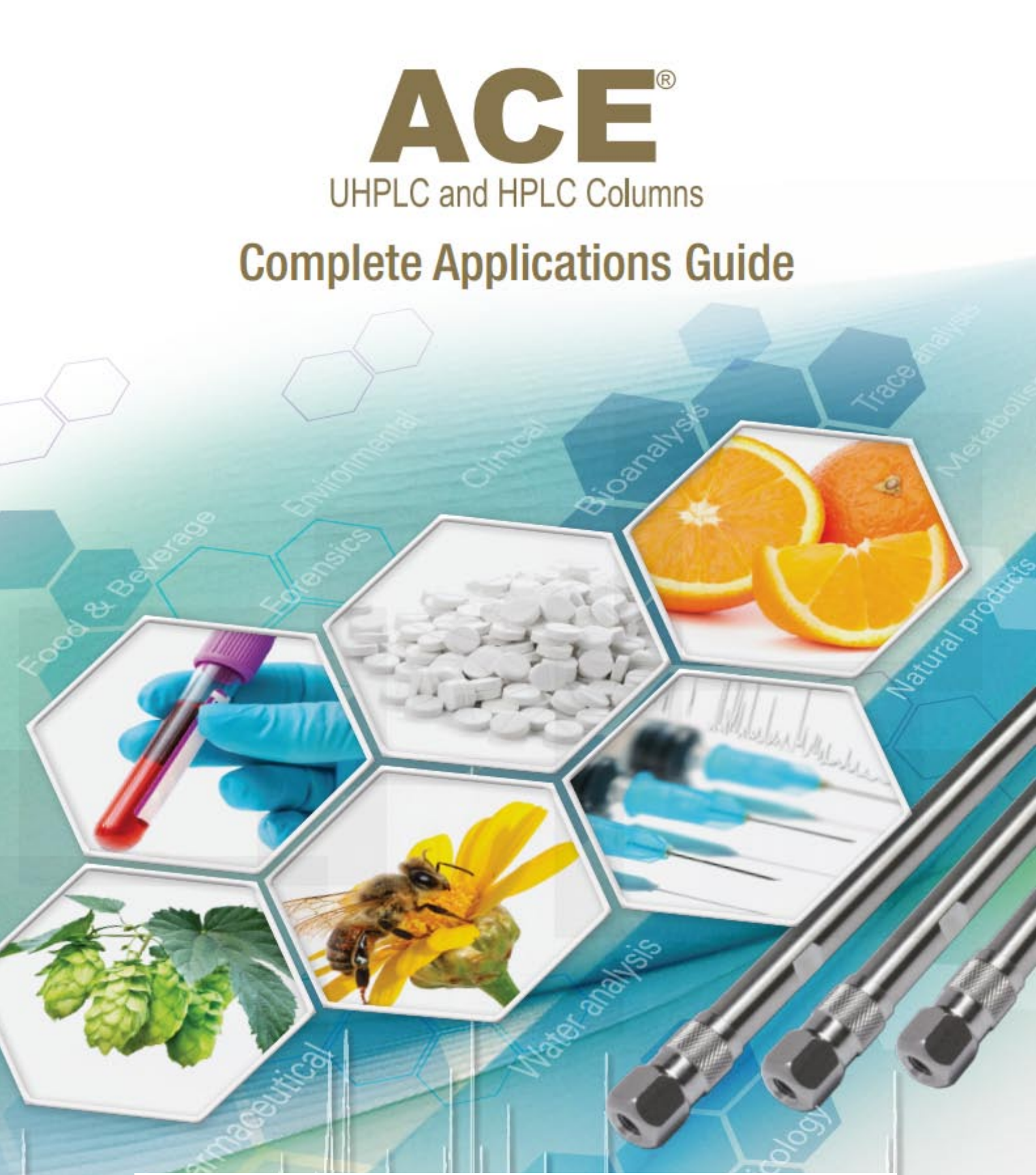
ACE®

UHPLC and HPLC Columns

Complete Applications Guide



MZ ANALYSENTECHNIK

AUTHORIZED DISTRIBUTOR

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

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

e-mail: info@mz-at.de, www.mz-at.de

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.

Contents

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.

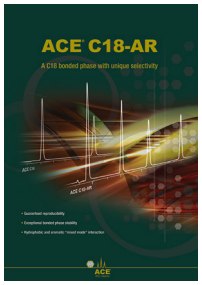
Recommended Applications

- 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

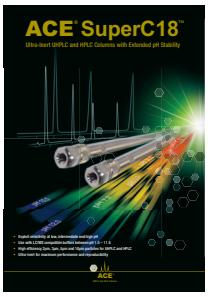
- Mixtures of very polar, polar and non-polar analytes
- Analytes with double and triple bonds
- Analytes differing in hydrophobicity
- Suitable for NP and RP separations
- Fully wettable - 100% aqueous buffer compatible
- Applications where a typical C18 column does not provide adequate separation
-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

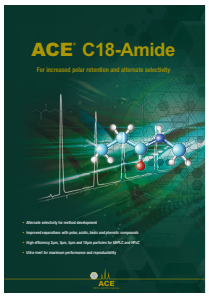
*Encapsulated Bonding Technology

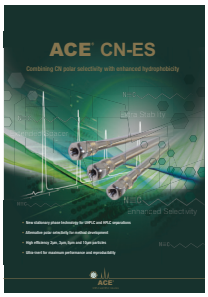
Additional information

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
HiPerSolv CHROMANORM
Acetonitrile
LiChrosolv
Reag. Ph Eur
Acetonitrile
gradient grade for liquid chromatography
Acetonitril
Acetonitrile
Acetonitrilo
MERCK
VWR
HITACHI

Application Index

	Page Number	Clinical, Forensics & Bioanalysis	Environmental	Food & Beverage	Pharmaceutical	LC-MS	Other
Acylcarnitines by LC-MS/MS	21	✓				✓	
Additives and Intense Sweeteners	22			✓			
Alcohol Biomarkers by UHPLC-MS/MS	22	✓				✓	
Alternative Selectivity Provided by ACE CN-ES	23						✓
Amino Acid Enantiomer Separation of Seawater Samples	24			✓		✓	
Amino Acid Profile of Edible Stink Bugs by LC-MS	23		✓	✓		✓	
Amino Acids and Biogenic Amines in Wine and Beer	25			✓			
Amino Acids Derivatised with Dabsyl Chloride	27	✓					
Amino Acids in Extracellular Matrix	26	✓				✓	
Amino Acids in Peas *(Pisum Sativum)* by HPLC-HRAM-MS	28	✓		✓		✓	
Aminoglycosides in Eggs	29	✓		✓		✓	
Amoxicillin Metabolites in Human Liver Microsomes	30	✓				✓	
Amphetamines from Drugs of Abuse Screen (#AN2190)	31	✓			✓	✓	
Amphetamines in Urine by LC-MS/MS	31	✓			✓	✓	
Anabolic Steroids from Horse Urine by LC-MS/MS	32	✓			✓	✓	
Analgesic Rapid Separation	32				✓		
Analgesics / Cough & Cold Medicine Ingredients	33				✓		
Analgesic Separation	33				✓		
Andrographis Paniculata Fingerprint Profile by RRLC-TOF-MS	34				✓	✓	
Angiotensin II Receptor Antagonists by LC-UV	34	✓			✓		
Angiotensin Peptides	35	✓					
Annatto	35			✓			
Anthocyanins from *Sambucus Nigra* (Elderberry)	36			✓			
Antihistamines	36	✓			✓		
Antihistamines and Expectorants	36				✓		
Antihistamines and Expectorants – Mobile Phase Effects	37				✓		
Antihistamines – Fast Analysis	37				✓		
Antimycins from Marine Sponge *Streptomyces* sp. by LC-HRMS	38	✓			✓	✓	
Antiretrovirals in Human Mononuclear Cell Extracts by LC-MS/MS	39	✓			✓	✓	
Anti-Ulcer Drugs in Basic Mobile Phase Conditions	37	✓			✓		
Appetite Suppressants by LC-MS	39	✓		✓	✓	✓	
Aromatic Nitrobenzenes	39						✓
Arsenolipids from Edible Seaweed *(Alaria Esculenta)* by LC-ICP-MS and LC-ESI-MS	40	✓	✓	✓		✓	
Artemisinin	41				✓		
Artificial Food Colours	41			✓			
Artificial Sweeteners Global Method	41			✓			
Artificial Sweeteners (Stevia Glycosides)	42			✓			
Aspirin and Related Substances (I)	42				✓		
Aspirin and Related Substances (II)	43				✓		
Avenacins	43			✓			
β-Antagonists and Diuretics	43	✓			✓		
β-Blockers	45	✓			✓		

Application Index

	Page Number	Clinical, Forensics & Bioanalysis	Environmental	Food & Beverage	Pharmaceutical	LC-MS	Other
β-Blockers at High pH	44	✓			✓		
β-Blockers at High pH – Fast Analysis	44	✓			✓		
β-Blockers by LC-MS/MS	45	✓			✓	✓	
Benzo(a)pyrene-7,8-quinone Derived Deoxynucleotide DNA Adducts	45	✓					
Benzodiazepines from Drugs of Abuse Screen (#AN2190)	46	✓			✓	✓	
Biomarker Analysis for Gaucher Disease by LC-MS/MS	46	✓				✓	
Biomarker for Niemann-Pick Type C1 Disease by LC-MS/MS	47	✓				✓	
Biomarker Profiling	47	✓					
Brazilian Red Propolis Biomarkers by LC-FTMS	48	✓		✓		✓	
Brompheniramine Maleate	48				✓		
BSA Tryptic Digest Profiling	48	✓		✓			
Bufotenine Extract from *Rhinella Jimi* Toad Skin Secretions	49	✓				✓	
Caffeine and Metabolites	50	✓		✓			
Caffeoylquinic and Dicaffeoylquinic Acids	50			✓			
Cannabinoids in Rat Plasma	52	✓			✓		
Cannabinoids (Synthetic) by LC-MS/MS	51	✓				✓	
Carglumic Acid in Human Plasma by LC-MS/MS	52	✓			✓	✓	
Catechins	53	✓					
Catecholamine Analysis (I)	53	✓					
Catecholamine Analysis (II)	53	✓					
Catecholamines and Metanephrines Separation (Gradient)	54	✓					
Catecholamines and Metanephrines Separation (Isocratic)	55	✓					
Catecholamines and their Metabolites in Urine by LC-MS/MS	54	✓				✓	
Catecholamines by LC-MS/MS	53	✓				✓	
Catecholamines from Plasma	55	✓					
Catecholamines from Urine	55	✓					
Catechols Mixture Separations (I) and (II)	56	✓					
Cathinone Psychoactive Substances by LC-UV and LC-Amperometry	56	✓			✓		
Cefquinome by LC-MS	57				✓	✓	
Chloramphenicol in Milk by LC-MS/MS	57	✓		✓	✓	✓	
Chocolate Analysis	58			✓			
Ciprofibrate from Human Plasma by LC-MS/MS	57	✓			✓	✓	
Clenbuterol in Equine Plasma by LC-MS/MS	58	✓			✓	✓	
Clonidine Hydrochloride Oral Solution Containing Preservatives	59	✓			✓		
Clopidogrel and Photodegradation Products	59	✓			✓		
Coffee Metabolite Profiling by LC-MS	60			✓		✓	
Cold Medicine Analytes (I) and (II)	61				✓		
Corticosteroids by LC-MS/MS	61	✓			✓	✓	
Cortisol in Urine by LC-MS/MS	62	✓			✓	✓	
Cyclodextrin-Encapsulated Flavour Compounds in Beer	62			✓			
Cyclosporin Mixture	62	✓					
Cytarabine Analogues by Ion-Pairing LC-MS/MS	63	✓			✓	✓	
Cytotoxic Agents by UHPLC-MS/MS	63	✓			✓	✓	

Application Index

	Page Number	Clinical, Forensics & Bioanalysis	Environmental	Food & Beverage	Pharmaceutical	LC-MS	Other
Decarboxylation of Sirohaem by Sirohaem Decarboxylase	64	✓					
Defensins (Human) in Saliva Matrix	64	✓		✓		✓	
Dermorphin in Equine Urine by LC-MS/MS	65	✓			✓	✓	
Didanosine	65				✓		
Diuretics	66	✓			✓		
Diuretics (Isocratic)	65	✓			✓		
^{68}Ga-DOTATATE PET Tracer by LC-MS/MS	67	✓			✓	✓	
^{68}Ga-DOTATATE QC Analysis by Radiometric Detection	66	✓			✓		
DOTATATE and Octreotide	66	✓					
Drugs of Abuse Screen (250 Analytes) in Urine by LC-MS/MS	69	✓			✓	✓	
Drugs of Abuse Screen by UHPLC-MS/MS	68	✓			✓	✓	
Echinacea	72			✓			
Entacapone	73				✓		
Epanolol	73				✓		
Epinastine	73				✓		
Ethanol Extract from Seed Cover *(Acacia Farnesiana)*	73			✓			
Ethyl Glucuronide in Water by LC-MS/MS	74			✓		✓	
Exploiting Selectivity by Adjusting pH	74						✓
Explosive Analytes (I)	75						✓
Explosive Analytes (II)	75						✓
Fingerprinting of *Cuscuta Chinensis* Flavonoids	75			✓			
Flavone and Dibucaine	76			✓			
Flavonoids	76			✓			
Flurbiprofen and Related Substances	76				✓		
Formoterol from Human Plasma by LC-MS/MS	76	✓			✓	✓	
Galanthamine	77				✓		
Gamma Hydroxybutyric Acid (GHB) and Gamma Butyrolactone (GBL) Separation	77	✓					
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		✓	✓		✓	

Application Index

	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

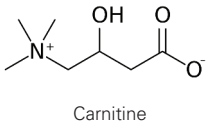
Gradient:

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

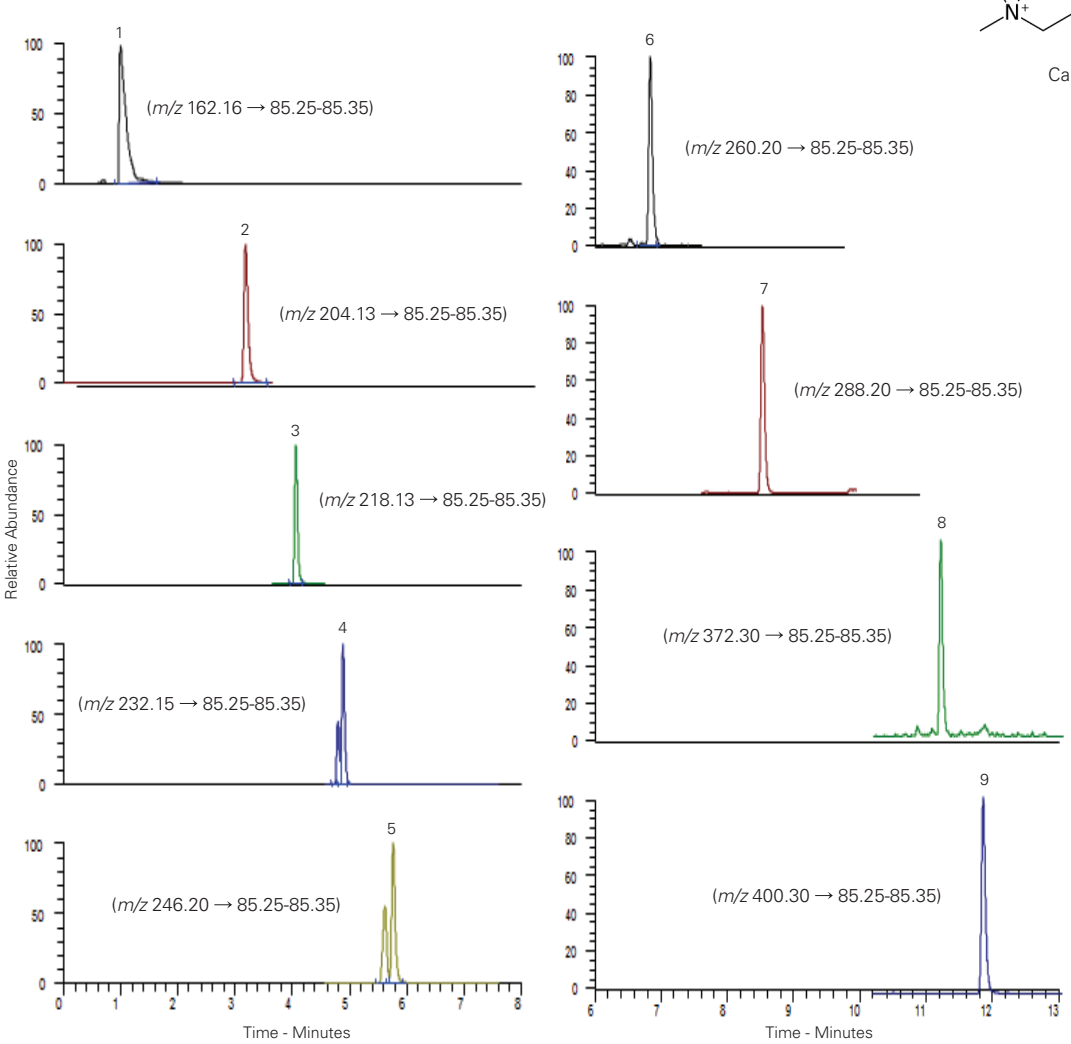
Flow Rate: 0.3 mL/min
Sample: Dried serum extract
Detection: Positive mode ESI

Analytes

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



Carnitine



Reproduced with permission of Department of Pathology, Immunology and Laboratory Medicine, University of Florida, USA

Additives and Intense Sweeteners

Application #AN2950

Conditions

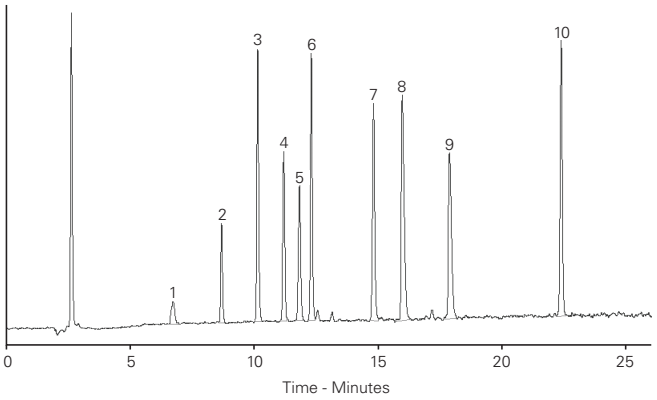
Column:	ACE 5 C18
Dimensions:	250 x 4.0 mm
Part Number:	ACE-121-2504
Mobile Phase:	A: H_2O
	B: MeCN
	C: 1% TFA in H_20

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



Reproduced with permission of Durham County Council, UK

Send us your application and receive a free ACE column

Your proven method will enable your chromatography colleagues to benefit and if we select your application for future publications we'll send you a FREE ACE analytical column of your choice.

To submit your application: email us at info@ace-hplc.com

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

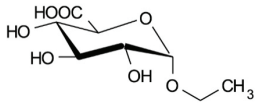
Gradient:	**Time (mins)**	**%B**
	0.0	0
	0.5	20
	1.5	20
	2.0	100
	4.0	100
	4.5	0

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

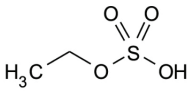
Fluoride counter-ion thought to enhance negative ESI response
Detection limit ~ 1 ng/mL in oral fluid

Analytes

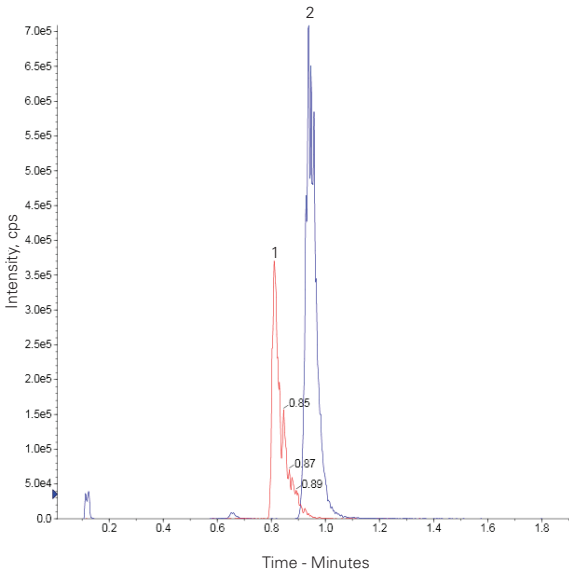
1. Ethyl glucuronide (EtG)
2. Ethyl sulphate (EtS)



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

Reproduced with permission of Biotage GB Ltd, UK

Alternative Selectivity Provided by ACE CN-ES

Application #AN2450

Conditions

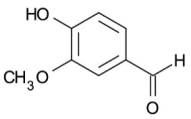
Column: ACE Excel 3 CN-ES
ACE Excel 3 CN
ACE Excel 3 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-1113-0502U (ACE Excel 3 CN-ES),
EXL-114-0502U (ACE Excel 3 CN),
EXL-111-0502U (ACE Excel 3 C18)
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeOH/H_2O (90:10 v/v)
Gradient:

Time (mins)	%B
0	3
5	100

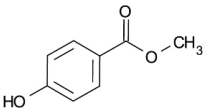
Flow Rate: 0.6 mL/min
Injection: 1 µL
Temperature: 40 °C
Detection: UV, 254 nm

Analytes

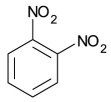
1. Metronidazole
2. Benzyl alcohol
3. Hydrochlorothiazide
4. Vanillin
5. Methyl paraben
6. 1,2-Dinitrobenzene



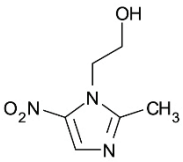
Vanillin



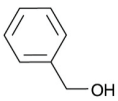
Methyl paraben



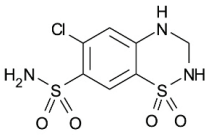
1,2-Dinitrobenzene



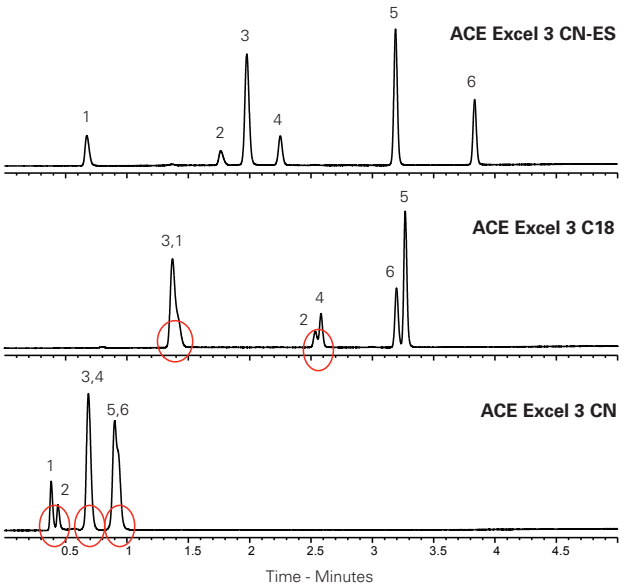
Metronidazole



Benzyl alcohol



Hydrochlorothiazide



Amino Acid Profile of Edible Stink Bugs by LC-MS

Application #AN3530

Conditions

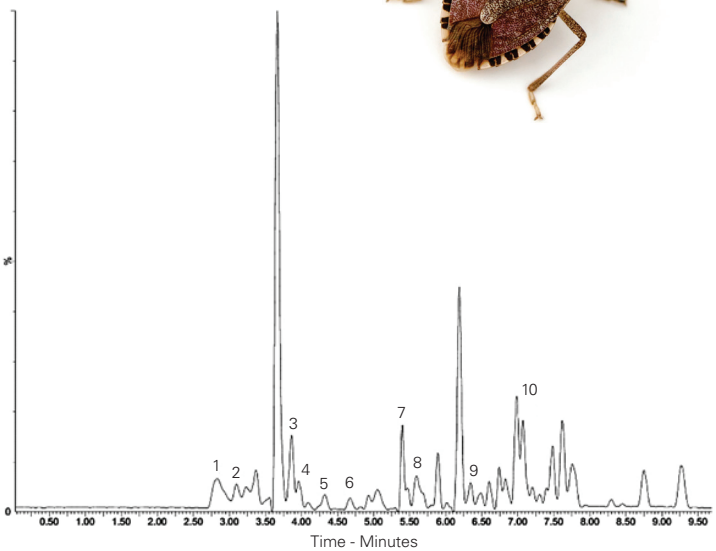
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.01% formic acid in H_2O
B: 0.01% formic acid in MeCN
Gradient:

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)

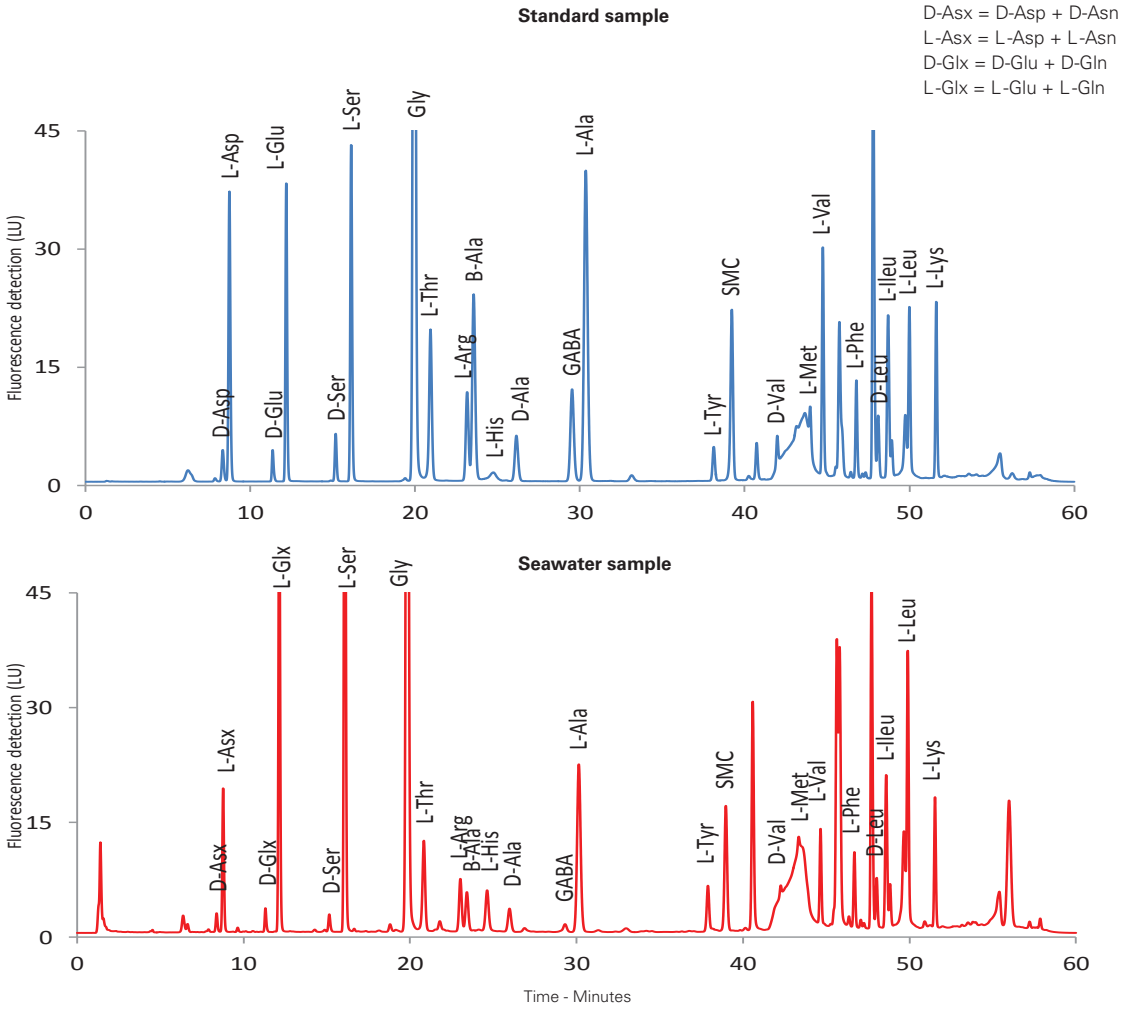
Conditions

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



Reproduced with permission of Department of Chemistry and Biochemistry, Université de Moncton, New Brunswick, Canada

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)

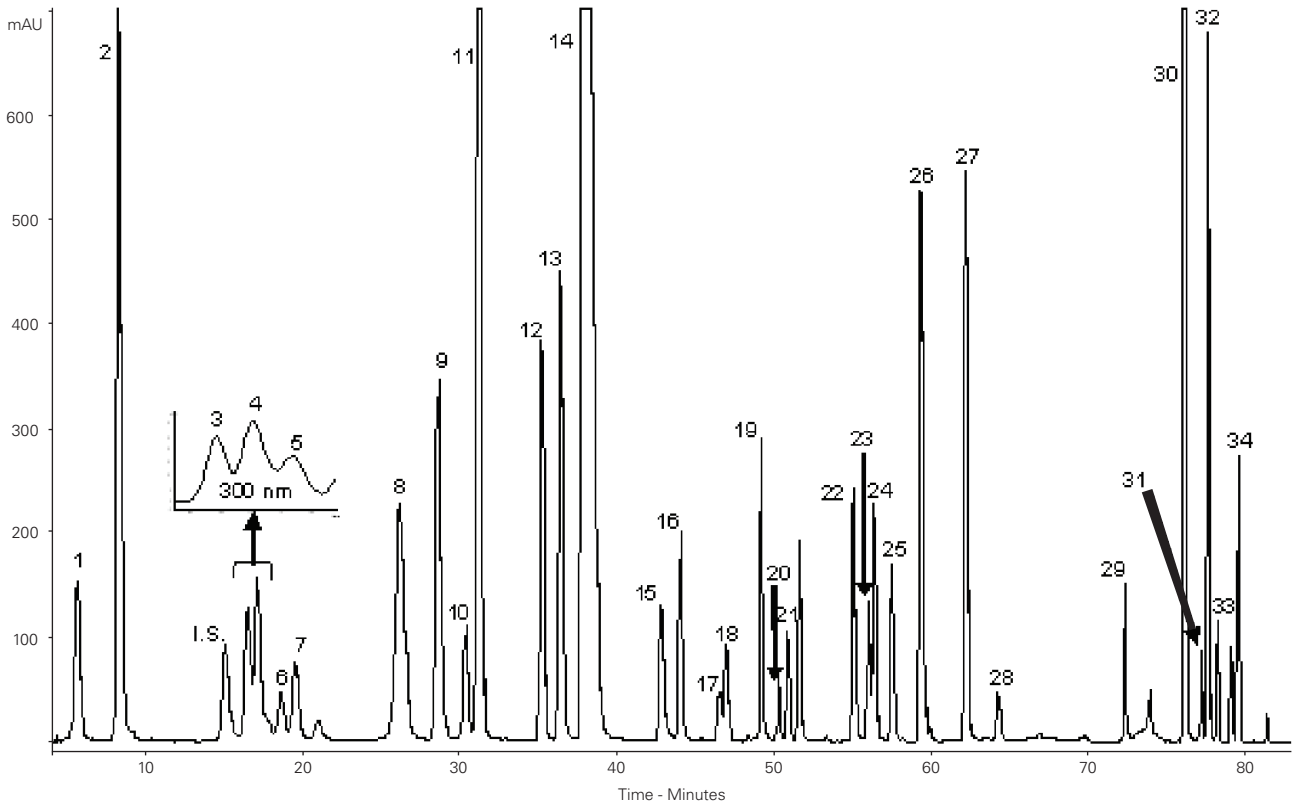
Gradient:

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



Reproduced with permission of Instituto de la Vid y el Vino de Castilla-La Mancha, Spain

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:

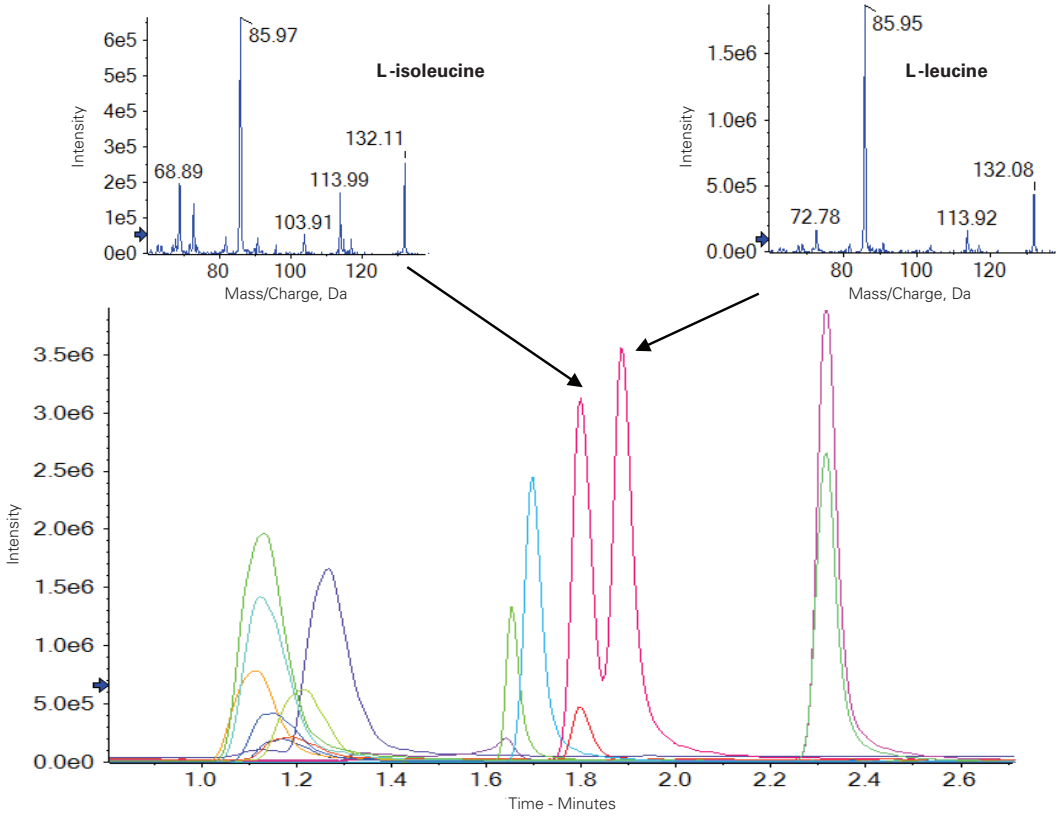
Time (mins)	%B
0	2
5	20

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

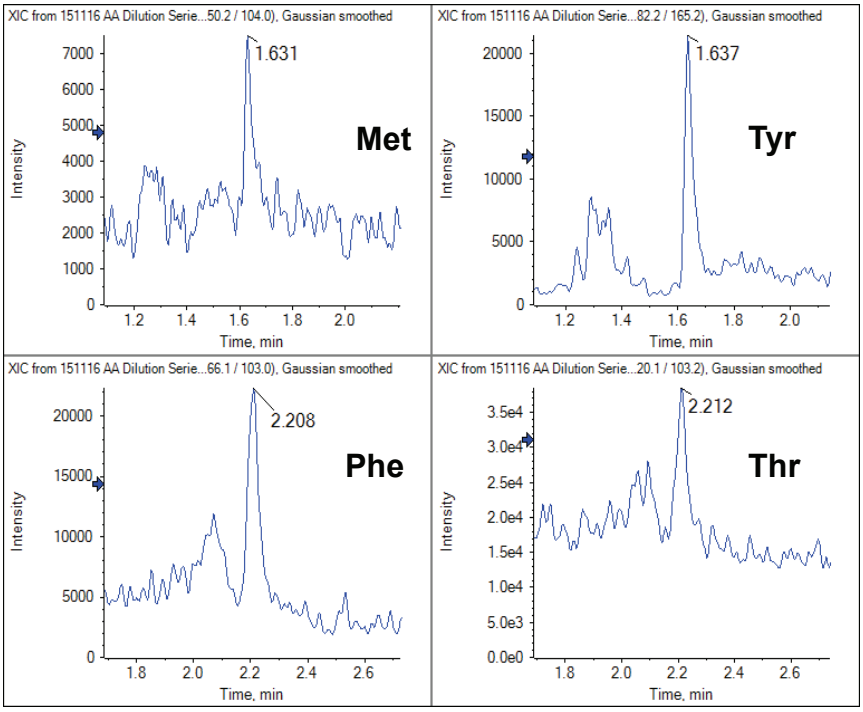
Full scan linear ion trap MS/MS data can distinguish isobaric amino acids L-isoleucine and L-leucine.



Reproduced with permission of SCIEX, Warrington, UK

Amino Acids in Extracellular Matrix (*Continued*)

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



Reproduced with permission of SCIEX, Warrington, UK

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)

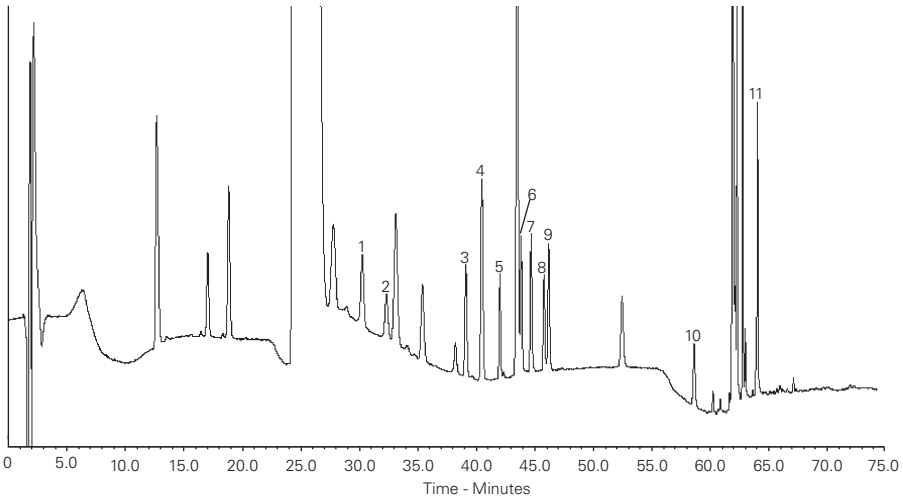
Gradient:

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



Reproduced with permission of Department of Veterinary Public Health, University of Veterinary Medicine, Vienna, Austria

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

Application #AN2660

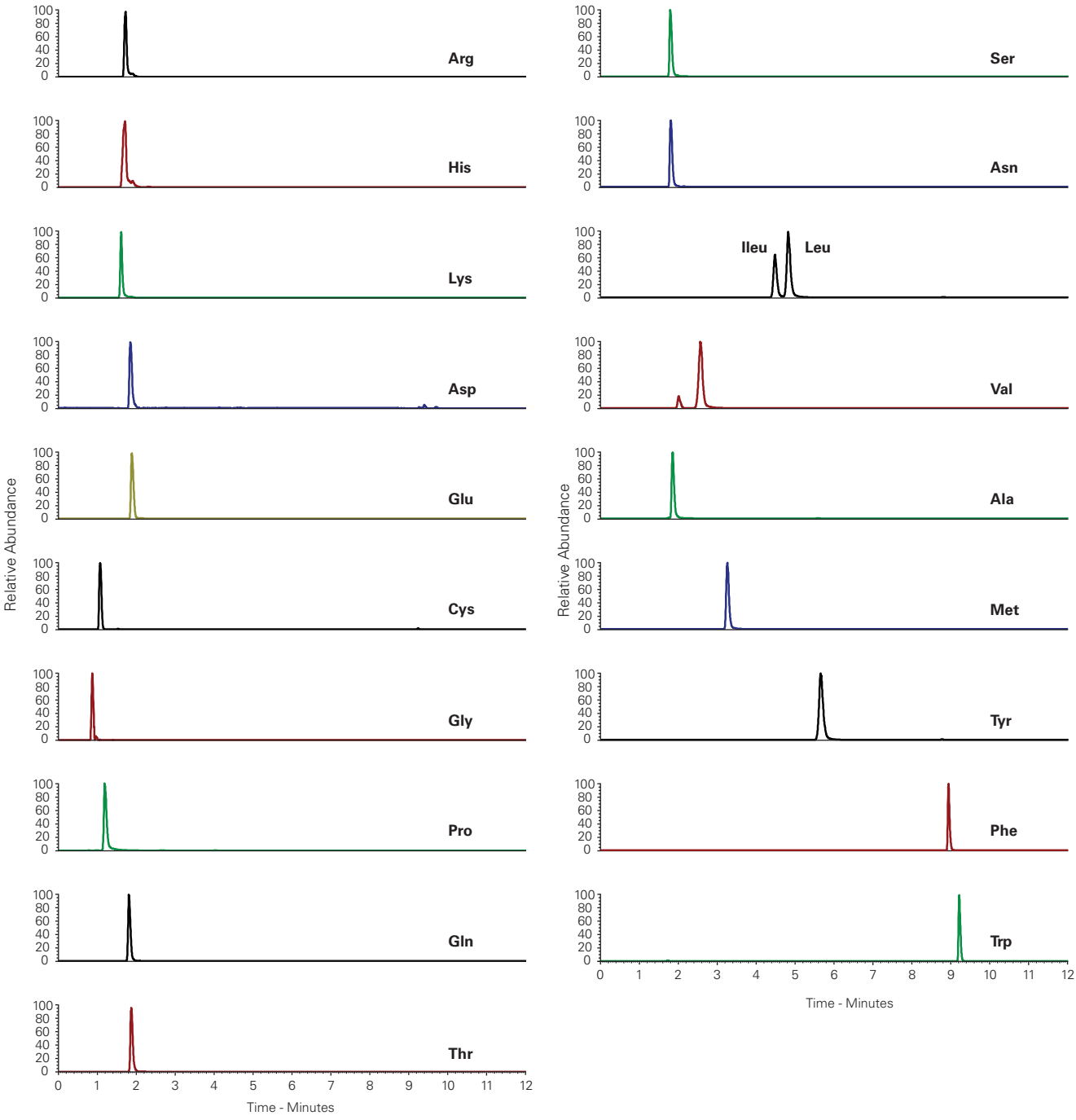
Conditions

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



Reproduced with permission of Fera Science Ltd, York, UK

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)

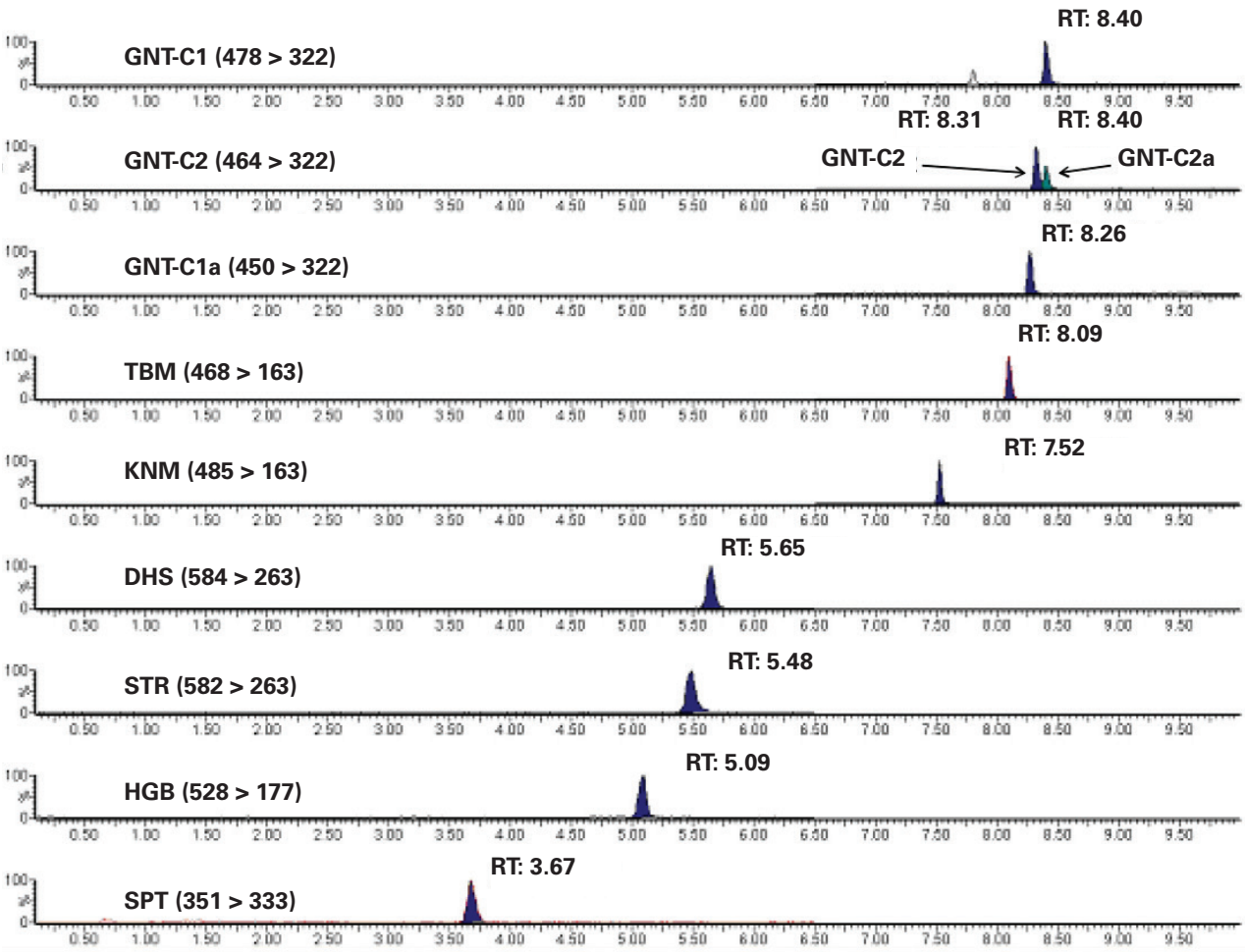
Gradient:

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



Reproduced with permission of Veterinary Drug Residues Department, Centro Nacional de Alimentación (CNA, AECOSAN), Madrid, Spain

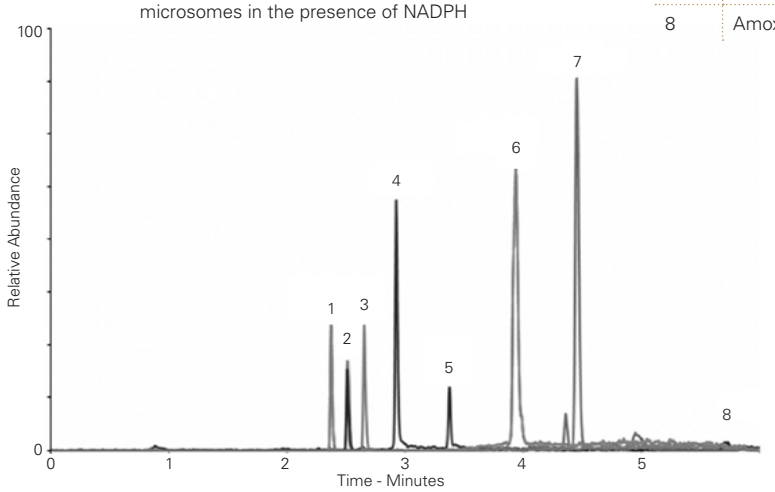
Amoxicillin Metabolites in Human Liver Microsomes

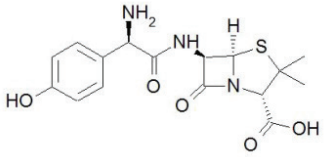
Application #AN4400

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

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

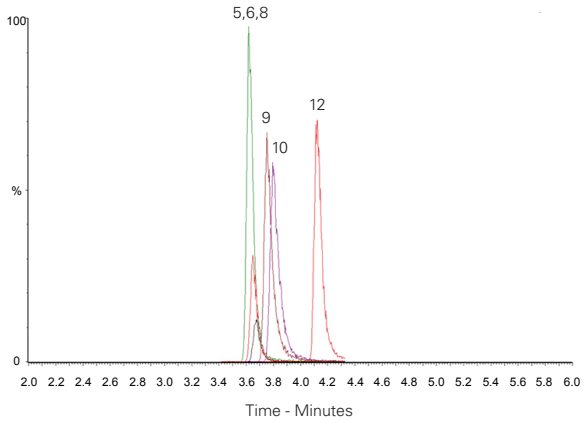
Gradient:

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)



Reproduced with permission of Biotage GB Ltd, UK

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)

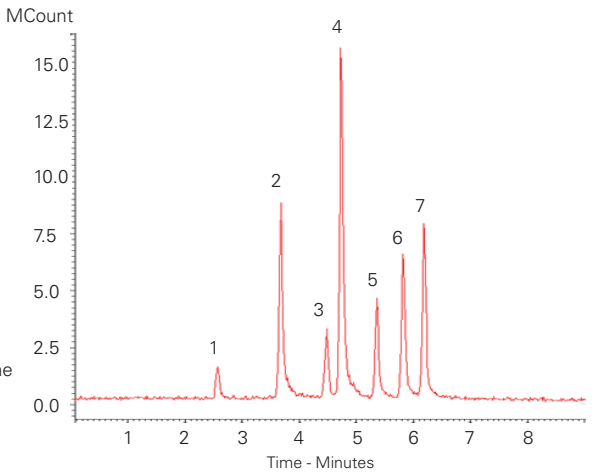
Gradient:

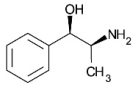
Time (mins)	%B
0	30
8	95

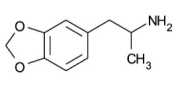
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: Varian 320 Triple Quadrupole MS
Electrospray voltage: +5 kV
Inlet capillary voltage: 30 V
CID with argon at 1.5 mTorr
Collision cell potential ranges from 5 to 17 V
Drying gas (nitrogen) temperature: 325 °C
Nebulizing gas (nitrogen)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

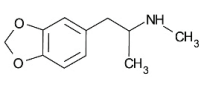
Analytes

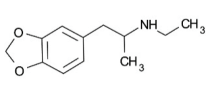
1. Phenylpropanolamine
LOD (est) 4 ppb
(*m/z* 151.6 → 134.0)
2. (l)-Ephedrine
LOD (est) 2 ppb
(*m/z* 166.2 → 148.0)
3. (dl)-3,4-MDA
LOD (est) 30 ppb
(*m/z* 179.7 → 163.0)
4. (d)-Amphetamine
LOD (est) 4 ppb
(*m/z* 135.8 → 90.9)
5. (dl)-3,4-MDMA
LOD (est) 2 ppb
(*m/z* 193.7 → 163.0)
6. 4-Methylthioamphetamine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

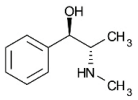


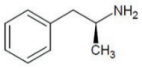

Phenylpropanolamine

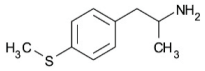

(dl)-3,4-MDA


(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

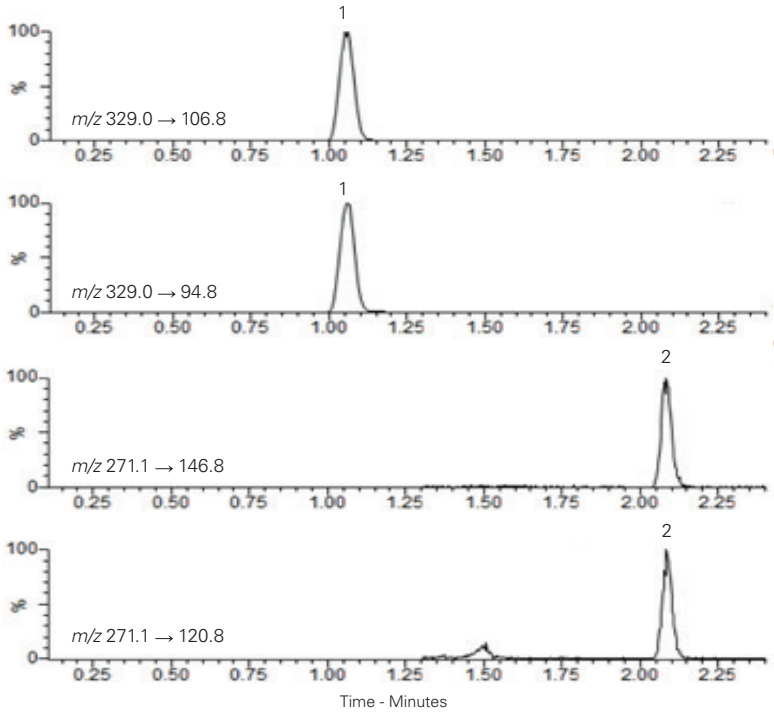
Gradient:

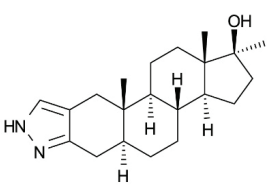
Time (mins)	%B
0.00	75
0.25	75
1.50	90
1.51	100
3.50	100
3.51	75
4.00	75

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

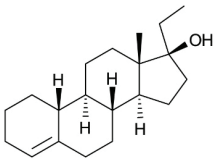
Analytes

1. Stanozolol
2. Ethylestrenol





Stanozolol



Ethylestrenol

Reproduced with permission of Biotage GB, Ltd. For extraction conditions see Biotage Application Note AN843

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

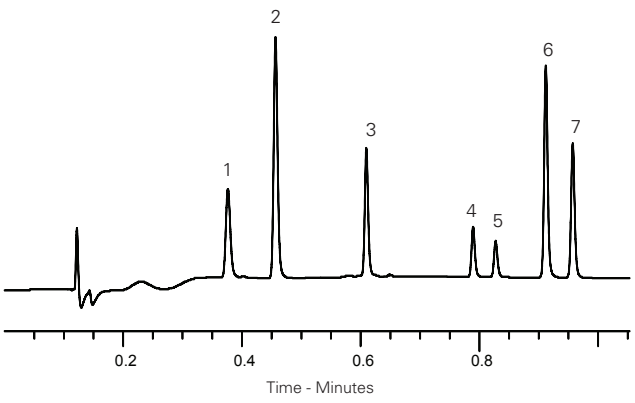
Gradient:

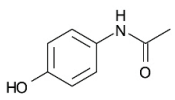
Time (mins)	%B
0.0	5
1.0	100
1.5	100
1.6	5
3.1	5

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

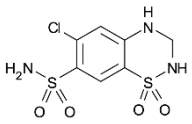
Analytes

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

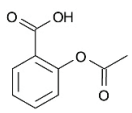




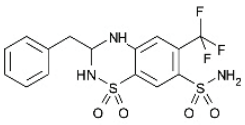
Paracetamol



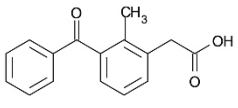
Hydrochlorothiazide



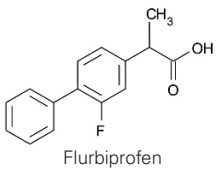
Aspirin



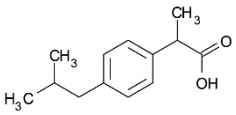
Bendroflumethiazide



Ketoprofen



Flurbiprofen



Ibuprofen

Analgesic Separation

Application #AN2490

Conditions

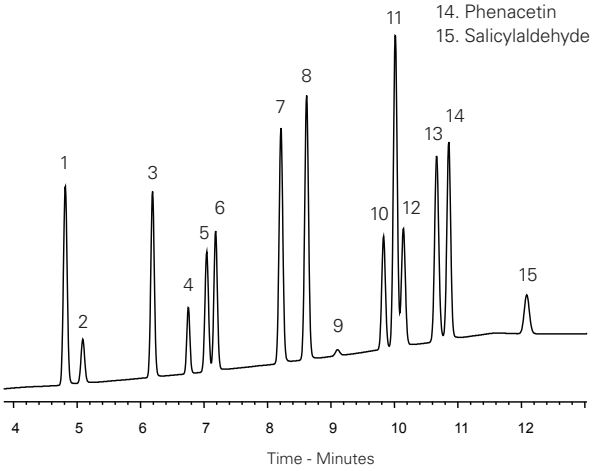
Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

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

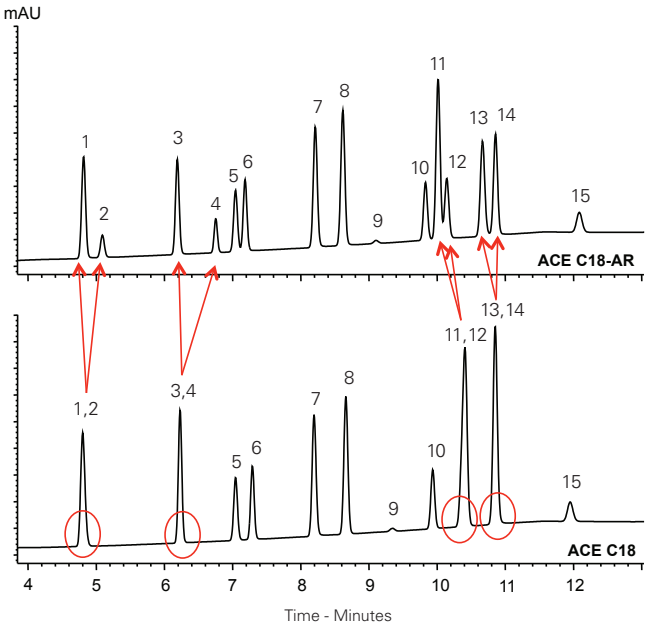
Column:	ACE 3 C18-AR
	ACE 3 C18
Dimensions:	150 x 4.6 mm
Part Numbers:	ACE-119-1546
	ACE-111-1546
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

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

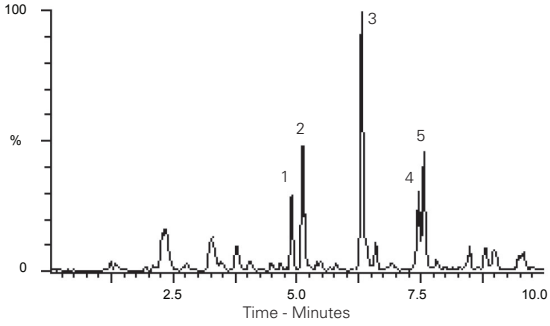
Application #AN3770

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

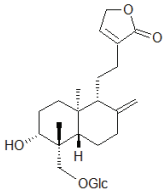
Gradient:	**Time (mins)**	**%B**
	0.0	30
	2.0	40
	8.0	75
	9.0	100
	9.5	30
	15.5	30

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

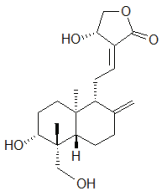


Analytes

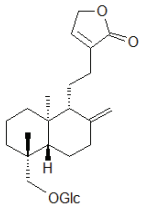
1. 14-Deoxyandrographiside
2. Andrographolide
3. Neoandrographolide
4. 14-Deoxyandrographolide
5. Dehydroandrographolide



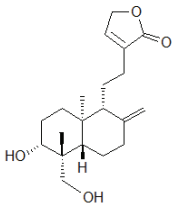
14-Deoxyandrographiside
(*Tentative assignment)



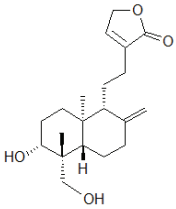
Andrographolide



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

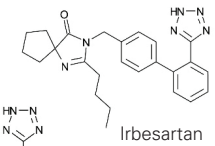
Application #AN3460

Conditions

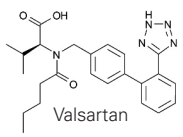
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	0.025 M KH_2PO_4 pH 6.0/MeCN (65:35 v/v)
Flow Rate:	1.5 mL/min
Temperature:	40 °C
Detection:	UV, 220 nm

Analytes

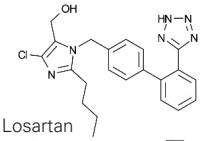
1. Valsartan
2. Losartan
3. Irbesartan
4. Telmisartan



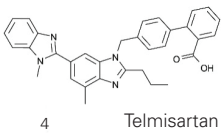
Irbesartan



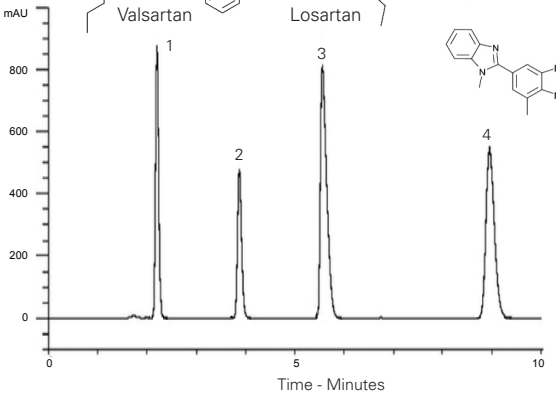
Valsartan



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

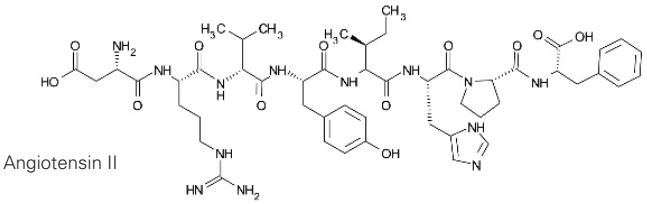
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H_2O
B: 0.1% TFA in H_2O/MeCN (80:20 v/v)
Gradient:

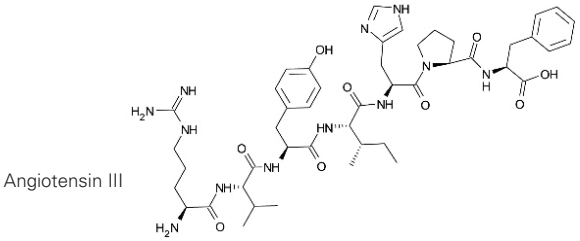
Time (mins)	%B
0	25
15	40

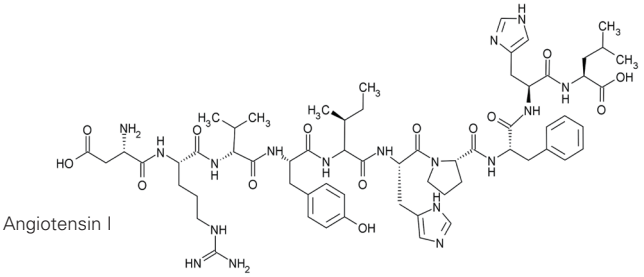
Flow Rate: 1.0 mL/min
Temperature: Ambient
Detection: UV, 215 nm

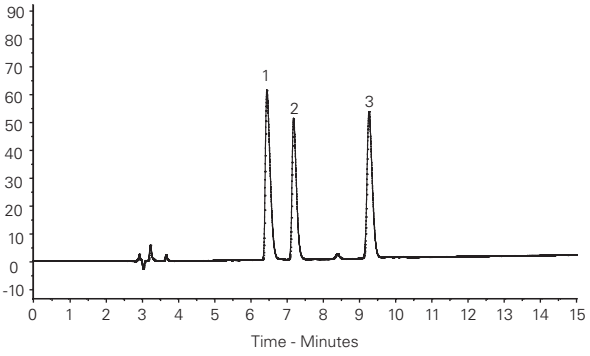
Analytes

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









Annatto

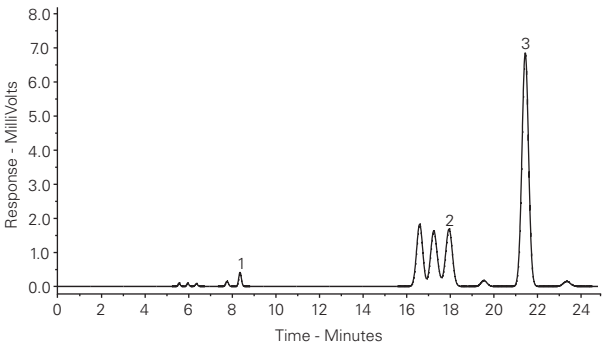
Application #AN2840

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



Reproduced with permission of Lincolne Sutton & Wood, Norwich, UK

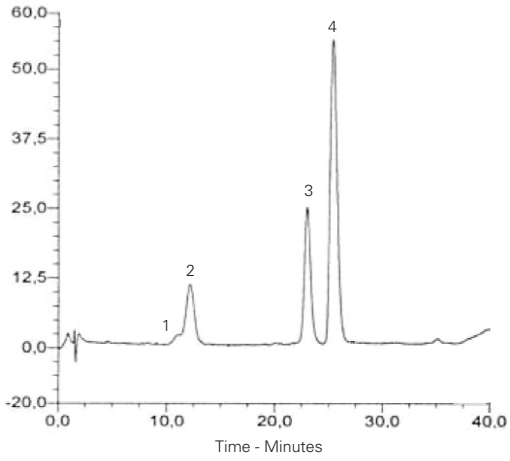
Annatto - An orange-red condiment and food colouring derived from the seeds of the achiote tree.

Anthocyanins from *Sambucus Nigra* (Elderberry)

Application #AN2750

Conditions

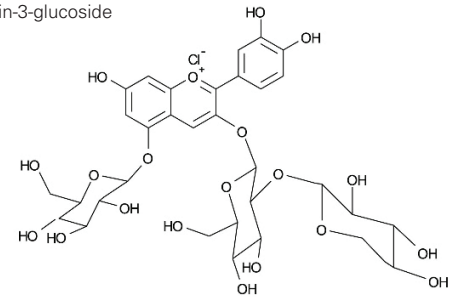
Column:	ACE UltraCore 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	CORE-5A-1546U
Mobile Phase:	A: 5% formic acid in H_2O
	B: MeOH
Gradient:	**Time (mins) %B**
	0 5
	35 10
	55 65
	65 65
Flow Rate:	1 mL/min
Temperature:	40 °C
Detection:	UV-Vis, 525 nm



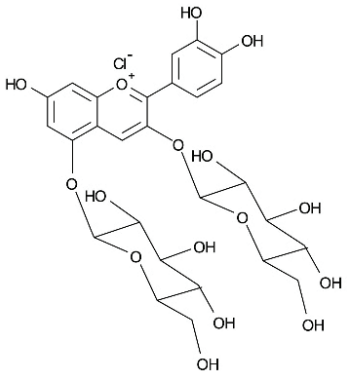
Reproduced with permission of University of Vila Real, Portugal

Analytes

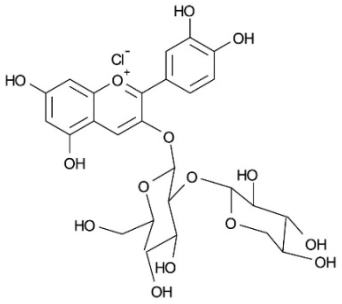
1. Cyanidin-3-sambubioside-5-glucoside
2. Cyanidin-3,5-diglucoside
3. Cyanidin-3-sambubioside
4. Cyanidin-3-glucoside



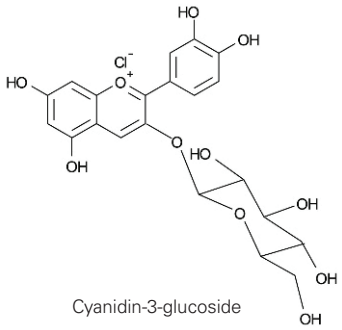
Cyanidin-3-sambubioside-5-glucoside



Cyanidin-3,5-diglucoside



Cyanidin-3-sambubioside



Cyanidin-3-glucoside

Antihistamines

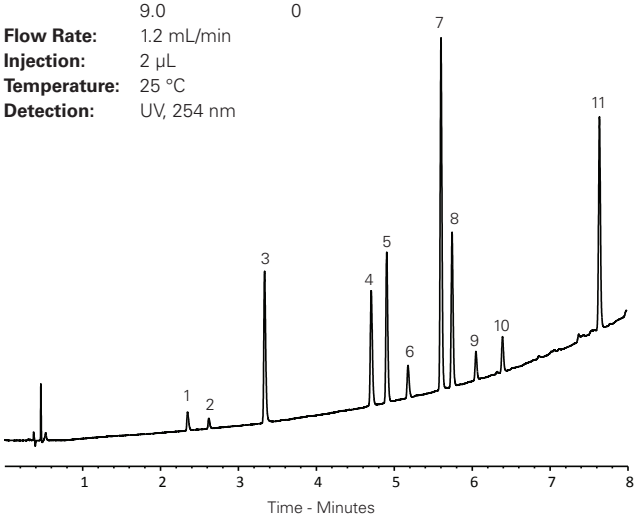
Application #AN1400

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

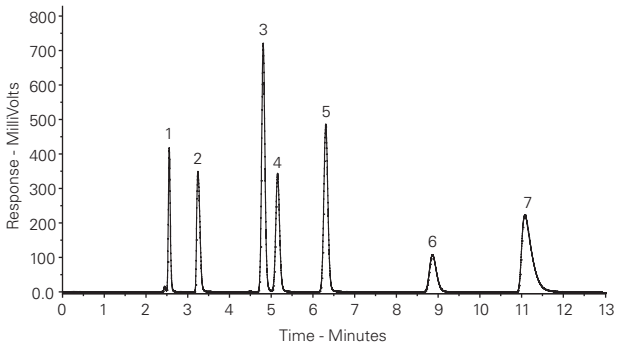
Application #AN3190

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

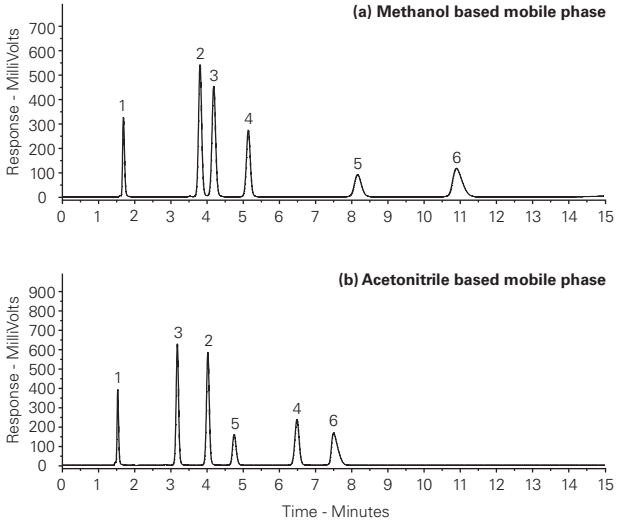
Application #AN3960

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

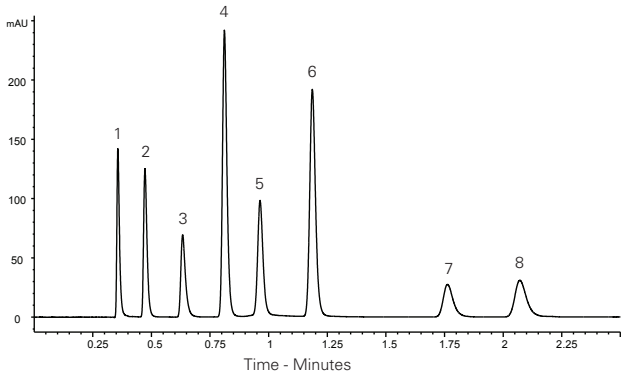
Application #AN4290

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)

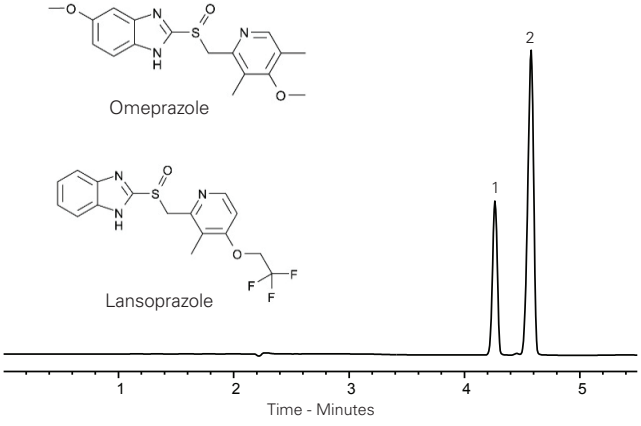
Gradient:

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



Need a custom column for your application?

Please enquire

email: info@ace-hplc.com

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

Application #AN4380

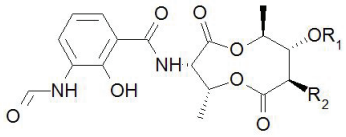
Conditions

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:

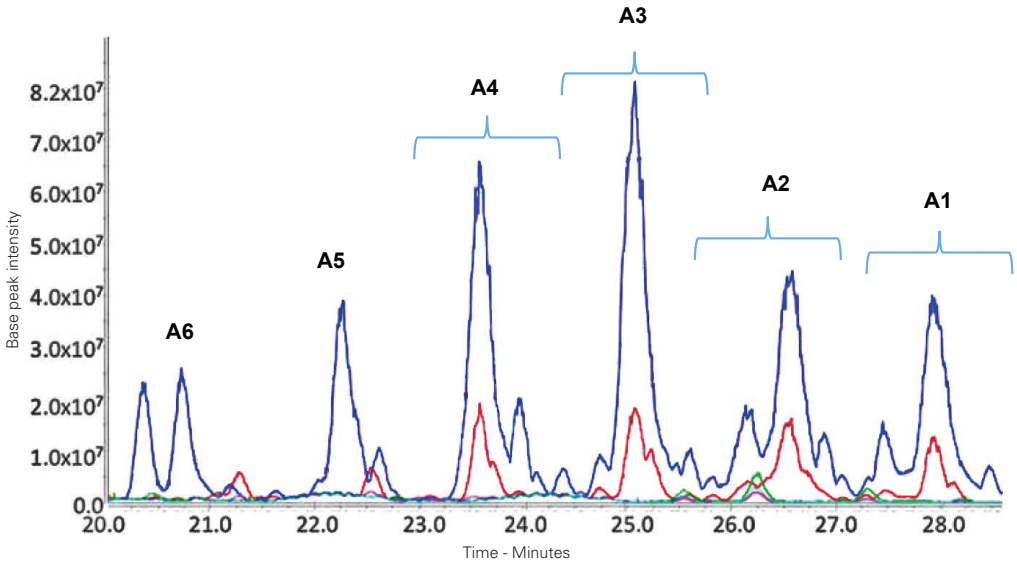
Time (mins)	%B
0	10
30	100
35	100

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

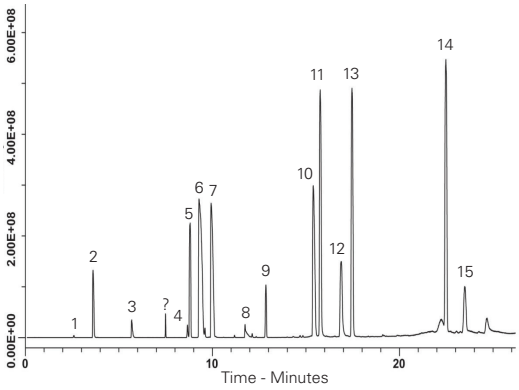
Application #AN1960

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



Reproduced with permission of US FDA

Aromatic Nitrobenzenes

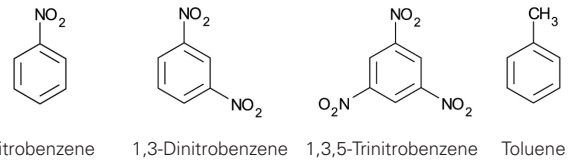
Application #AN2480

Conditions

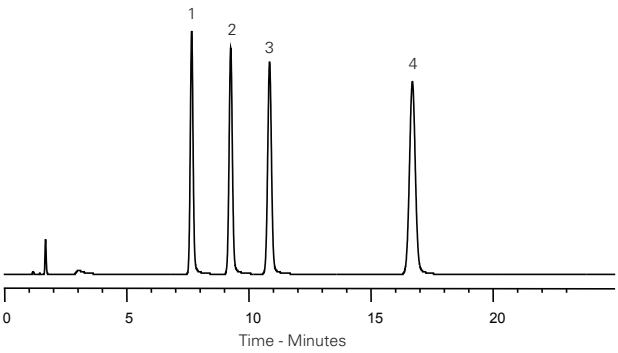
Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	H_2O/MeOH (50:50 v/v)
Flow Rate:	1 mL/min
Temperature:	40 °C
Detection:	UV, 210 nm

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

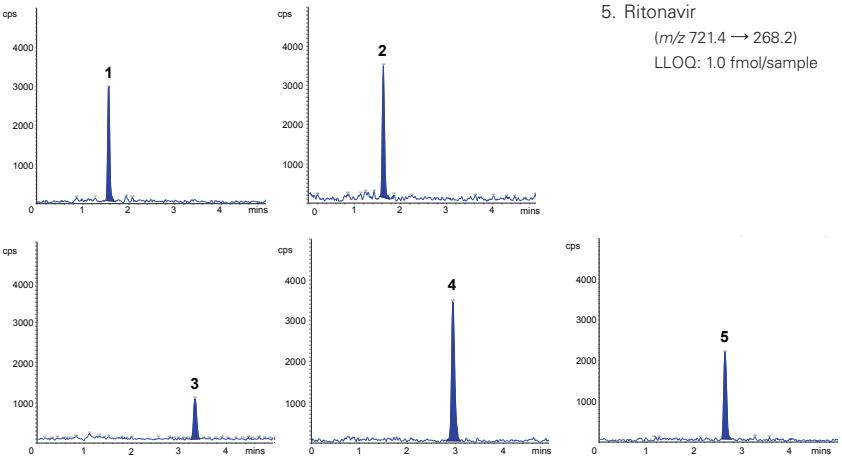
Application #AN3470

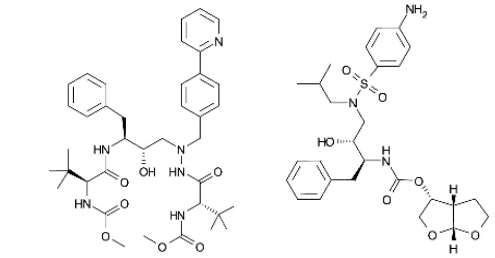
Conditions

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)

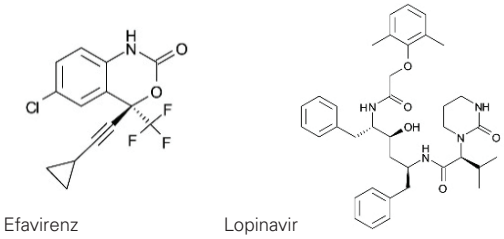
Analytes

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

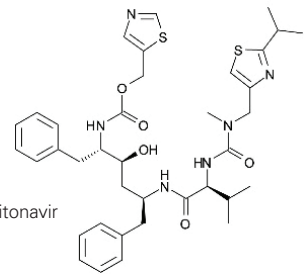




Atazanavir Darunavir



Efavirenz Lopinavir



Ritonavir

Reproduced with permission of Antiviral Pharmacology Laboratory, College of Pharmacy, University of Nebraska Medical Centre, Nebraska, USA

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

Application #AN1970

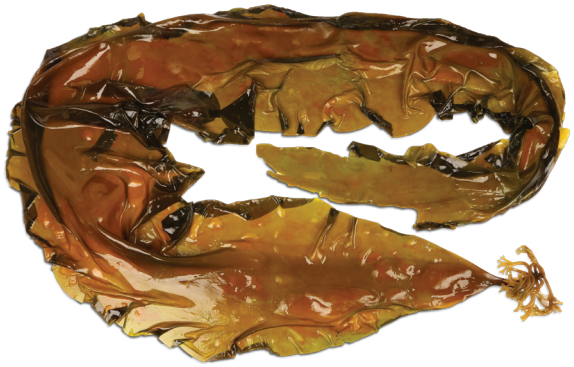
Conditions

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



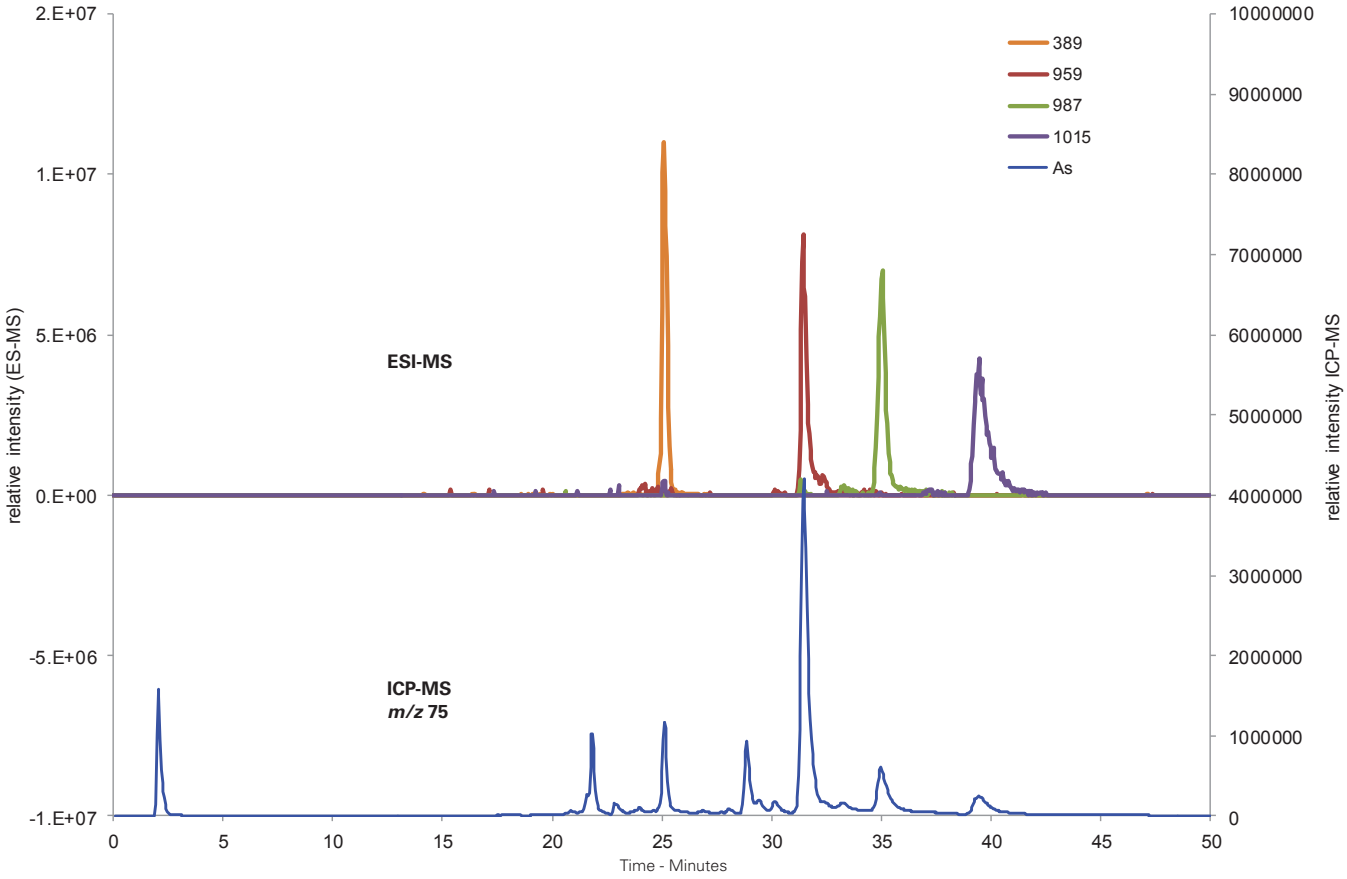
Alaria esculenta is an edible seaweed. It is a traditional food found along the coasts of the far north Atlantic Ocean.

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)



Reproduced with permission of Trace Element Speciation Laboratory, University of Aberdeen, UK

Artemisinin

Application #AN3140

Conditions

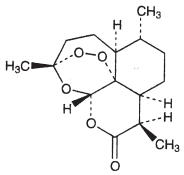
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: H_2O
	B: MeOH

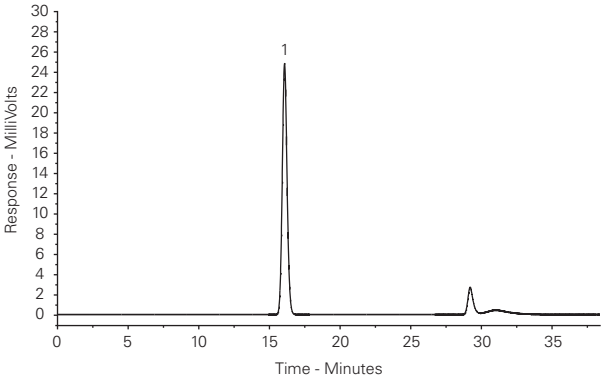
Gradient:	**Time (mins)**	**%B**
	0	50
	25	100
	35	100

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

Analyte

1. Artemisinin





Reproduced with permission of Neem Biotech, Cardiff, UK

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

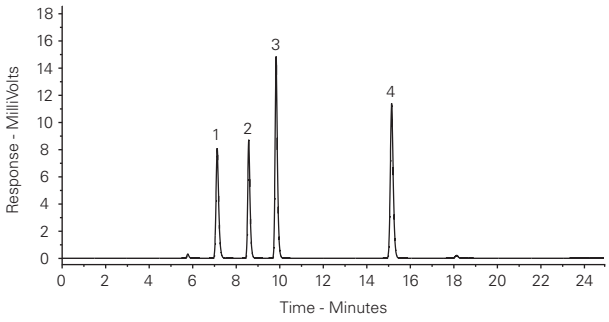
Gradient:	**Time (mins)**	**%B**
	0	45
	12	60
	25	45

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



Reproduced with permission of Lincolne Sutton & Wood, Norwich, UK

Artificial Sweeteners Global Method

Application #AN1980

Conditions

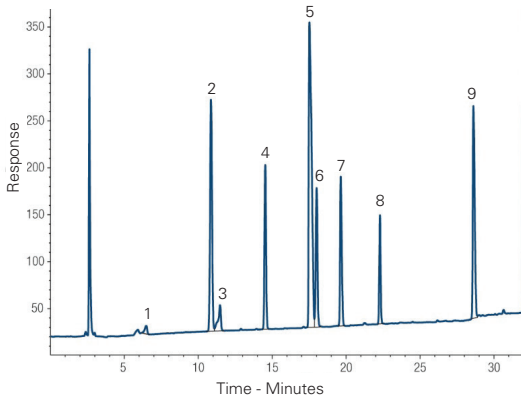
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: H_2O
	B: MeCN
	C: 0.1% TFA

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



Reproduced with permission of Durham County Council Scientific Services, UK

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

email: info@ace-hplc.com

Artificial Sweeteners (Stevia Glycosides)

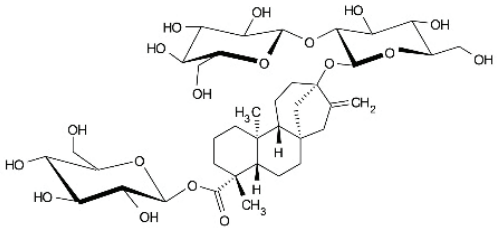
Application #AN1020

Conditions

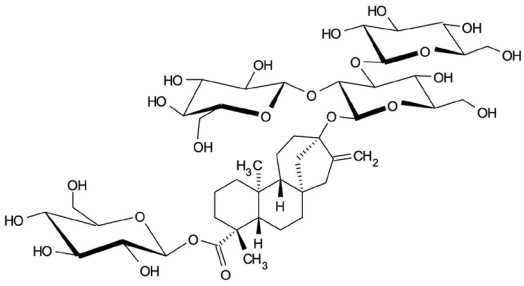
Column:	ACE Excel 2 SuperC18
Dimensions:	150 x 2.1 mm
Part Number:	EXL-1011-1502U
Mobile Phase:	A: 10 mM sodium dihydrogen phosphate pH 2.8 in H_2O
	B: 10 mM sodium dihydrogen phosphate pH 2.8 in H_2O/MeCN (20:80 v/v)
Gradient:	**Time (mins) %B**
	0 39.5
	4 48.0
Flow Rate:	0.6 mL/min
Injection:	1 µL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

Analytes

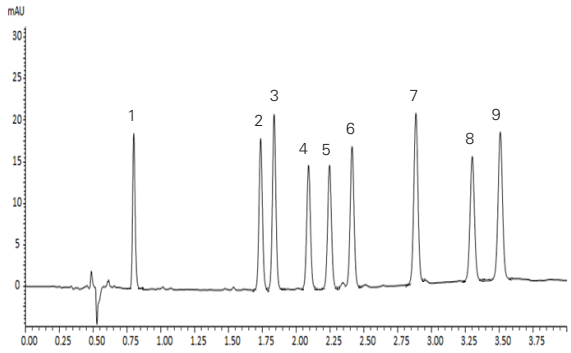
1. Rebaudioside D
2. Rebaudioside A
3. Stevioside
4. Rebaudioside F
5. Rebaudioside C
6. Dulcoside A
7. Rubusoside
8. Rebaudioside B
9. Steviolbioside



Stevioside
MW 804.87



Rebaudioside A
MW 967.01



Reproduced with permission of Shimadzu Europe GmbH. Analysed on Shimadzu Nexera X2. http://images2.advanstar.com/PixelMags/lcgc-eu/pdf/2013-10-sp.pdf

Aspirin and Related Substances (I)

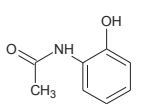
Application #AN1050

Conditions

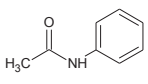
Column:	ACE Excel 3 CN-ES
	ACE Excel 3 C18
	ACE Excel 3 CN
Dimensions:	50 x 2.1 mm
Part Numbers:	EXL-1113-0502U,
	EXL-111-0502U,
	EXL-114-0502U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH
Gradient:	**Time (mins) %B**
	0.00 5
	3.75 38
	5.00 38
Flow Rate:	0.6 mL/min
Temperature: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

Analytes

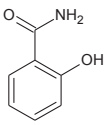
1. 2-Acetamidophenol
2. Acetanilide
3. Salicylamide
4. Aspirin
5. Phenacetin
6. Salicylic acid



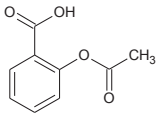
2-Acetamidophenol



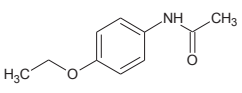
Acetanilide



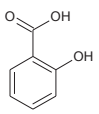
Salicylamide



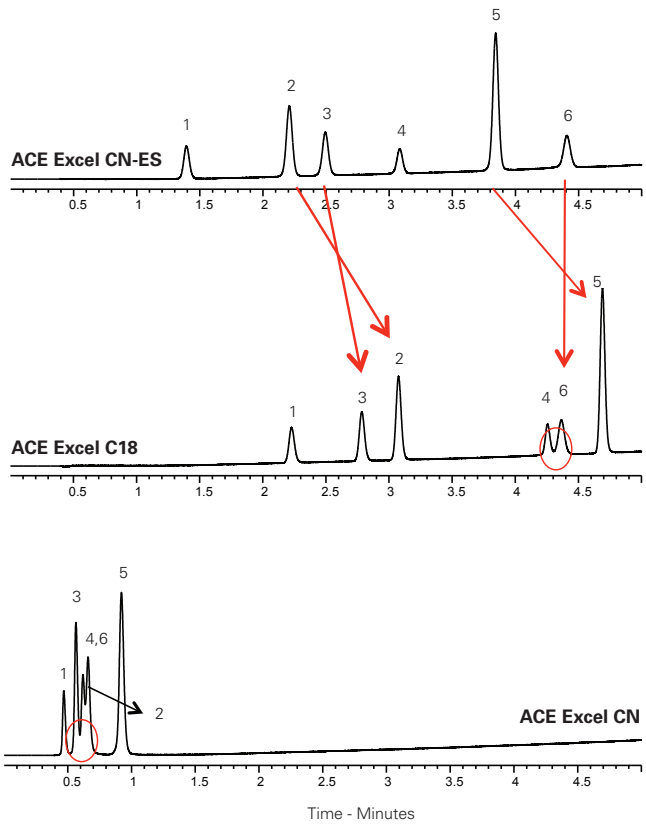
Aspirin



Phenacetin



Salicylic acid



Aspirin and Related Substances (II)

Application #AN2280

Conditions

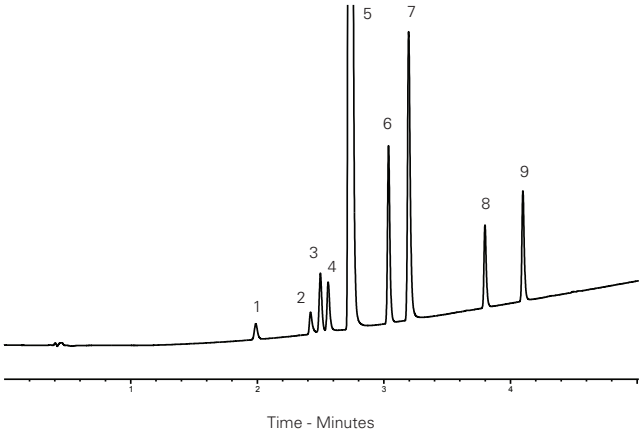
Column:	ACE Excel 1.7 CN-ES
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1713-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

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

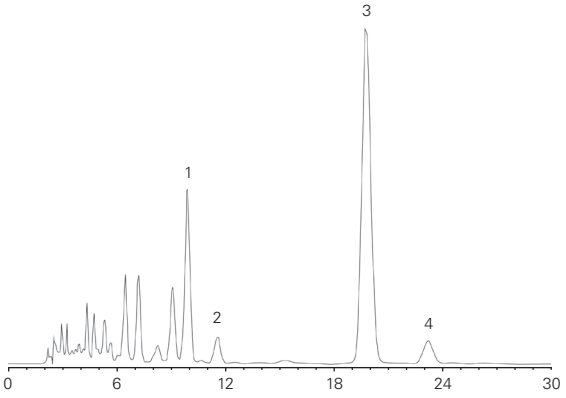
Application #AN2740

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



Reproduced with permission of Sainsbury Laboratory, John Innes Centre, UK

β-Antagonists and Diuretics

Application #AN1410

Conditions

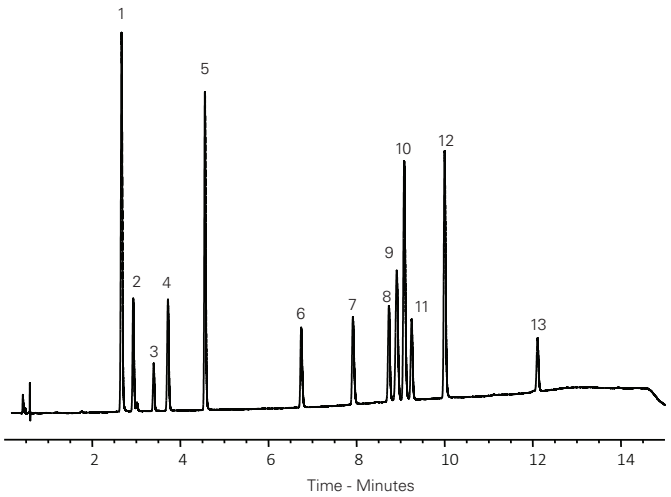
Column:	ACE 3 C18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-111-1002
Mobile Phase:	A: 20 mM KH_2PO_4, pH 2.7
	B: 20 mM KH_2PO_4, pH 2.7
	in MeCN/H_2O (65:35 v/v)

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

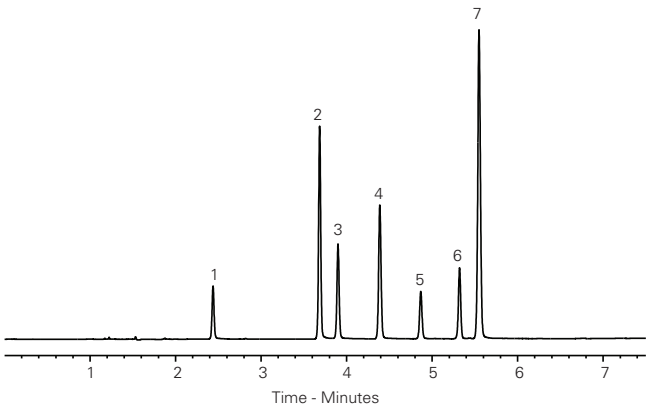
Application #AN1420

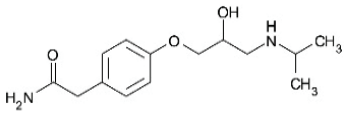
Conditions

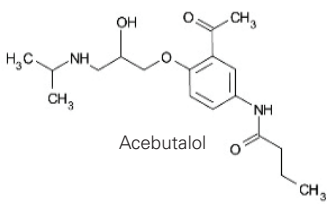
Column:	ACE Excel 5 SuperC18	
Dimensions:	150 x 4.6 mm	
Part Number:	EXL-1211-1546U	
Mobile Phase:	A: 0.1% ammonia in H_2O	
	B: 0.1% ammonia in MeCN	
Gradient:	**Time (mins)**	**%B**
	0.0	30
	5.0	90
	7.0	90
	7.5	30
	22.5	30
Flow Rate:	1 mL/min	
Injection:	5 µL	
Temperature:	35 °C	
Detection:	UV, 230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

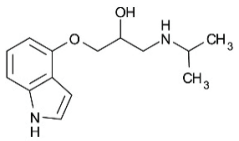
Analytes

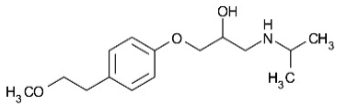
1. Atenolol
2. Acebutalol
3. Pindolol
4. Metoprolol
5. Oxprenolol
6. Carvedilol
7. Propranolol

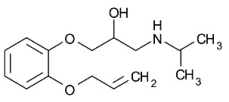


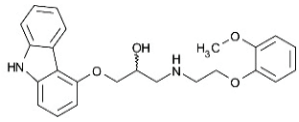

Atenolol

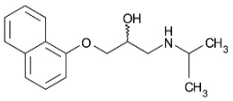

Acebutalol


Pindolol


Metoprolol


Oxprenolol


Carvedilol


Propranolol

β-Blockers at High pH – Fast Analysis

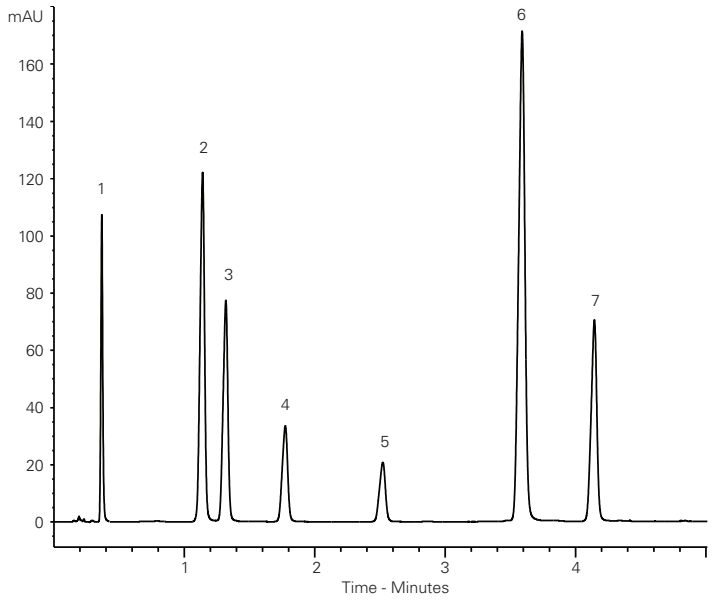
Application #AN2160

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

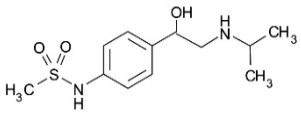
Gradient:

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

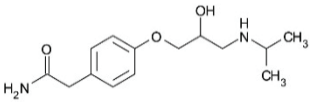
Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: MS/MS ESI in positive ion mode
Sample: 2.5 pg/µL

Analytes

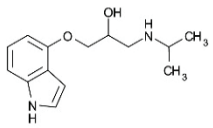
1. Sotalol (*m/z* 272.9 → 212.8)
2. Atenolol (*m/z* 267.0 → 189.8)
3. Pindolol (*m/z* 248.9 → 115.8)
4. Nadolol diastereomers (*m/z* 310.0 → 253.9)
5. Metoprolol (*m/z* 268.0 → 115.8)
6. Labetalol (*m/z* 329.1 → 161.8)
7. Propranolol (*m/z* 260.0 → 115.7)
8. Alprenolol (*m/z* 250.0 → 115.8)



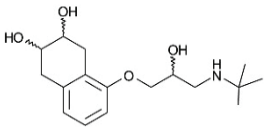
Sotalol



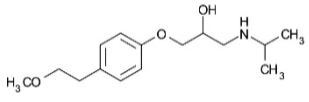
Atenolol



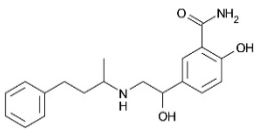
Pindolol



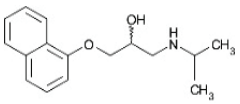
Nadolol diastereomers



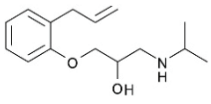
Metoprolol



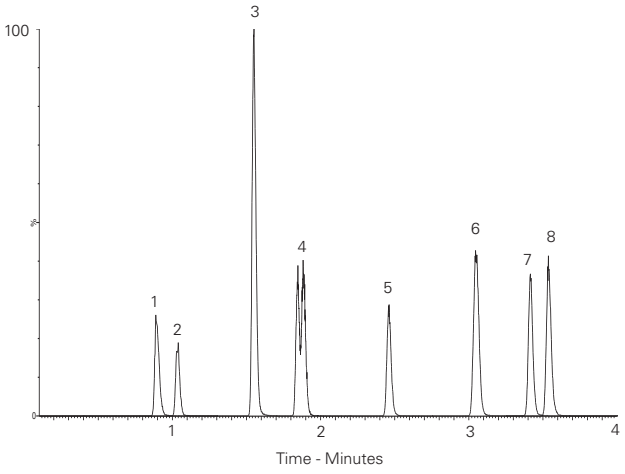
Labetalol



Propranolol



Alprenolol



Reproduced with permission of Biotage GB Ltd, UK

β-Blockers

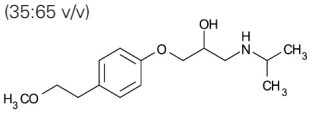
Application #AN3160

Conditions

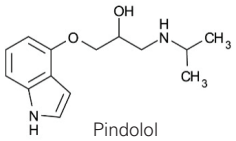
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM 1-methylpiperidine pH 11/MeOH (35:65 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 215 nm

Analytes

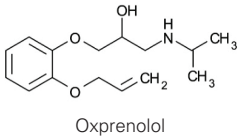
1. Pindolol
2. Metoprolol
3. Oxprenolol
4. Propranolol



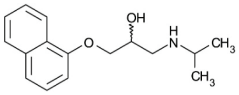
Metoprolol



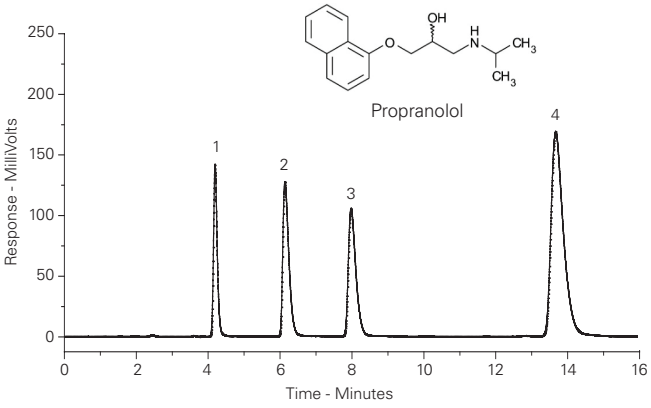
Pindolol



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

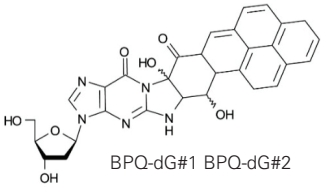
Gradient:

Time (mins)	%B
0	25
8	55

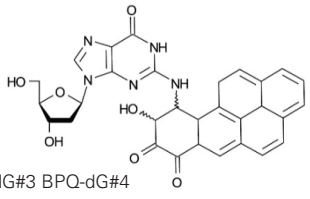
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 35 °C
Detection: UV, 285 nm

Analytes

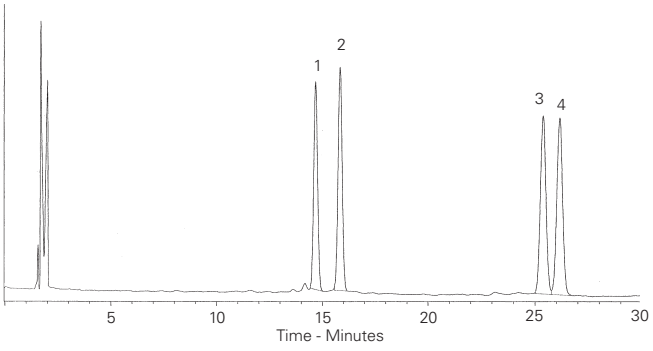
1. BPQ-dG#1
2. BPQ-dG#2
3. BPQ-dG#3
4. BPQ-dG#4



BPQ-dG#1 BPQ-dG#2



BPQ-dG#3 BPQ-dG#4



Reproduced with permission of Institute of Cancer Research, Sutton, Surrey, UK

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

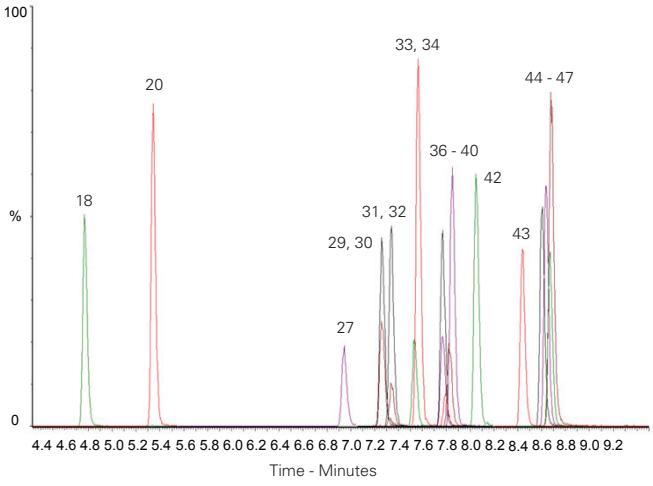
Gradient:

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)



Reproduced with permission of Biotage GB Ltd, UK

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)

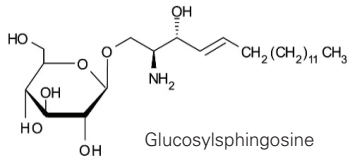
Gradient:

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

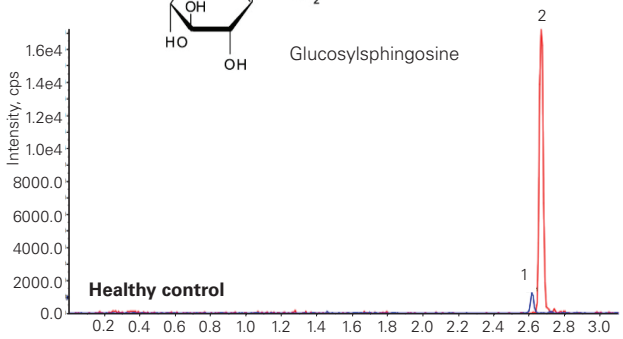
Flow Rate: 0.9 mL/min
Injection: 5 µL
Temperature: 60 °C
Detection: API 4000 triple quad MS
ESI in positive ion mode
Temperature: 500 °C

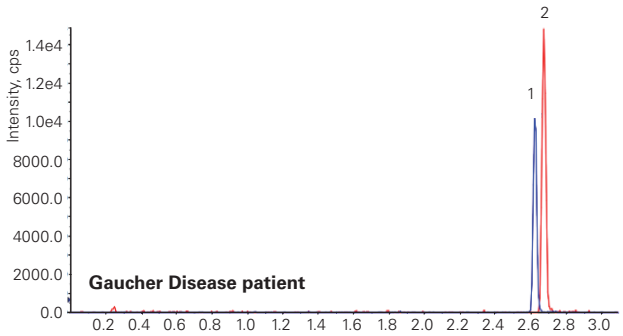
Analytes

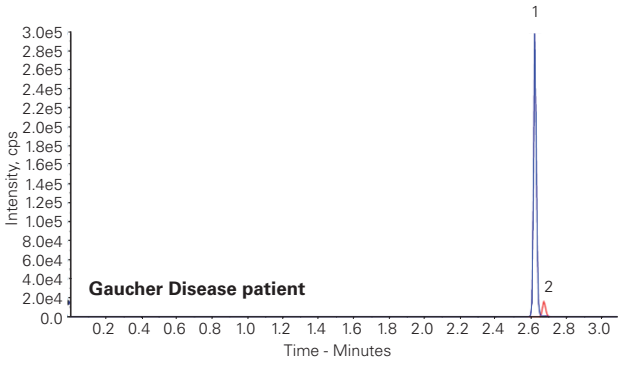
1. Glucosylsphingosine (*m/z* 462 → 282)
2. Lyso-Gb2 (IS) (*m/z* 624 → 282)



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)

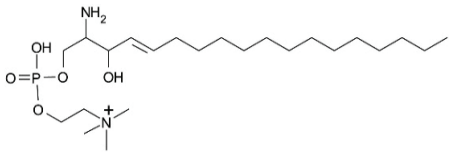
Gradient:

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

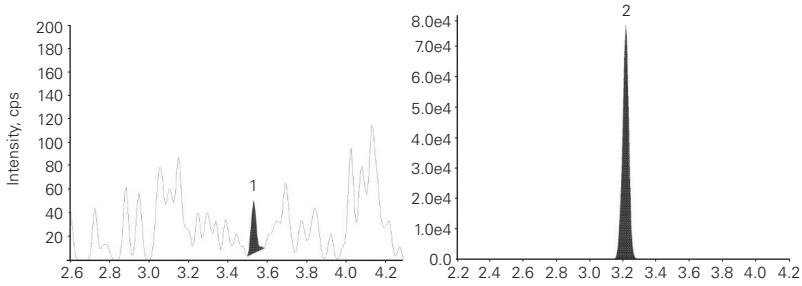
Analytes

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

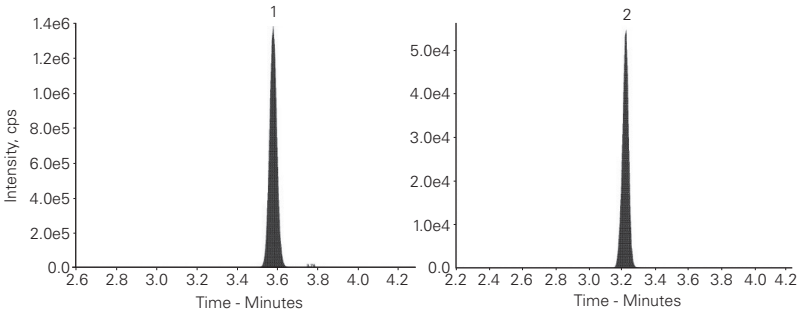


Lyso-SM (lyso-sphingomyelin)

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

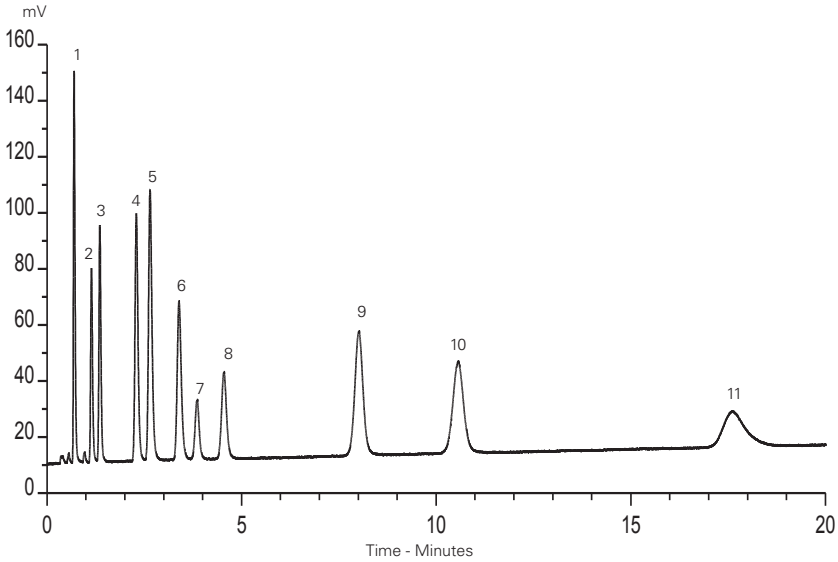
Application #AN1990

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



Reproduced with permission of Department of Medical Biochemistry and Biophysics, Umeå University, Sweden

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

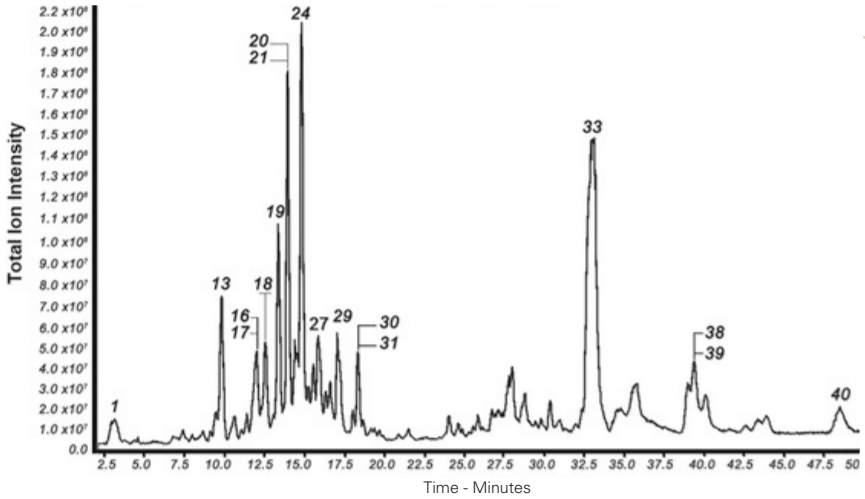
Gradient:

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

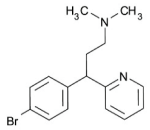
Conditions

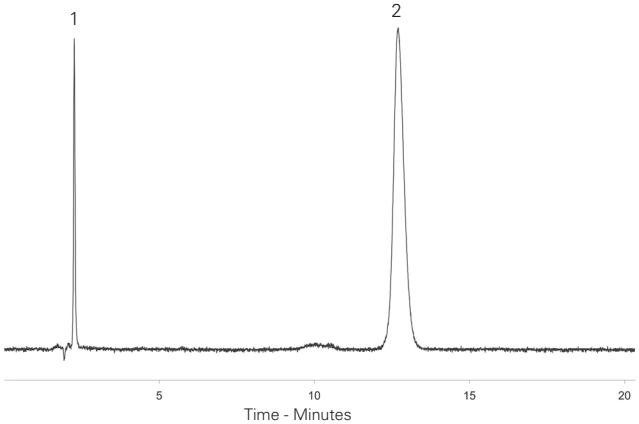
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: 20 mM ammonium formate pH 3.0 in H_2O/MeOH (95:5 v/v)
Flow Rate: 1.0 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV, 265 nm

Analytes

1. Maleic acid
2. Brompheniramine


Maleic acid


Brompheniramine



Reproduced with permission of School of Pharmacy, University of Sunderland, UK

BSA Tryptic Digest Profiling

Application #AN2000

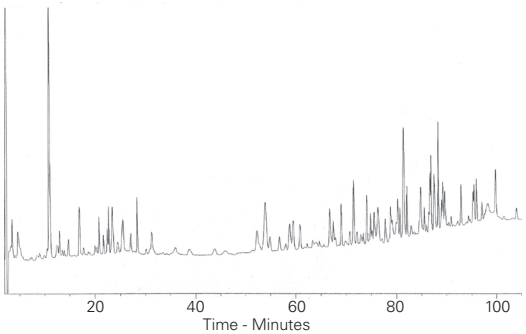
Conditions

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



Reproduced with permission of Department of Food Science, University of Reading, UK

Bufotenine Extract from *Rhinella Jimi* Toad Skin Secretions

Application #AN3800

Conditions

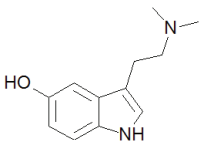
Column: ACE 5 C18
Dimensions: 250 x 7.75 mm (semi-preparative separation) and 250 x 4.6 mm (analytical)
Part Number: ACE-121-2508 and ACE-121-2546
Mobile Phase: A: 0.1% TFA in H_2O
B: 0.1% TFA in H_2O/MeCN (10:90 v/v)

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

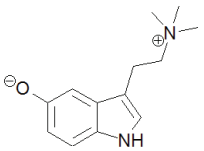
Flow Rate: 1.7 mL/min (semi-preparative) and 1.1 mL/min (analytical)
Temperature: 4 °C
Detection: UV, 214 nm
MS positive ESI mode for peak identification
Sample: Aqueous extract from liquid-liquid partition of toad skin secretion Fraction* from semi-preparative separation injected into analytical system.

Analytes

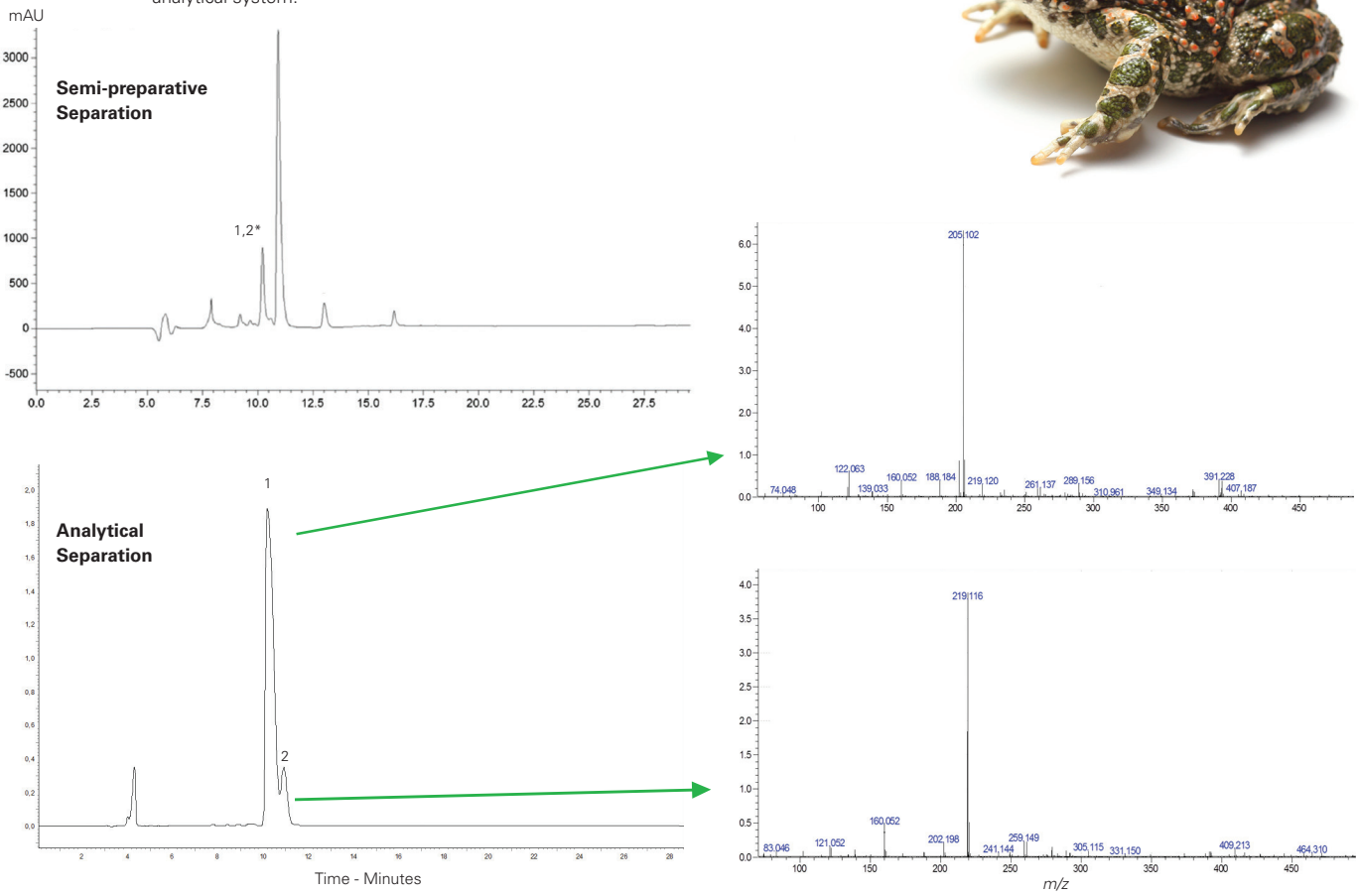
1. Bufotenine ([M+H]$^+$ *m/z* 205)
2. Bufotenidine (5-HTQ)



Bufotenine



Bufotenidine (5-HTQ)



AUTHORIZED DISTRIBUTOR
MZ-Analysentechnik GmbH, Barcelona-Allee 17 • D-55129 Mainz
Tel +49 6131 880 96-0, Fax +49 6131 880 96-20
e-mail: info@mz-at.de, www.mz-at.de

Caffeine and Metabolites

Application #AN2010

Conditions

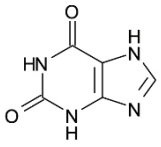
Column:	ACE Excel 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1211-1546U
Mobile Phase:	A: 20 mM ammonium acetate pH 7.0 in H_2O B: 20 mM ammonium acetate pH 7.0 in MeCN/H_2O (90:10 v/v)

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

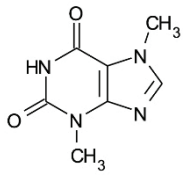
Flow Rate:	1 mL/min
Injection:	1 µL
Temperature:	60 °C
Detection:	UV, 273 nm

Analytes

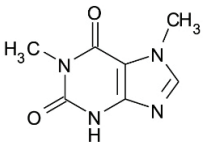
1. Xanthine
2. Theobromine
3. Paraxanthine
4. Theophylline
5. Caffeine



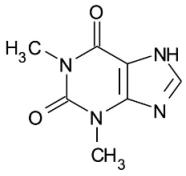
Xanthine



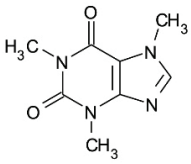
Theobromine



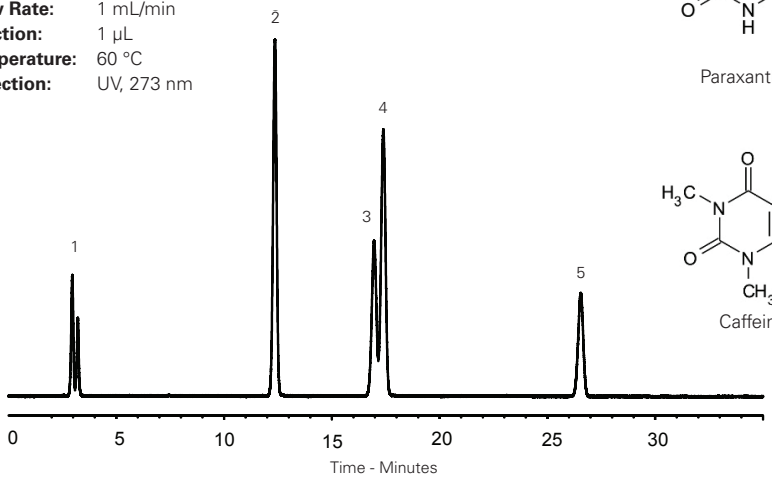
Paraxanthine



Theophylline



Caffeine



Caffeoylquinic and Dicaffeoylquinic Acids

Application #AN3520

Conditions

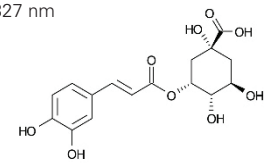
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	100 x 4.6 mm
Part Number:	CORE-25A-1046U
Mobile Phase:	A: 0.2% phosphoric acid in H_2O B: MeCN

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

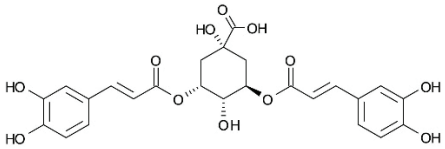
Flow Rate:	0.8 mL/min
Temperature:	35 °C
Detection:	UV-Vis, 327 nm

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)