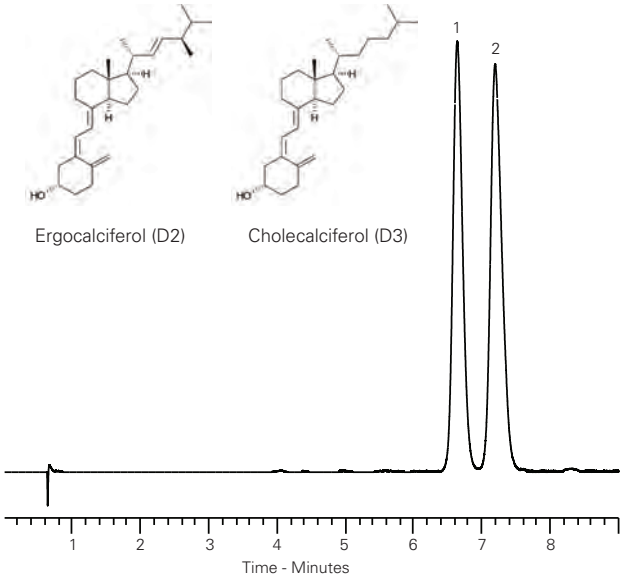
Column: ACE Excel 2 C18-Amide
Dimensions: 50 x 3.0 mm
Part Number: EXL-1012-0503U
Mobile Phase: 100% MeCN
Flow Rate: 0.43 mL/min
Injection: 2 µL
Temperature: 20 °C
Detection: UV, 265 nm

Analytes

1. Ergocalciferol (D2)
2. Cholecalciferol (D3)

Ergocalciferol (D2)

Cholecalciferol (D3)



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email: info@ace-hplc.com

25-Hydroxy Vitamin D in Serum by LC-MS/MS

Application #AN2390

Conditions

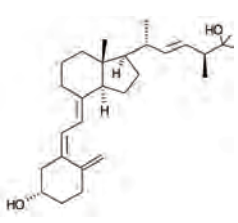
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H_2O
B: 0.1% formic acid in MeOH
Gradient:

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

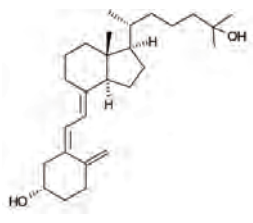
Flow Rate: 0.4 mL/min
Injection: 15 µL
Temperature: 40 °C
Detection: Quattro Premier XE triple quad MS
MRM positive ESI mode
Desolvation temperature: 450 °C
Ion source temperature: 150 °C

Analytes

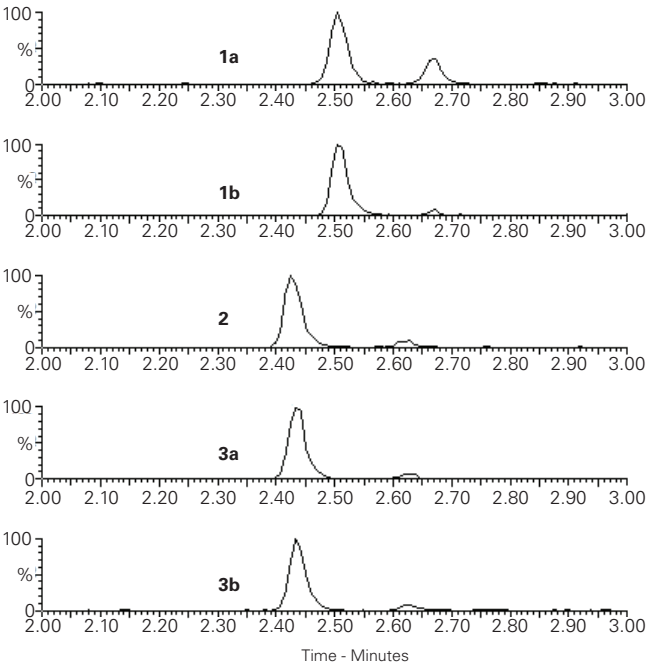
1a. 25-OH Vitamin D2
(*m/z* 395.5 → 269.5)
1b. 25-OH Vitamin D2
(*m/z* 395.5 → 119.2)
2. d6-25-OH Vitamin D3 (IS)
(*m/z* 389.6 → 263.5)
3a. 25-OH Vitamin D3
(*m/z* 383.5 → 257.5)
3b. 25-OH Vitamin D3
(*m/z* 383.5 → 107.2)



25-OH Vitamin D2



25-OH Vitamin D3



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1,25-Dihydroxyvitamins D2 and D3 in Serum by LC-MS/MS

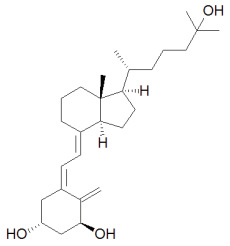
Application #AN4070

Conditions

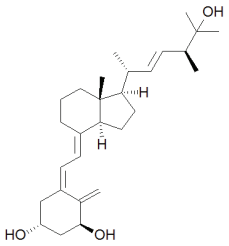
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: MeCN/H_2O (50:50 v/v) containing 30 µL methylamine per 500 mL
Flow Rate: 0.5 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: AB Sciex 5500 triple quad MS
ESI in positive ion mode
IonSpray Voltage: 5500 V
Temperature: 550 °C
Sample: 1,25 diOH vitamin D2 and 1,25 diOH vitamin D3 metabolites are extracted from serum using supported liquid extraction. Sensitivity of LC-MS/MS analysis is maximised through use of PTAD (9-phenyl-1,2,4-triazole-3,5-dione) derivatisation and complexation with methylamine.

Analytes

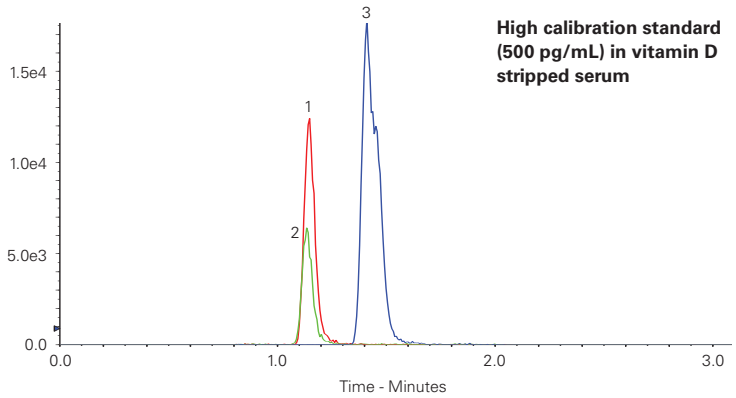
1. 1,25-diOH vitamin D3-PTAD-methylamine complex
(*m/z* 623.4 ⟶ 314.1)
2. d3-1,25-diOH vitamin D3-PTAD-methylamine complex (I.S.)
(*m/z* 626.4 ⟶ 317.1)
3. 1,25-diOH vitamin D2-PTAD-methylamine complex
(*m/z* 635.4 ⟶ 314.1)



1,25-dihydroxy vitamin D3

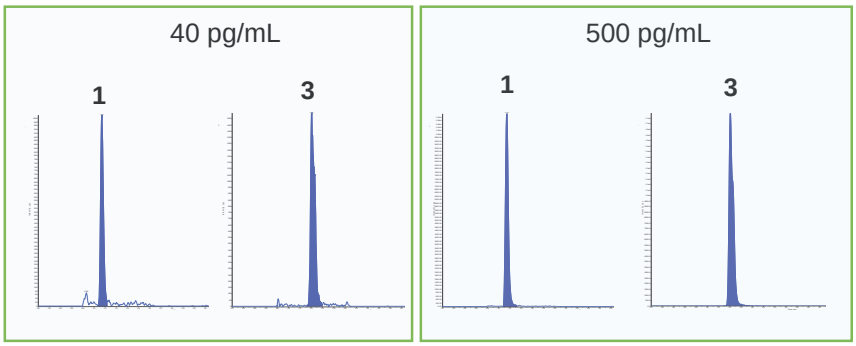


1,25-dihydroxy vitamin D2



High calibration standard (500 pg/mL) in vitamin D stripped serum

Low and high calibration standards in charcoal stripped (vitamin D free) serum, analysed as PTAD-methylamine complexes



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Vitamins – Fat Soluble

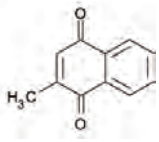
Application #AN2420

Conditions

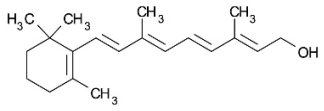
Column:	ACE Excel 3 C18-Amide
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1112-1546U
Mobile Phase:	MeOH/MeCN (90:10 v/v)
Flow Rate:	1 mL/min
Temperature:	20 °C
Detection:	UV, 280 nm

Analytes

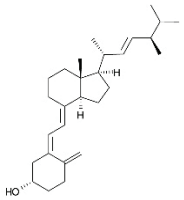
1. Menadione (Vitamin K3)
2. Retinol (Vitamin A)
3. Vitamin A acetate
4. Ergocalciferol (Vitamin D2)
5. Cholecalciferol (Vitamin D3)
6. Vitamin E acetate
7. α-Tocopherol (Vitamin E)
8. Vitamin K1



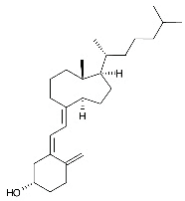
Menadione (Vitamin K3)



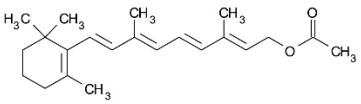
Retinol (Vitamin A)



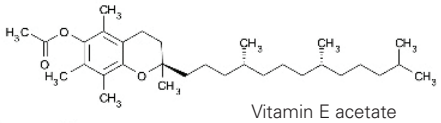
Ergocalciferol (Vitamin D2)



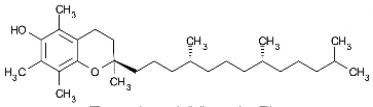
Cholecalciferol (Vitamin D3)



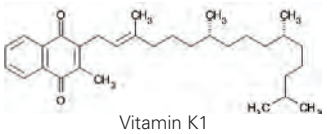
Vitamin A acetate



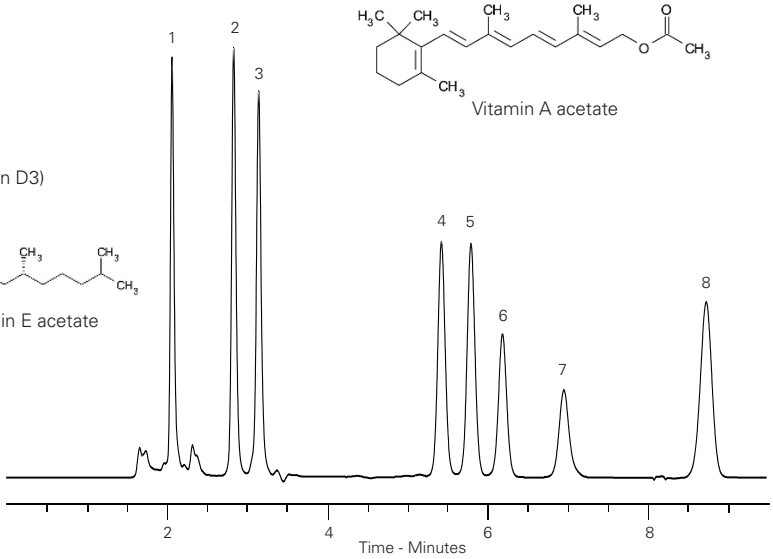
Vitamin E acetate



α-Tocopherol (Vitamin E)



Vitamin K1



Vitamins – Water Soluble (Gradient I)

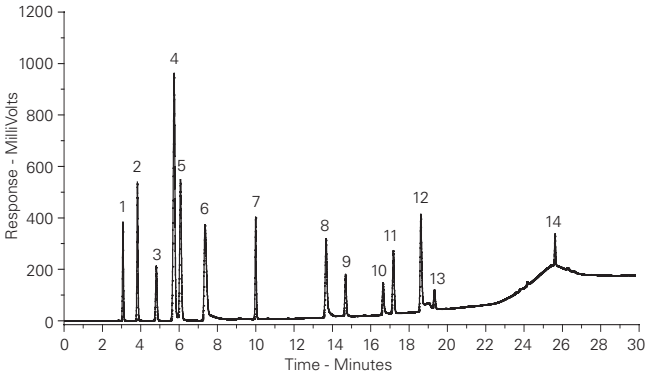
Application #AN2940

Conditions

Column:	ACE 5 C8	
Dimensions:	250 x 4.6 mm	
Part Number:	ACE-122-2546	
Mobile Phase:	A: 50 mM KH_2PO_4 pH 2.5 in H_2O	
	B: MeOH	
Gradient:	**Time (mins)**	**%B**
	0.0	0
	3.0	0
	16.5	45
	19.5	80
Flow Rate:	1 mL/min	
Temperature:	Ambient	
Detection:	UV, 205 nm	

Analytes

1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Niacinamide (Vitamin B3)
5. Nicotinic acid
6. Pyridoxal
7. Pyridoxine
8. p-Aminobenzoic acid
9. Pantothenic acid (Vitamin B5)
10. Folic acid (Vitamin B9)
11. Cyanocobalamin (Vitamin B12)
12. Riboflavin (Vitamin B2)
13. d-Biotin (Vitamin B7)
14. Thioctic acid



Vitamins – Water Soluble (Gradient II)

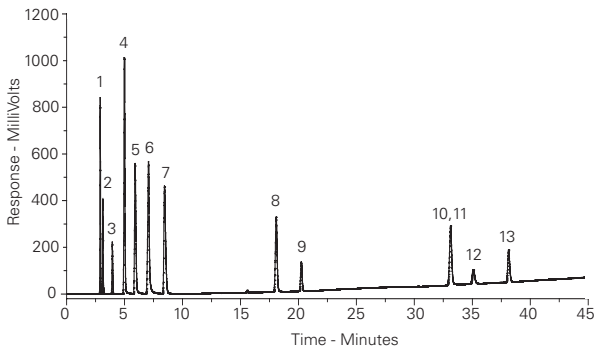
Application #AN2930

Conditions

Column:	ACE 5 C18	
Dimensions:	250 x 4.6 mm	
Part Number:	ACE-121-2546	
Mobile Phase:	A: 50 mM KH_2PO_4 pH 3.0 in H_2O	
	B: MeOH	
Gradient:	**Time (mins)**	**%B**
	0	3
	5	3
	45	45
	50	80
Flow Rate:	1 mL/min	
Temperature:	Ambient	
Detection:	UV, 205 nm	

Analytes

1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Nicotinic acid
5. Pyridoxal
6. Impurity
7. Pyridoxine
8. p-Aminobenzoic acid
9. Pantothenic acid (Vitamin B5)
10. Folic acid (Vitamin B9)
11. Cyanocobalamin (Vitamin B12)
12. d-Biotin (Vitamin B7)
13. Riboflavin (Vitamin B2)



Vitamins – Water Soluble (Gradient III)

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)

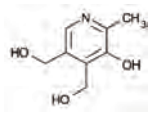
Gradient:

Time (mins)	%B
0	20
15	70

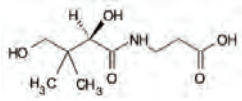
Flow Rate: 1.5 mL/min
Injection: 1 µL
Temperature: 40 °C
Detection: UV, 205 nm

Analytes

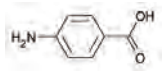
1. Pyridoxine (Vitamin B6)
2. Pantothenic acid (Vitamin B5)
3. p-Aminobenzoic acid
4. Folic acid (Vitamin B9/ Vitamin M)
5. D-Biotin (Vitamin B7/ Vitamin H)
6. Cyanocobalamin (Vitamin B12)
7. Riboflavin (Vitamin B2)



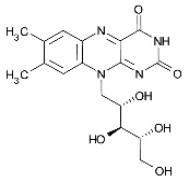
Pyridoxine (Vitamin B6)



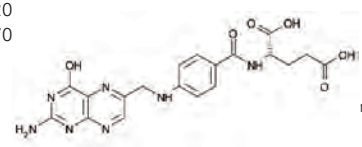
Pantothenic acid (Vitamin B5)



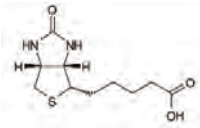
p-Aminobenzoic acid



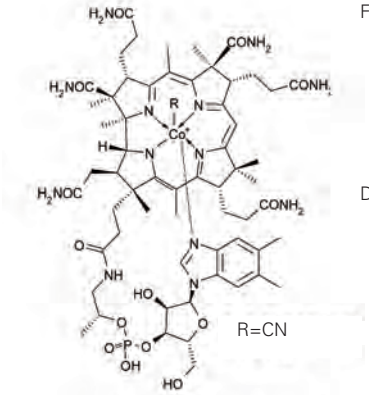
Riboflavin (Vitamin B2)



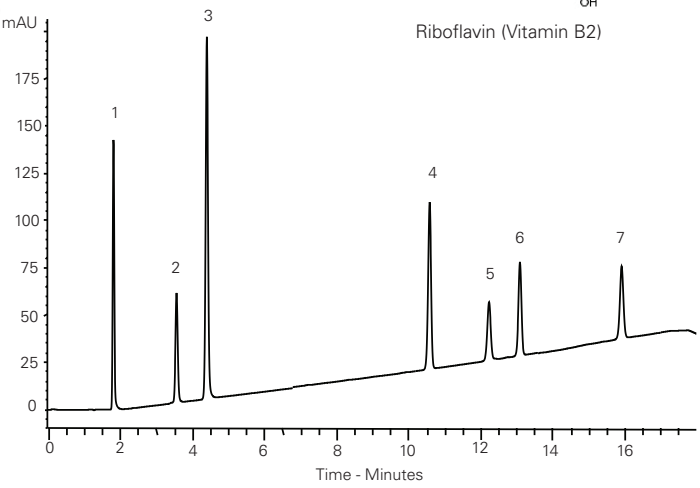
Folic acid (Vitamin B9/ Vitamin M)



D-Biotin (Vitamin B7/ Vitamin H)



Cyanocobalamin (Vitamin B12)



Vitamins – Water Soluble (Gradient IV)

Application #AN1880

Conditions

Column: ACE Ultracore 2.5 SuperPhenylHexyl
Dimensions: 50 x 2.1 mm
Part Number: CORE-25B-0502U
Mobile Phase: A: 20 mM KH_2PO_4, pH 2.7
B: 20 mM KH_2PO_4, pH 2.7 in MeOH/H_2O (50:50 v/v)

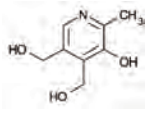
Gradient:

Time (mins)	%B
0.00	20
1.50	60
3.00	70
3.75	70
4.50	20
9.00	20

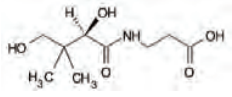
Flow Rate: 0.4 mL/min
Injection: 1 µL
Temperature: 40 °C
Detection: UV, 205 and 254 nm

Analytes

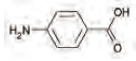
1. Pyridoxine
2. Pantothenic acid
3. p-Aminobenzoic acid
4. Folic acid
5. D-Biotin
6. Cyanocobalamin
7. Riboflavin



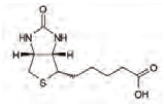
Pyridoxine



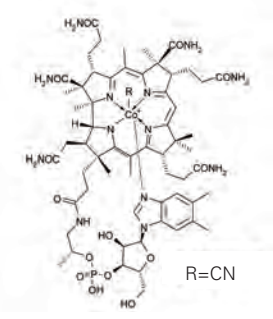
Pantothenic acid



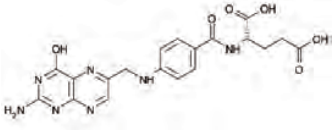
p-Aminobenzoic acid



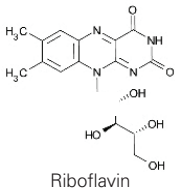
D-Biotin



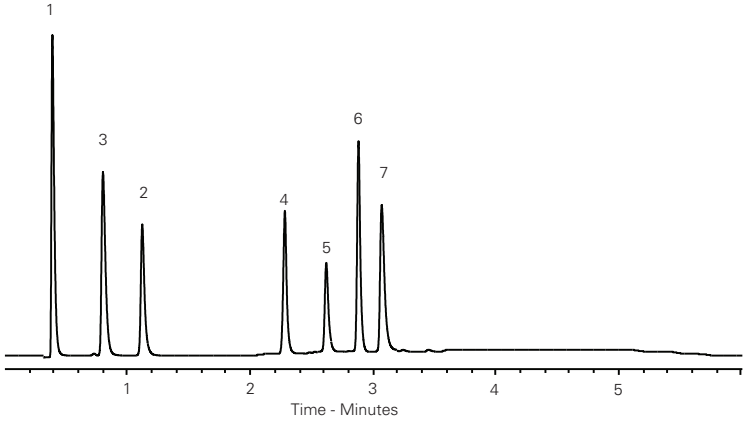
Cyanocobalamin



Folic acid



Riboflavin



Vitamins – Water Soluble (Isocratic I)

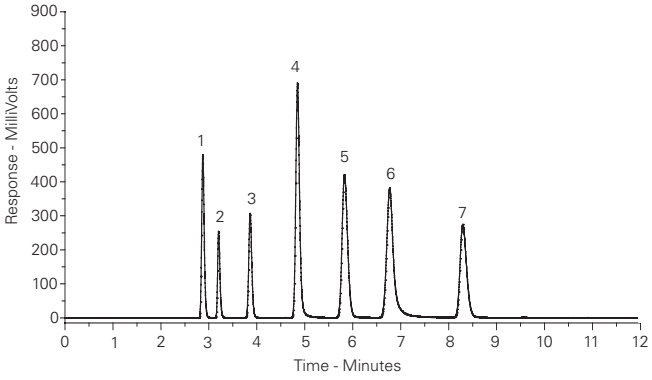
Application #AN2990

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	50 mM KH_2PO_4 pH 3.0 in H_2O/MeOH (97:3 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 205 nm

Analytes

1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Nicotinic acid
5. Pyridoxal
6. Impurity
7. Pyridoxine



Vitamins – Water Soluble (Isocratic II)

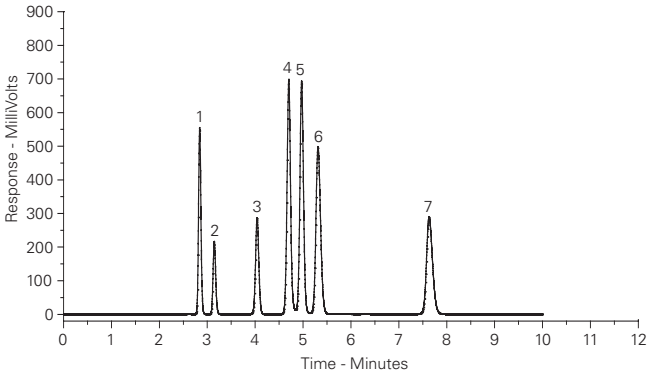
Application #AN2980

Conditions

Column:	ACE 5 C8
Dimensions:	250 x 4.6 mm
Part Number:	ACE-122-2546
Mobile Phase:	50 mM KH_2PO_4 pH 2.5 in H_2O/MeOH (97:3 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 205 nm

Analytes

1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Niacinamide (Vitamin B3)
5. Pyridoxal
6. Nicotinic acid
7. Pyridoxine



Vitamins in Fruit Juice by Fast LC-MS

Application #AN2610

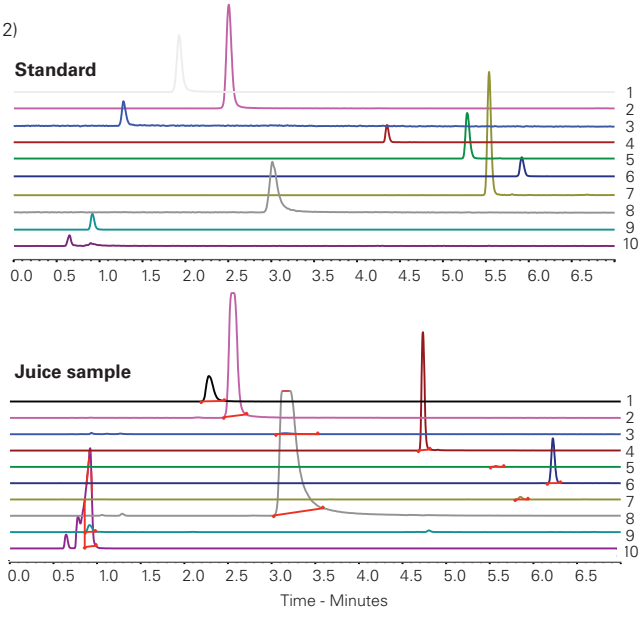
Conditions

Column:	ACE Excel 3 C18-PFP	
Dimensions:	100 x 2.1 mm	
Part Number:	EXL-1110-1002U	
Mobile Phase:	A: 15 mM formic acid, adjusted to pH 3.8 with ammonia solution B: MeOH	
Gradient:	**Time (mins)**	**%B**
	0.00	1
	1.00	1
	3.00	8
	3.10	25
	6.00	50
	6.50	50
	6.51	1
	9.00	1
Flow Rate:	0.4 mL/min	
Temperature:	30 °C	
Detection:	LCMS-8040 triple quad MS ESI positive mode (ESI negative for ascorbic and citric acid) DL temperature: 250 °C Heat block temperature: 400 °C	

Analytes

1. Thiamine (Vitamin B1)
   (*m/z* 266.10 → 122.15)
2. Pyridoxine (Vitamin B6)
   (*m/z* 170.20 → 152.15)
3. Nicotinic acid (Vitamin B3)
   (*m/z* 124.00 → 78.00)
4. Pantothenic acid (Vitamin B5)
   (*m/z* 220.30 → 90.05)
5. Cyanocobalamin (Vitamin B12)
   (*m/z* 678.50 → 147.05)
6. Riboflavin (Vitamin B2)
   (*m/z* 377.20 → 243.10)
7. Biotin (Vitamin B7)
   (*m/z* 245.10 → 227.05)
8. Nicotinamide (Vitamin B3)
   (*m/z* 123.20 → 80.05)
9. Ascorbic acid (Vitamin C)
   (*m/z* 175.10 → 114.80)
10. Citric acid
    (*m/z* 191.10 → 87.15)





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Vitamins in Green Vegetables by LC-MS/MS - Water Soluble

Application #AN1860

Conditions

Column: ACE 3 C4-300
Dimensions: 150 x 2.1 mm
Part Number: ACE-213-1502
Mobile Phase: A: 10 mM ammonium acetate pH 4.5 in H_2O
B: 0.1% acetic acid in MeOH
C: 0.3% acetic acid in MeOH

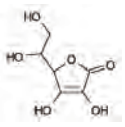
Gradient:

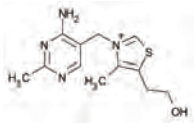
Time (mins)	%A	%B	%C
0	90	10	0
3	90	10	0
4	50	0	50
7	50	0	50
10	0	100	0

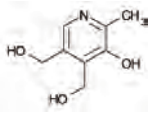
Flow Rate: 0.2 mL/min
Injection: 10 µL
Temperature: 20 °C
Detection: TSQ triple quad MS; SRM mode
-ESI for vitamin C
+ESI for vitamin B

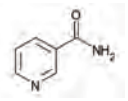
Analytes

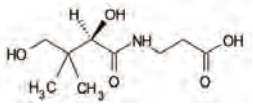
1. Ascorbic acid
2. Thiamine
3. Pyridoxine
4. Nicotinamide
5. Pantothenic acid
6. Hippuric acid (IS)
7. Folic acid
8. Riboflavin

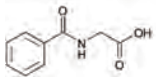

Ascorbic acid

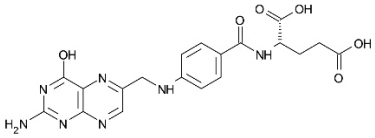

Thiamine

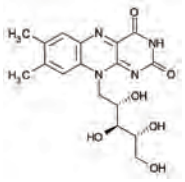

Pyridoxine

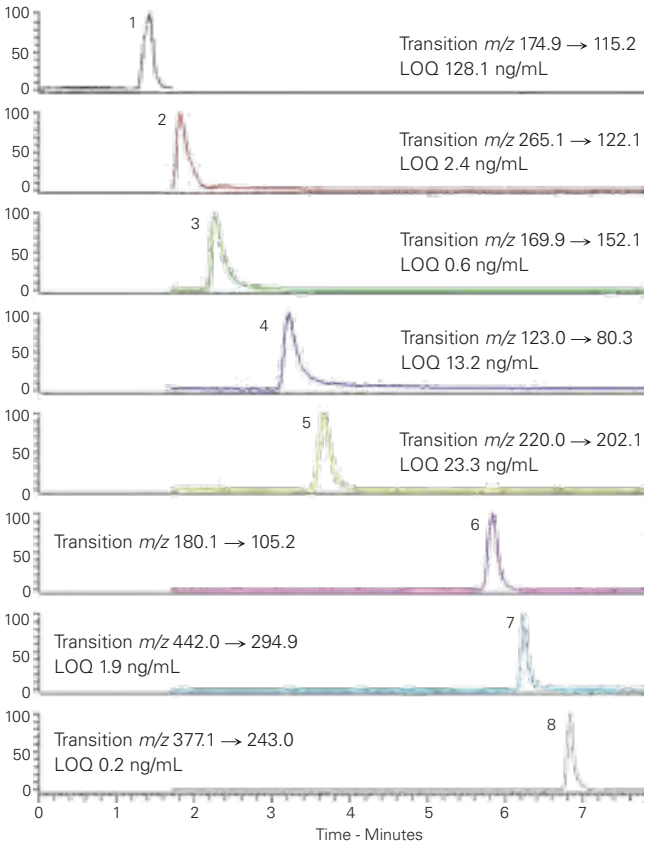

Nicotinamide


Pantothenic acid


Hippuric acid (IS)


Folic acid


Riboflavin





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Vitamins and Polar Molecules - Water Soluble

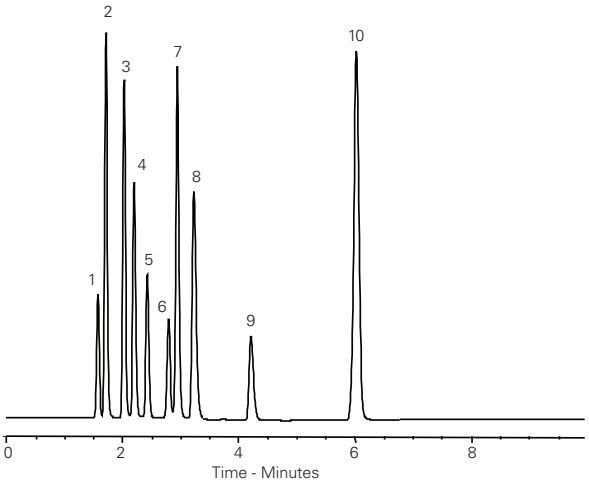
Application #AN1850

Conditions

Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	0.1 % phosphoric acid in H_2O/MeOH (96.5:3.5 v/v)
Flow Rate:	1 mL/min
Injection:	2 µL
Temperature:	22 °C
Detection:	UV, 260 nm

Analytes

1. Pyridoxamine (Vitamin B6)
2. Thiamine (Vitamin B1)
3. Isonicotinamide
4. Nicotinamide
5. L-Ascorbic acid (Vitamin C)
6. Orotic Acid
7. Hypoxanthine
8. Pyridoxal (Vitamin B6)
9. Pyridoxine (Vitamin B6)
10. p-Aminobenzoic acid



Water Soluble Artificial Colours

Application #AN3010

Conditions

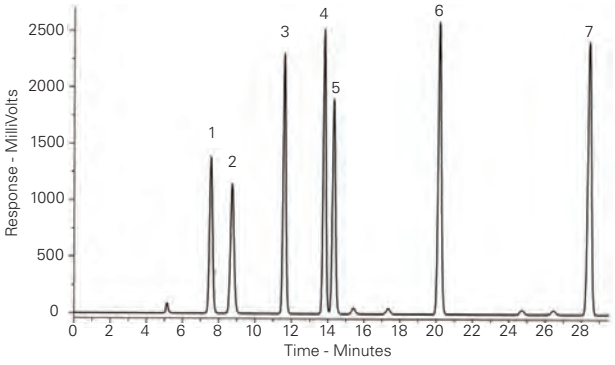
Column:	ACE 3 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-111-1046
Mobile Phase:	A: 3 mM tetrabutylammonium bromide and 5 mM KH_2PO_4 in H_2O B: 5 mM tetrabutylammonium bromide in MeOH

Gradient:	**Time (mins)**	**%B**
	0	45
	20	70
	30	45
	40	45

Flow Rate:	0.8 mL/min
Injection:	10 µL
Temperature:	Ambient
Detection:	UV-Vis, 420 nm, 520 nm and 600 nm

Analytes

1. Amaranth
2. Sunset Yellow
3. Allura Red
4. Red 2G
5. Ponceau 4R
6. Carmoisine
7. Erythrosine



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Whey Proteins from Whole Milk

Application #AN3000

Conditions

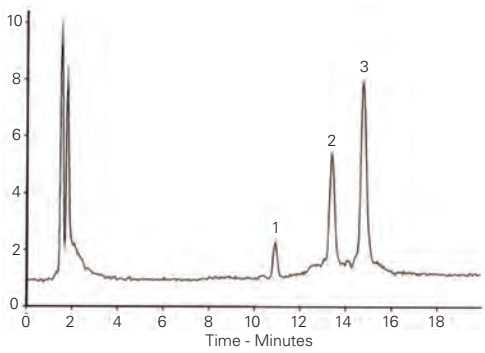
Column:	ACE 3 C4-300
Dimensions:	150 x 2.1 mm
Part Number:	ACE-213-1502
Mobile Phase:	A: 0.5% formic acid in H_2O B: 0.5% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0	35
	16	43
	17	80
	20	80
	21	35
	31	35

Flow Rate:	0.4 mL/min
Injection:	10 µL
Temperature:	40 °C
Detection:	ESI-MS (+ve)

Analytes

1. α-Lactalbumin
2. β-Lactoglobulin B
3. β-Lactoglobulin A



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Wine Acid Analysis

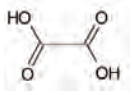
Application #AN1890

Conditions

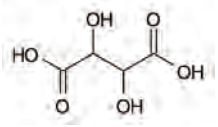
Column:	ACE Excel 3 C18-Amide
Dimensions:	250 x 2.1 mm
Part Number:	EXL-1112-2502U
Mobile Phase:	40 mM ammonium phosphate pH 2.5 in H_2O
Flow Rate:	0.21 mL/min
Injection:	5 µL
Temperature:	25 °C
Detection:	UV, 214 nm

Analytes

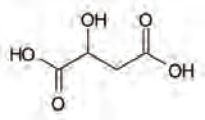
1. Oxalic acid
2. Tartaric acid
3. Malic acid
4. Lactic acid
5. Ascorbic acid
6. Citric acid



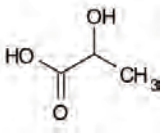
Oxalic acid



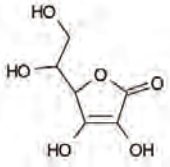
Tartaric acid



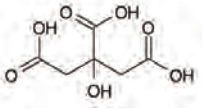
Malic acid



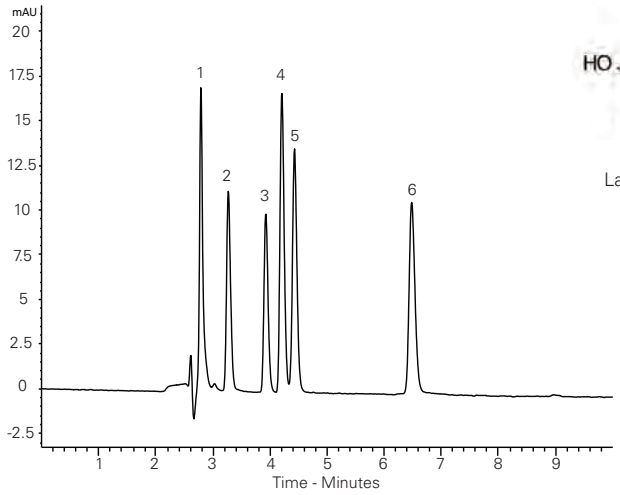
Lactic acid



Ascorbic acid



Citric acid





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