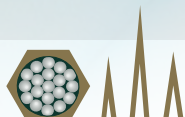


ACE[®]

UHPLC and HPLC Columns

Complete Applications Guide



ACE[®]

UHPLC and HPLC Columns

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

Preface

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

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

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



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

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

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

ACE performance
guarantee 

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



Contents

Page

| | |
|--|---------|
| ACE UHPLC/HPLC Columns, Product Specifications | 4 |
| Method Development Kits | 5–11 |
| Index by Application Type | 13–20 |
| A–Z Applications | 21–185 |
| Index by Analyte | 186–194 |

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 | *

3 PORE SIZES

90 Å | 100 Å | 300 Å

*New phases - launching soon.

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

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

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

| 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





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-AR | ACE C18-PFP |
|--|---|--|
| <p>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.</p> <p>Recommended Applications</p> <ul style="list-style-type: none"> • 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 | <p>ACE C18-AR combines the excellent performance and advantages of the ACE C18 phase with the added selectivity of an integral phenyl group.</p> <p>Recommended Applications</p> <ul style="list-style-type: none"> • 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. | <p>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.</p> <p>Recommended Applications</p> <ul style="list-style-type: none"> • 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 • Structural 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) | | | | | | |
|---|-----------------|---------------|-----------------|---------------|-----------------|---------------|
| Column Dimensions | 2 μm | | 3 μm | | 5 μm | |
| | 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, reusable 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 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

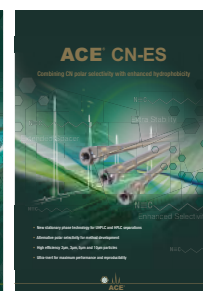
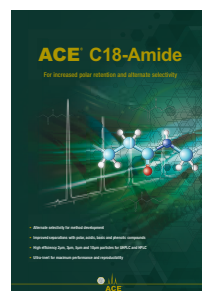
| ACE SuperC18 | ACE C18-Amide | ACE CN-ES |
|--|---|--|
| <p>ACE SuperC18 is a uniquely bonded, EBT™* endcapped C18 phase which offers unprecedented inertness, excellent efficiency and uncompromising durability over an extended pH range of 1.5 – 11.5.</p> <p>Recommended Applications</p> <ul style="list-style-type: none"> • 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 | <p>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.</p> <p>Recommended Applications</p> <ul style="list-style-type: none"> • 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 | <p>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.</p> <p>Recommended Applications</p> <ul style="list-style-type: none"> • 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) | | | | | | |
|---|-----------------|---------------|-----------------|---------------|-----------------|---------------|
| Column Dimensions | 2 μm | | 3 μm | | 5 μm | |
| | 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, reusable 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) | | | (UHPLC/HPLC hardware format with 1000 bar/15000 psi pressure limit) | | |
|---|---------------|--------------|---|---------------|--------------|
| Column Dimensions | 2.5 µm | 5 µm | Column Dimensions | 2.5 µm | 5 µm |
| 2.1 x 20 mm | MDKU-25-0202U | MDKU-5-0202U | 3.0 x 100 mm | MDKU-25-1003U | MDKU-5-1003U |
| 2.1 x 30 mm | MDKU-25-0302U | MDKU-5-0302U | 3.0 x 125 mm | MDKU-25-1203U | MDKU-5-1203U |
| 2.1 x 35 mm | MDKU-25-3502U | MDKU-5-3502U | 3.0 x 150 mm | MDKU-25-1503U | MDKU-5-1503U |
| 2.1 x 50 mm | MDKU-25-0502U | MDKU-5-0502U | 3.0 x 250 mm | - | MDKU-5-2503U |
| 2.1 x 75 mm | MDKU-25-7502U | MDKU-5-7502U | 4.6 x 20 mm | MDKU-25-0246U | MDKU-5-0246U |
| 2.1 x 100 mm | MDKU-25-1002U | MDKU-5-1002U | 4.6 x 30 mm | MDKU-25-0346U | MDKU-5-0346U |
| 2.1 x 125 mm | MDKU-25-1202U | MDKU-5-1202U | 4.6 x 35 mm | MDKU-25-3546U | MDKU-5-3546U |
| 2.1 x 150 mm | MDKU-25-1502U | MDKU-5-1502U | 4.6 x 50 mm | MDKU-25-0546U | MDKU-5-0546U |
| 2.1 x 250 mm | - | MDKU-5-2502U | 4.6 x 75 mm | MDKU-25-7546U | MDKU-5-7546U |
| 3.0 x 20 mm | MDKU-25-0203U | MDKU-5-0203U | 4.6 x 100 mm | MDKU-25-1046U | MDKU-5-1046U |
| 3.0 x 30 mm | MDKU-25-0303U | MDKU-5-0303U | 4.6 x 125 mm | MDKU-25-1246U | MDKU-5-1246U |
| 3.0 x 35 mm | MDKU-25-3503U | MDKU-5-3503U | 4.6 x 150 mm | MDKU-25-1546U | MDKU-5-1546U |
| 3.0 x 50 mm | MDKU-25-0503U | MDKU-5-0503U | 4.6 x 250 mm | - | MDKU-5-2546U |
| 3.0 x 75 mm | MDKU-25-7503U | MDKU-5-7503U | | | |

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) | | | | |
|---|---------------|----------------|--------------|---------------|
| Column Dimensions | 2.5 µm | | 5 µm | |
| | 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

- 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) | | | | |
|---|--------------|---------------|--------------|---------------|
| Column Dimensions | 3 µm | | 5 µm | |
| | 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, reusable 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

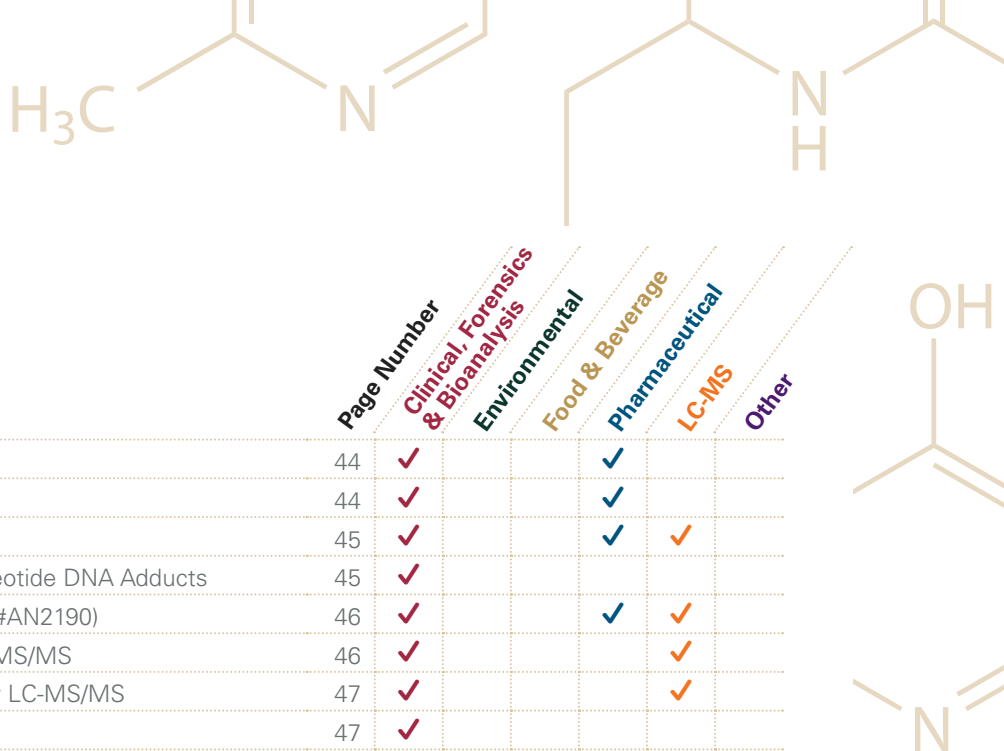
Please enquire for details of our
chromatography training, technical advice,
applications support, batch reservation
service and custom packing facility

email: info@ace-hplc.com



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 Derivatized with Dabsyl Chloride | 27 | ✓ | | | | | |
| Amino Acids in Extracellular Matrix | 26 | ✓ | | | | ✓ | |
| Amino Acids in Peas (<i>Pisum Sativum</i>) 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 | | | | ✓ | | |
| <i>Andrographis Paniculata</i> Fingerprint Profile by RRLC-TOF-MS | 34 | | | | ✓ | ✓ | |
| Angiotensin II Receptor Antagonists by LC-UV | 34 | ✓ | | | ✓ | | |
| Angiotensin Peptides | 35 | ✓ | | | | | |
| Annatto | 35 | | ✓ | | | | |
| Anthocyanins from <i>Sambucus Nigra</i> (Elderberry) | 36 | | ✓ | | | | |
| Antihistamines | 36 | ✓ | | | ✓ | | |
| Antihistamines and Expectorants | 36 | | | | ✓ | | |
| Antihistamines and Expectorants – Mobile Phase Effects | 37 | | | | ✓ | | |
| Antihistamines – Fast Analysis | 37 | | | | ✓ | | |
| Antimycins from Marine Sponge <i>Streptomyces</i> 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 (<i>Alaria Esculenta</i>) 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 | ✓ | | | ✓ | | |

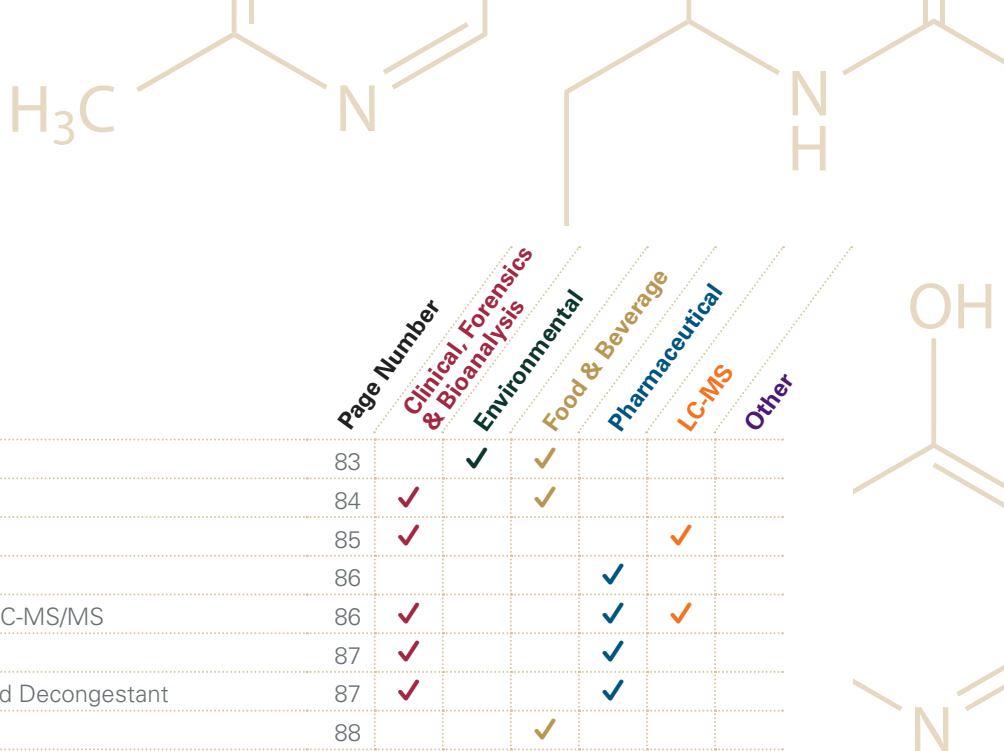


Application Index

| | 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 <i>Rhinella Jimi</i> Toad Skin Secretions | 49 | ✓ | | | | ✓ | |
| Caffeine and Metabolites | 50 | ✓ | ✓ | | | | |
| Caffeoylquinic and Dicafeoylquinic 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 (<i>Acacia Farnesiana</i>) | 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 <i>Cuscuta Chinensis</i> 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 | | ✓ | | | | |
| <i>Ginkgo Biloba</i> – Ultra Resolution | 78 | | ✓ | ✓ | | | |
| Ginseng Extract | 79 | | ✓ | | | | |
| Ginsenosides from Chinese Medicine by UHPLC-MS/MS | 78 | | ✓ | ✓ | ✓ | ✓ | |
| Gliotoxin from <i>Aspergillus Fumigatus</i> Liquid Culture | 80 | ✓ | ✓ | | | | |
| Glyphosate and Related Compounds as FMOX Derivatives (Gradient) | 80 | | ✓ | | | | |
| Glyphosate and Related Compounds as FMOX 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 | | ✓ | ✓ | | | |

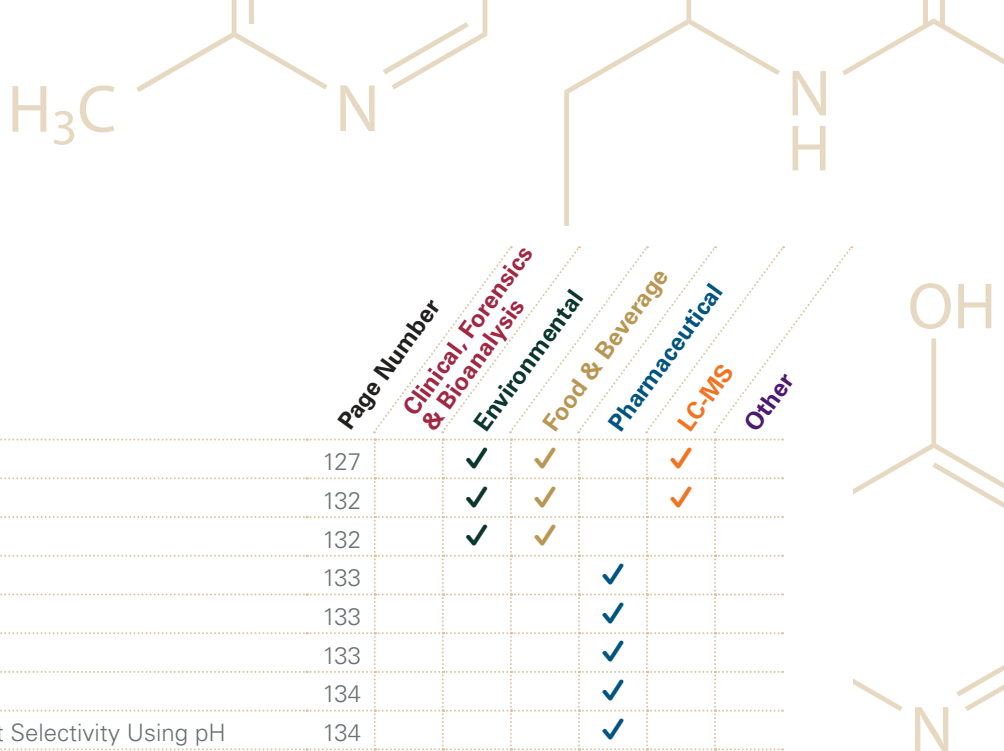


Application Index

| | 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 <i>Drosophila Melanogaster</i> | 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 ₂ EDTA Human Plasma by LC-MS/MS | 100 | ✓ | | | ✓ | ✓ | |
| 17 α -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 | | | | ✓ | | |
| <i>Paeonia Lactiflora</i> 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 | | ✓ | ✓ | | ✓ | |

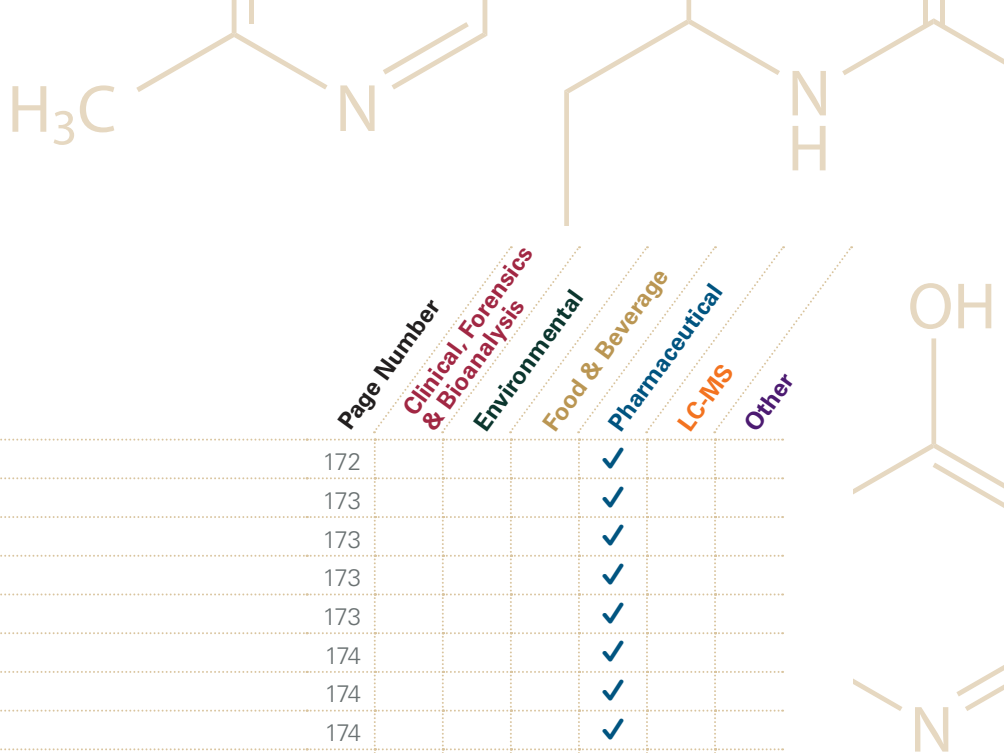


Application Index

| | 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 (<i>Echinacea Purpurea</i>) | 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 <i>Escherichia Coli</i> | 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 <i>Crotalus Durissus Terrificus</i> | 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 <i>Amanita Phalloides</i> 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 – 17 α -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

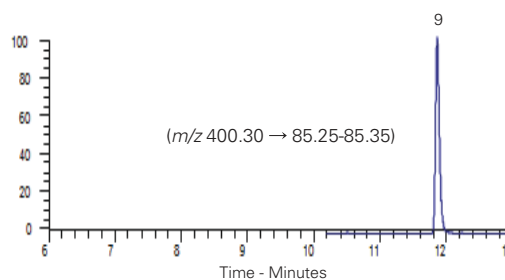
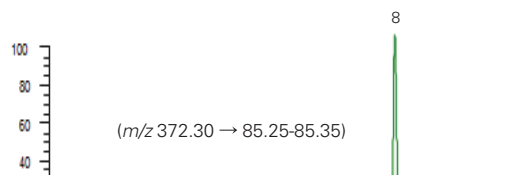
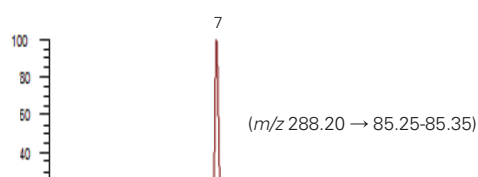
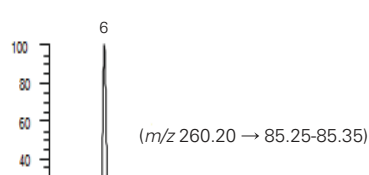
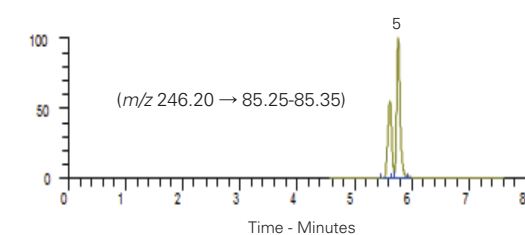
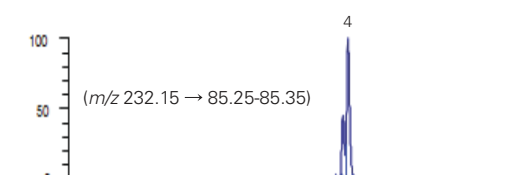
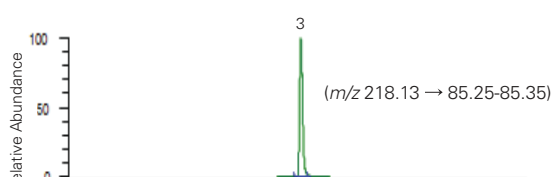
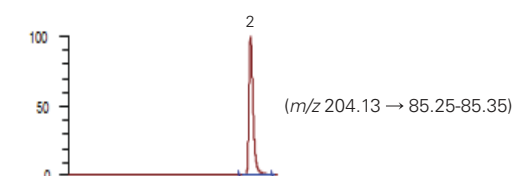
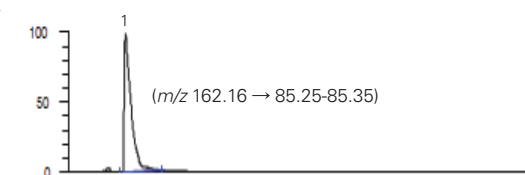
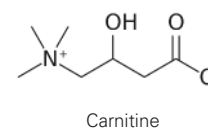
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

| 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



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





Additives and Intense Sweeteners

Application #AN2950

Conditions

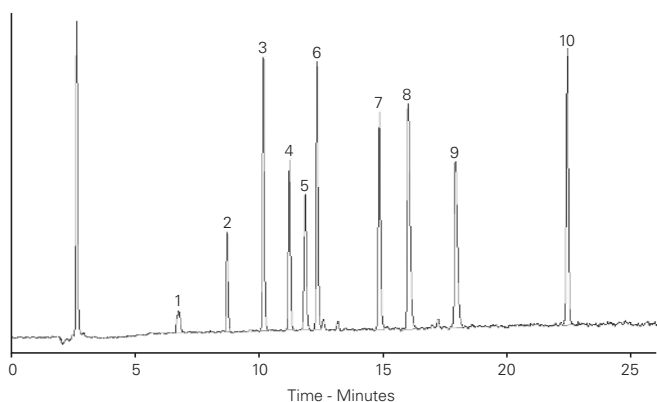
Column: ACE 5 C18
Dimensions: 250 x 4.0 mm
Part Number: ACE-121-2504
Mobile Phase: A: H₂O
 B: MeCN
 C: 1% TFA in H₂O
Gradient:

| 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

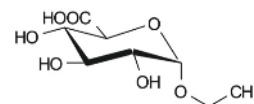
Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 1 mM ammonium fluoride
 B: MeCN
Gradient:

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

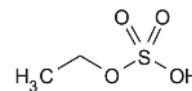
Flow Rate: 0.4 mL/min
Injection: 1 µL
Temperature: 40 °C
Detection: AB SCIEX triple quad 5500
 Negative ESI MRM
 Source temperature: 750 °C
 IonSpray voltage: -4500 V

Analytes

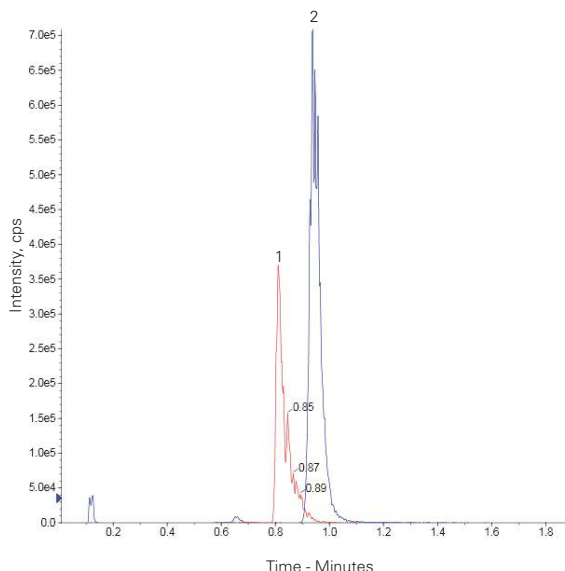
1. Ethyl glucuronide (EtG)
2. Ethyl sulphate (EtS)



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

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

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 H₂O
B: 0.1% formic acid in MeOH/H₂O (90:10 v/v)

Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 3 |
| 5 | 100 |

Flow Rate: 0.6 mL/min

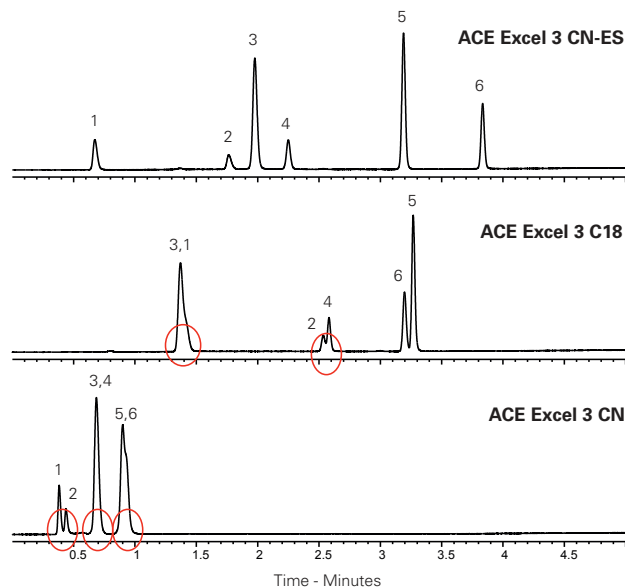
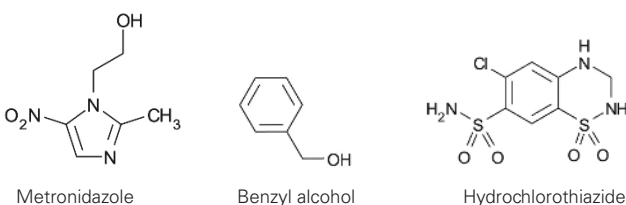
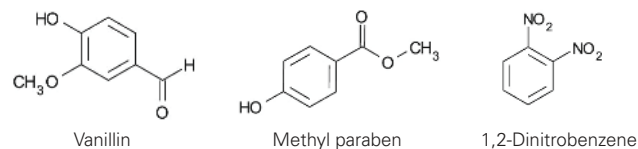
Injection: 1 µL

Temperature: 40 °C

Detection: UV, 254 nm

Analytes

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



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 H₂O
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

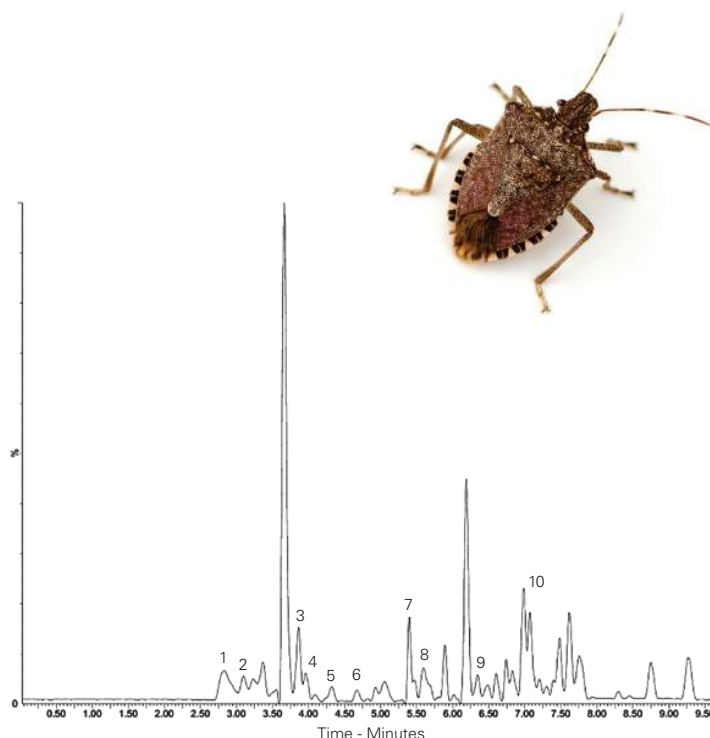
Injection: 1 µL

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



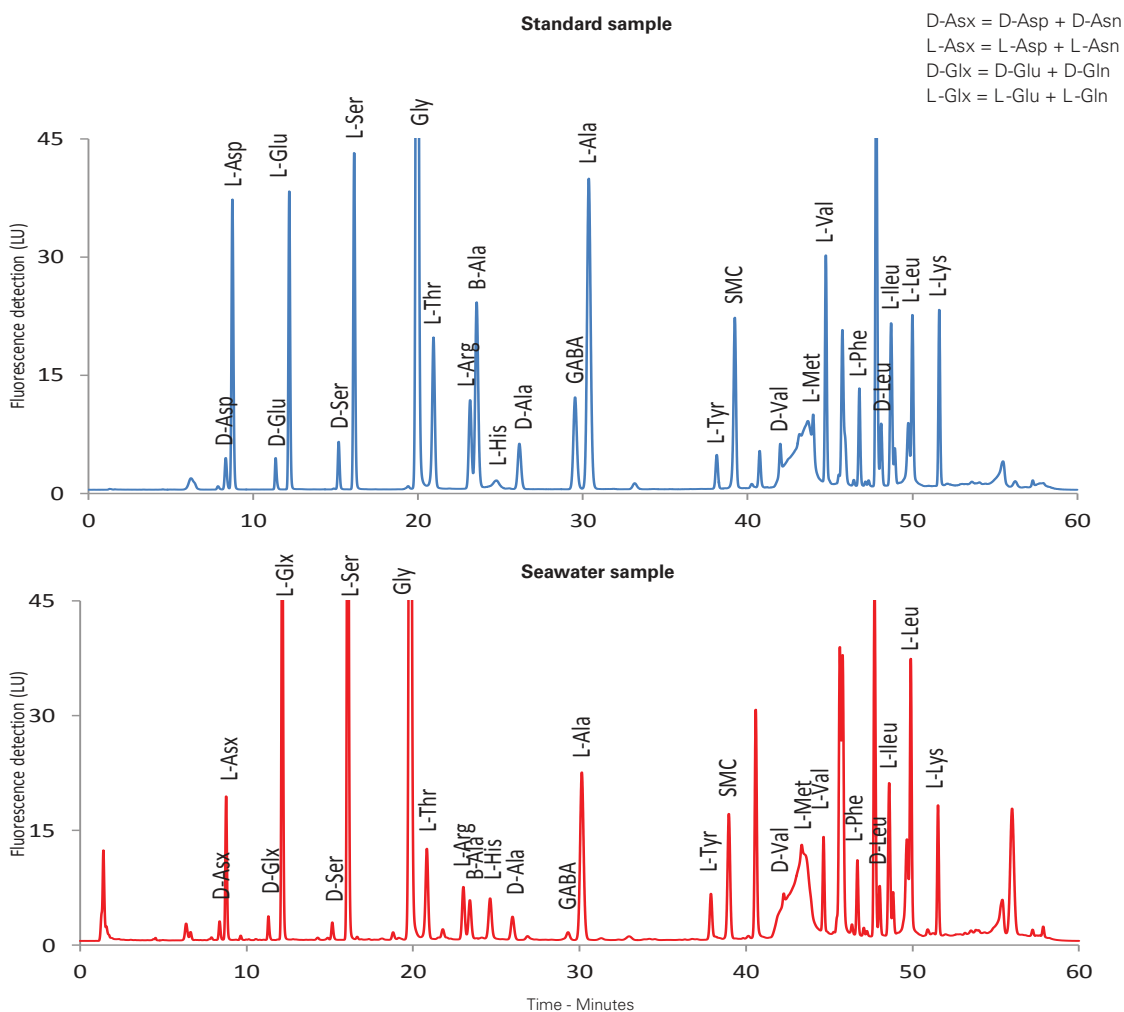
Amino Acid Enantiomer Separation of Seawater Samples

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-L-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: | <table border="1"> <thead> <tr> <th>Time (mins)</th> <th>%B</th> </tr> </thead> <tbody> <tr><td>0.0</td><td>0</td></tr> <tr><td>13.0</td><td>27</td></tr> <tr><td>33.0</td><td>36</td></tr> <tr><td>38.0</td><td>58</td></tr> <tr><td>54.0</td><td>92</td></tr> <tr><td>55.0</td><td>100</td></tr> <tr><td>57.5</td><td>0</td></tr> <tr><td>60.0</td><td>0</td></tr> </tbody> </table> | 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 |
| 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

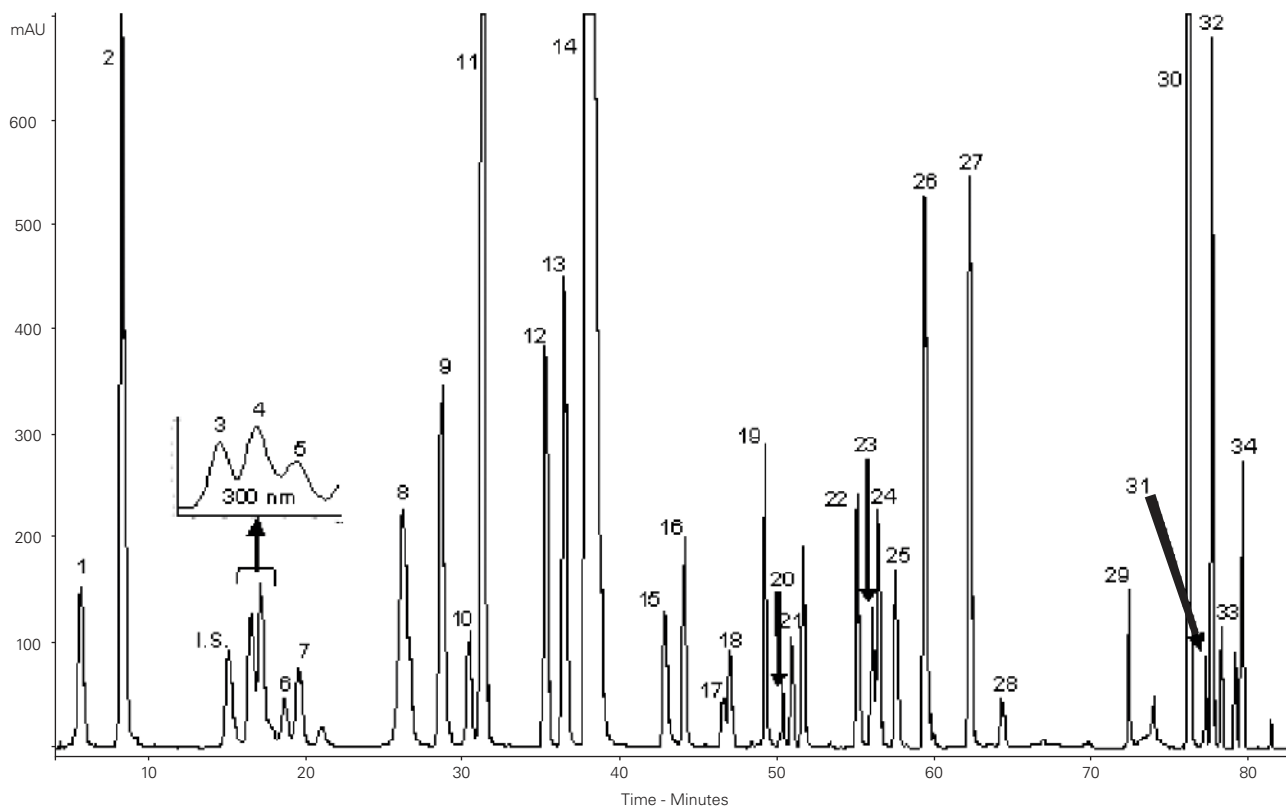
Temperature: 16 °C

Detection: DAD, 269, 280 and 300 nm

Sample: Derivatisation with diethyl ethoxymethylmalonate

Analytes

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



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 Page 1 of 2
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 H₂O
 B: 0.1% (v/v) formic acid in MeCN
Gradient:

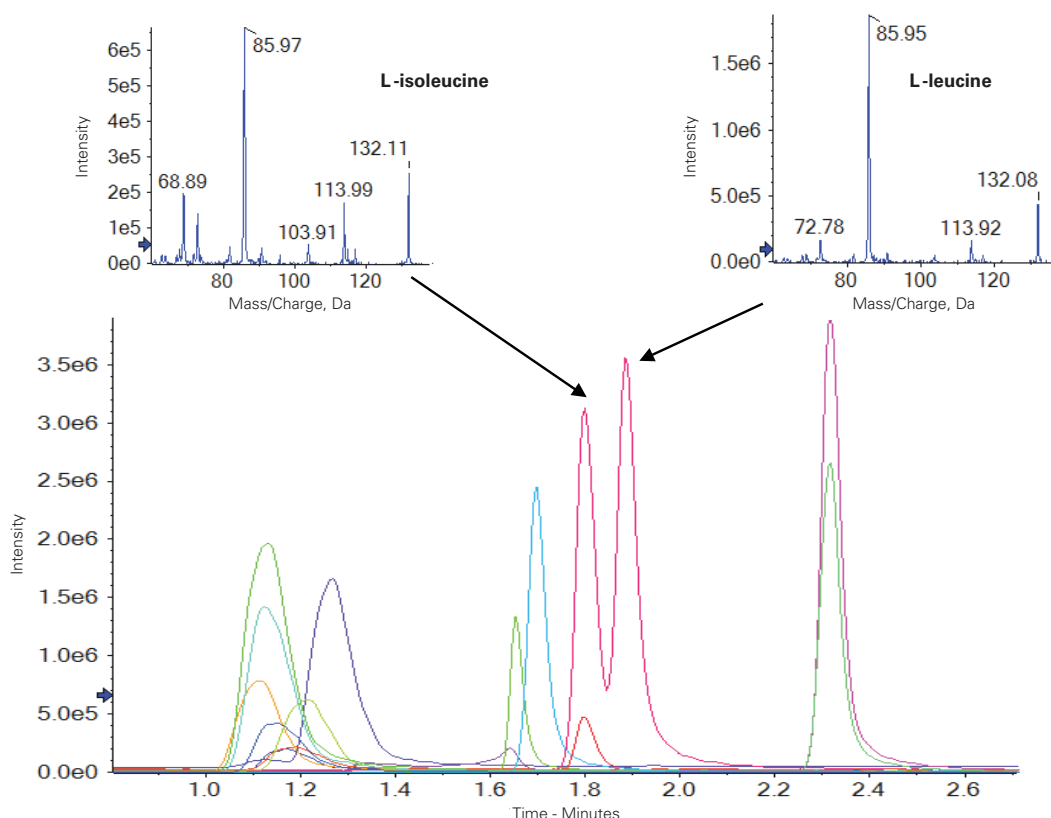
| Time (mins) | %B |
|-------------|----|
| 0 | 2 |
| 5 | 20 |

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.



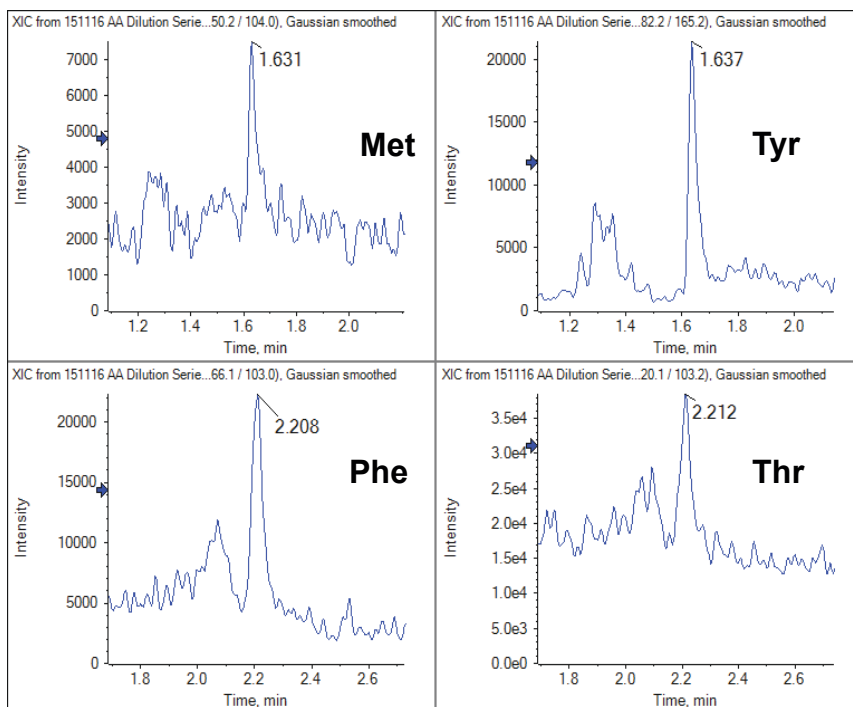
Reproduced with permission of SCIEX, Warrington, UK

Amino Acids in Extracellular Matrix (Continued)

Page 2 of 2

Application #AN4410

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



Reproduced with permission of SCIEX, Warrington, UK

Amino Acids Derivatized with Dabsyl Chloride

Application #AN3420

Conditions

Column: ACE 3 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-111-1503
Mobile Phase: A: 10 mM KH₂PO₄ buffer (pH 6.55)
 B: MeCN/2-Propanol (70:30 v/v)

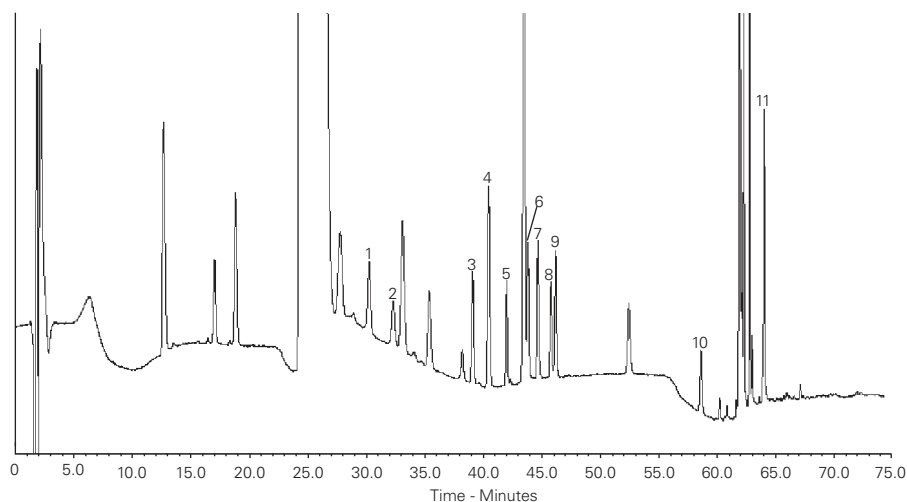
Gradient:

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



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



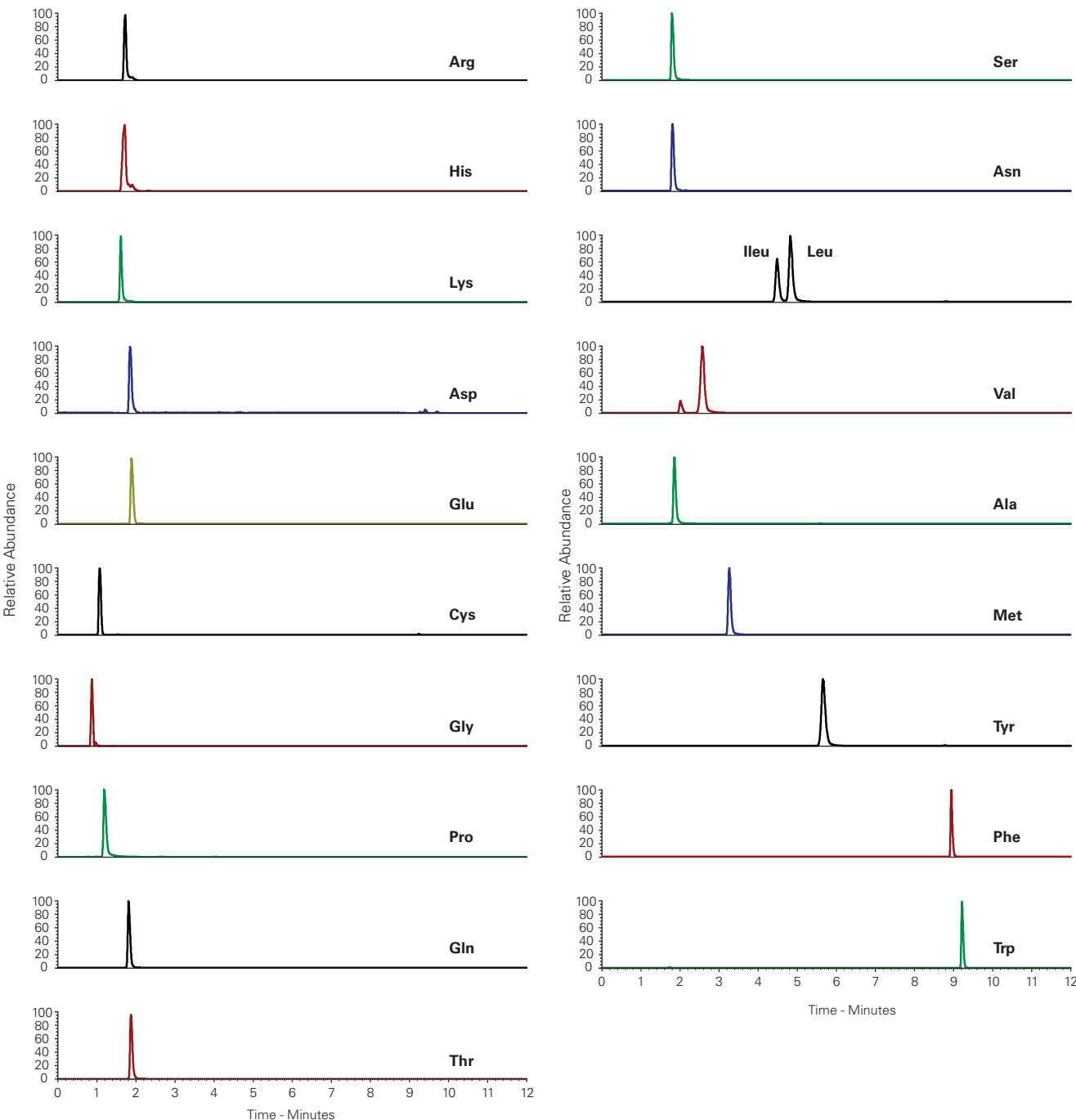
Amino Acids in Peas (*Pisum Sativum*) by HPLC-HRAM-MS Application #AN2660

Conditions

Column: ACE 3 AQ
Dimensions: 150 x 3.0 mm
Part Number: ACE-116-1503
Mobile Phase: A: 0.1% formic acid in H₂O
 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: Exacte 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 H₂O/MeCN (98:2 v/v)
 B: 20 mM HFBA in MeCN/H₂O (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

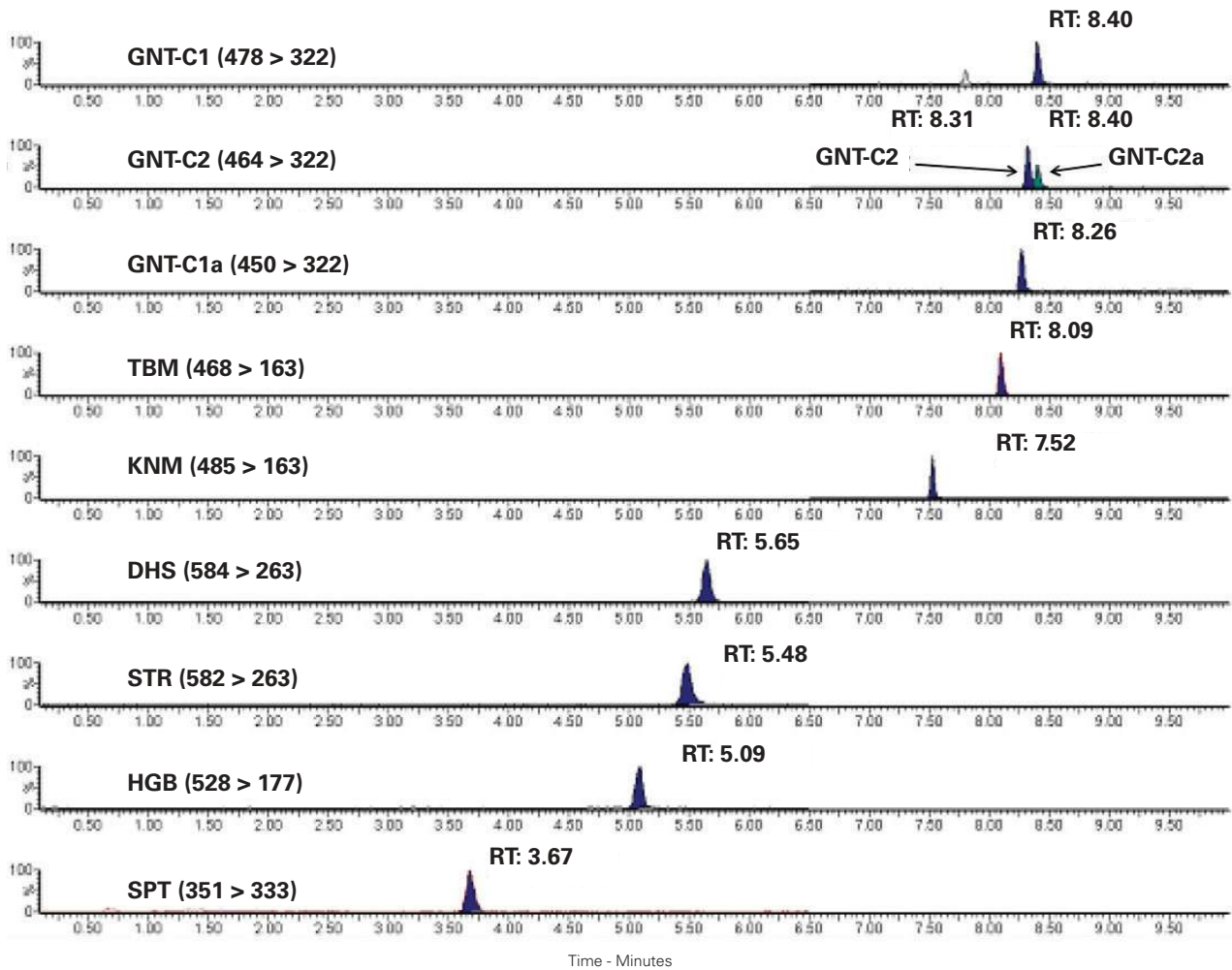
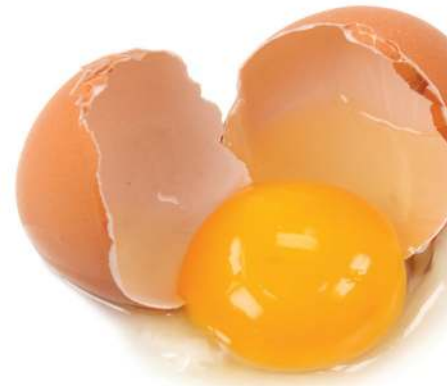
Temperature: 40 °C

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 Higmomycin-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

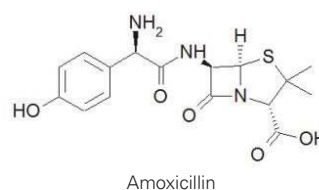
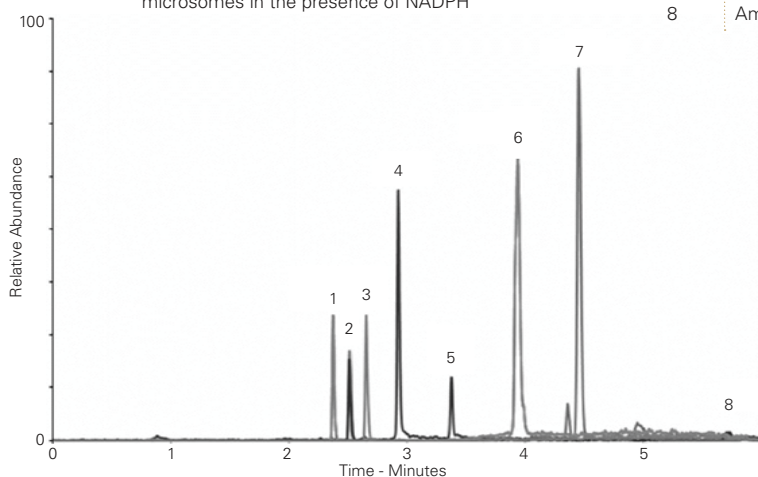
Application #AN4400

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 H₂O/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 ₃ O ₆ S | Hydroxylation |
| 2 | M2 | 379 | C ₁₇ H ₁₉ N ₂ O ₇ S | Oxidative deamination |
| 3 | M3 | 382 | C ₁₆ H ₂₀ N ₃ O ₆ S | Oxidation of aliphatic chain |
| 4 | M4 | 380 | C ₁₆ H ₁₈ N ₃ O ₆ S | Oxidation of aliphatic chain |
| 5 | M5 | 396 | C ₁₆ H ₂₀ N ₃ O ₇ S | Oxidation of aliphatic chain |
| 6 | M6 | 322 | C ₁₅ H ₁₉ N ₃ O ₅ S | Decarboxylation |
| 7 | M7 | 542 | C ₂₅ H ₂₈ N ₃ O ₁₁ S | Glucuronidation |
| 8 | Amoxicillin | 366 | C ₁₆ H ₂₀ N ₃ O ₅ S | |



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

ACE Method Development Kits

Intelligent Solutions for Method Development



- **Highly cost effective** - 2 and 3 column kits available for the same price as a single column
- **4 different Method Development Kits** available in dimensions from microbore (0.5 mm id) through to analytical (4.6 mm id) for rapid, systematic method development.
- Carefully selected ACE phases enabling the power of selectivity to be fully exploited
- Each ACE phase provides different selectivity due to differing interactions

FREE Application Support and FREE Method Development Service

Learn more: www.ace-hplc.com or email: info@ace-hplc.com

Amphetamines from Drugs of Abuse Screen (#AN2190)

Application #AN2350

Conditions

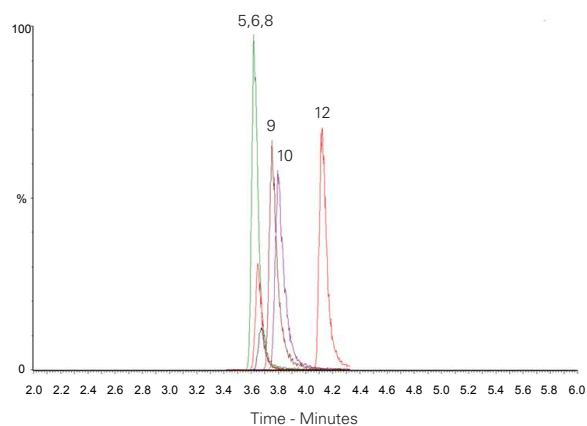
Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 5 mM ammonium acetate in H₂O
 B: 5 mM ammonium acetate in MeOH
Gradient:

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

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

Analytes

- Amphetamine-d5
(*m/z* 141.0 → 123.9)
- Amphetamine
(*m/z* 136.0 → 118.9)
- MDA
(*m/z* 180.1 → 105.0)
- MDMA
(*m/z* 194.1 → 163.0)
- Methamphetamine
(*m/z* 150.0 → 90.9)
- MDEA
(*m/z* 208.2 → 163.0)



Amphetamines in Urine by LC-MS/MS

Application #AN1010

Conditions

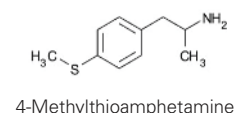
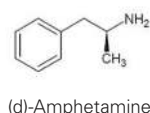
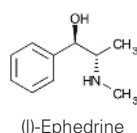
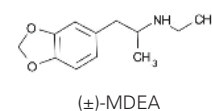
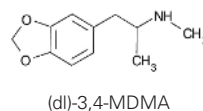
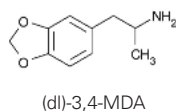
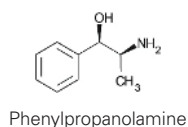
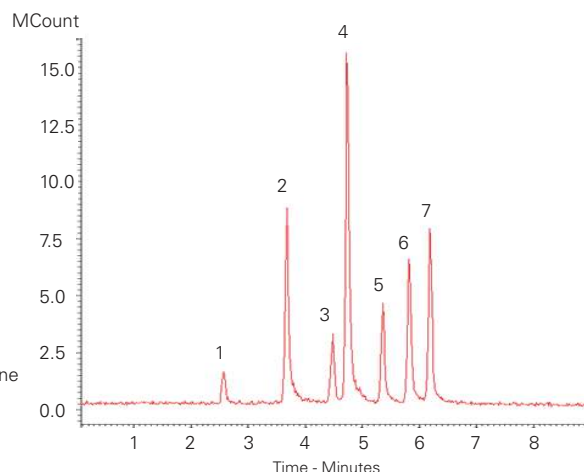
Column: ACE Excel 3 SuperC18
Dimensions: 75 x 2.1 mm
Part Number: EXL-1111-7502U
Mobile Phase: A: 5 mM ammonium hydroxide
 pH 10.8 in H₂O
 B: 5 mM ammonium hydroxide pH 10.8
 in MeOH/H₂O (90:10 v/v)
Gradient:

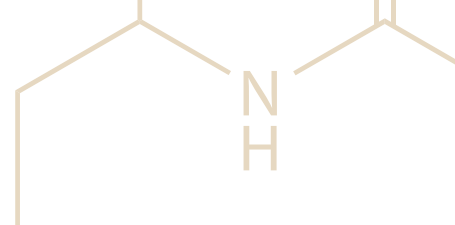
| Time (mins) | %B |
|-------------|----|
| 0 | 30 |
| 8 | 95 |

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

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





Anabolic Steroids from Horse Urine by LC-MS/MS

Application #AN2360

Conditions

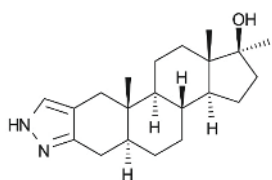
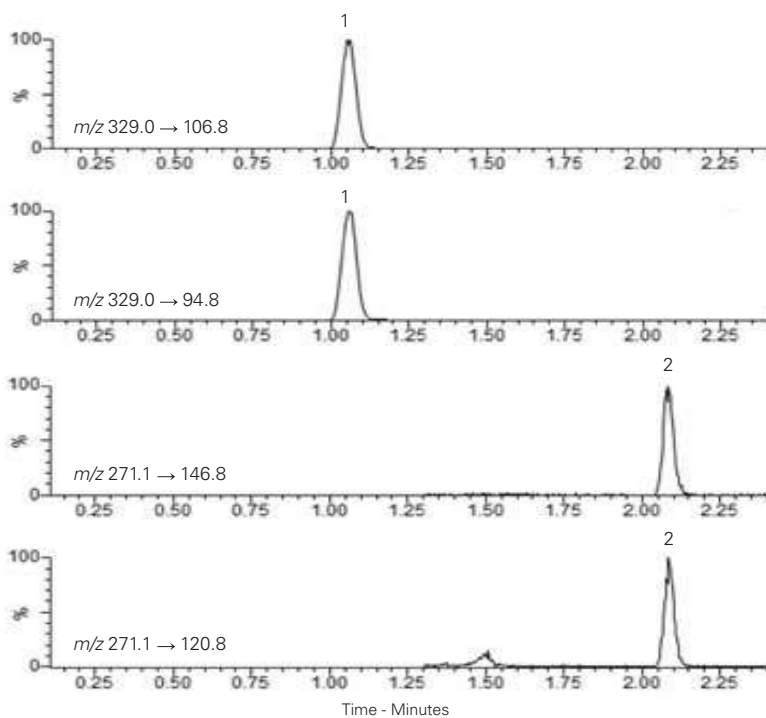
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O
 B: 2 mM ammonium acetate, 0.1% formic acid in MeOH
Gradient:

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

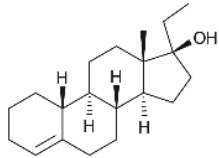
Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: Premier XE triple quad MS
 MRM positive ion mode
 Desolvation temperature: 450 °C
 Ion Source temperature: 120 °C

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

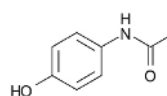
Column: ACE Excel 2 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: EXL-1011-0502U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

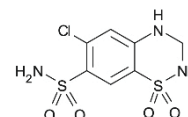
Flow Rate: 1.2 mL/min
Injection: 0.5 µL
Temperature: 50 °C
Detection: UV, 214 nm

Analytes

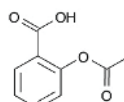
1. Paracetamol
2. Hydrochlorothiazide
3. Aspirin
4. Bendroflumethiazide
5. Ketoprofen
6. Flurbiprofen
7. Ibuprofen



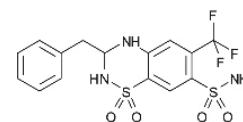
Paracetamol



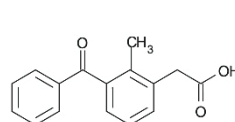
Hydrochlorothiazide



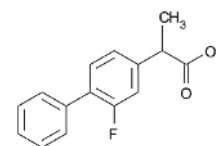
Aspirin



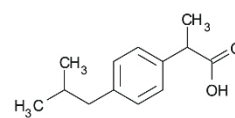
Bendroflumethiazide



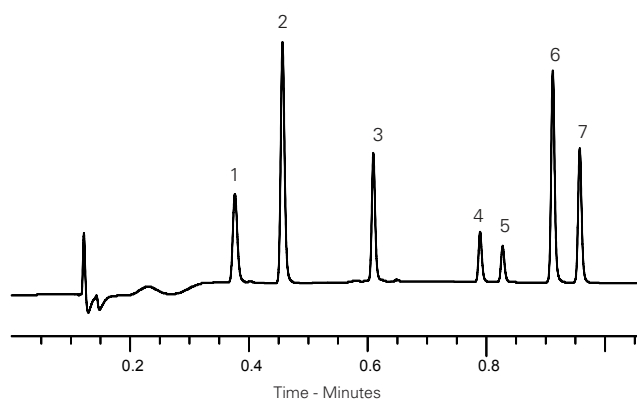
Ketoprofen



Flurbiprofen



Ibuprofen



Analgesic Separation

Application #AN2490

Conditions

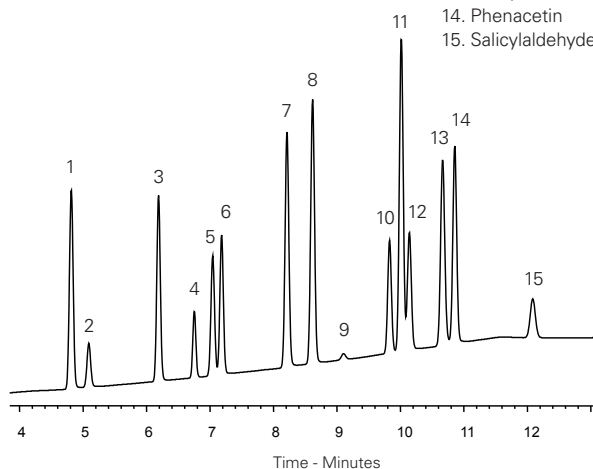
Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| 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

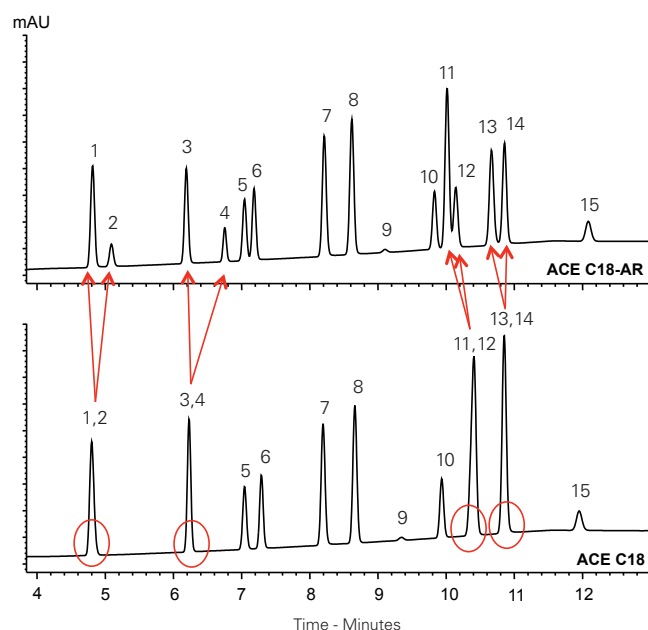
Column: ACE 3 C18-AR
 ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Numbers: ACE-119-1546
 ACE-111-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| 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

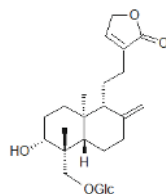
Column: ACE Excel 3 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: EXL-1111-1002U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN

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

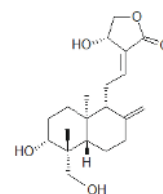
Flow Rate: 0.2 mL/min
Injection: 2 µL
Temperature: 35 °C
Detection: Waters Premier Q-TOF-MS
 ESI in positive ion mode
 Scan Range *m/z* 100-1000 Da

Analytes

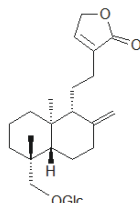
- 14-Deoxyandrographiside
- Andrographolide
- Neoandrographolide
- 14-Deoxyandrographolide
- Dehydroandrographolide



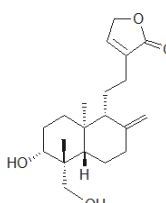
14-Deoxyandrographiside
 (*Tentative assignment)



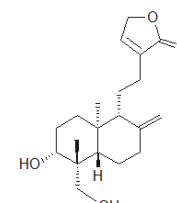
Andrographolide



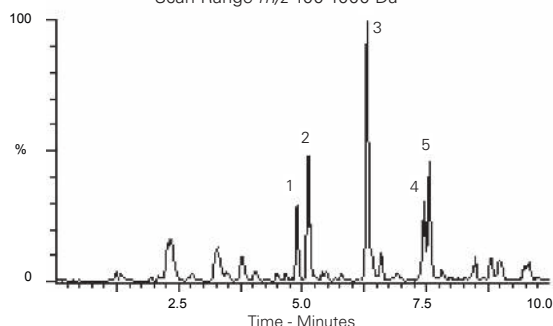
Neoandrographolide



14-Deoxyandrographolide
 (*Tentative assignment)



Dehydroandrographolide



Andrographis Paniculata -
 used in Chinese medicine.



Song YX, 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

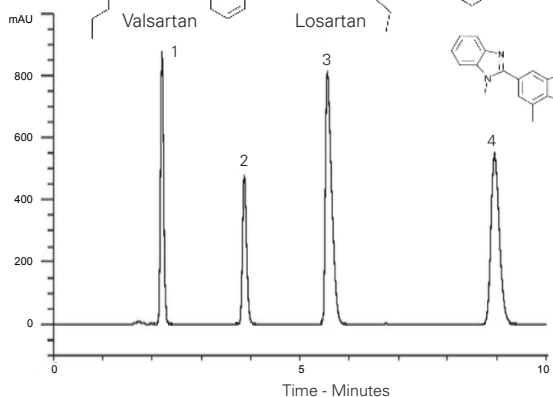
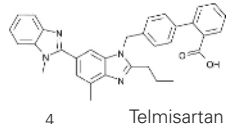
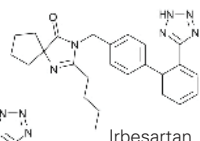
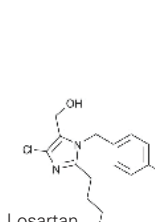
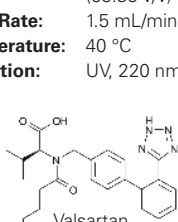
Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 0.025 M KH₂PO₄ 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



For further applications

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

Elshawanawane 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

Angiotensin Peptides

Application #AN2150

Conditions

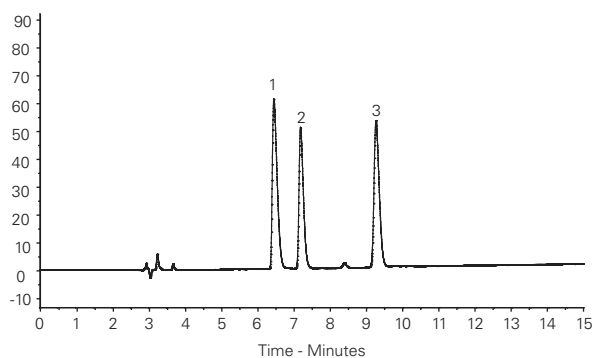
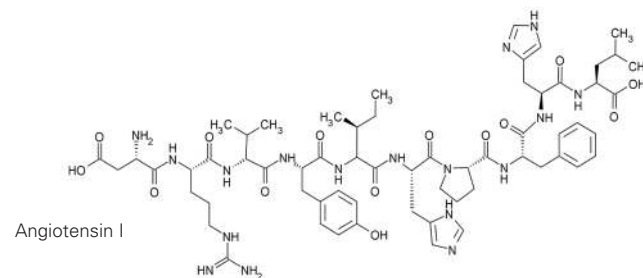
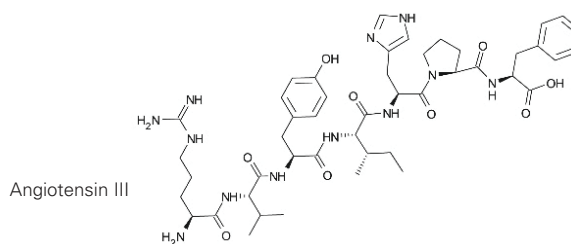
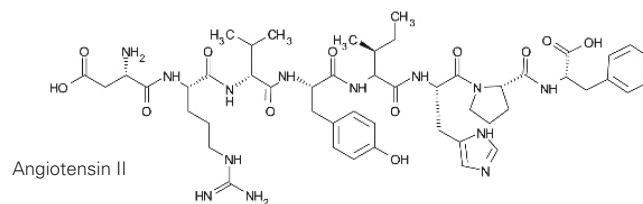
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in H₂O/MeCN (80:20 v/v)
Gradient:

| 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

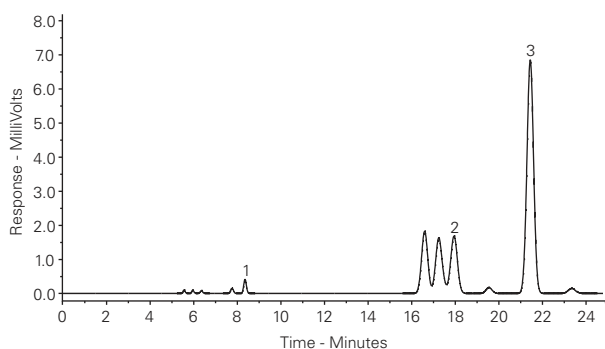
Application #AN2840

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/0.16% acetic acid in H₂O (70:30 v/v)
Flow Rate: 1.2 mL/min
Temperature: Ambient
Detection: UV-VIS, 478 nm

Analytes

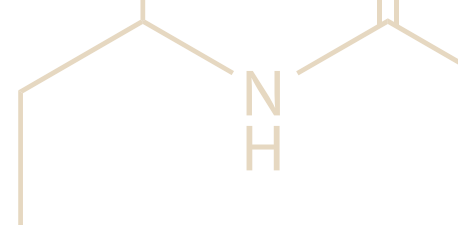
1. Norbixin
2. 9'-trans-Bixin
3. 9'-cis-Bixin



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

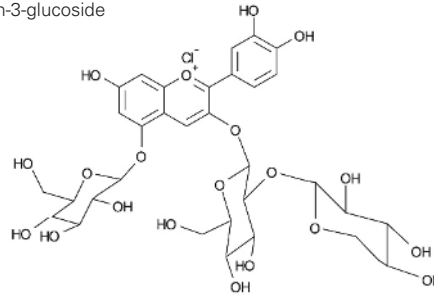
Column: ACE UltraCore 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: CORE-5A-1546U
Mobile Phase: A: 5% formic acid in H₂O
 B: MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 5 |
| 35 | 10 |
| 55 | 65 |
| 65 | 65 |

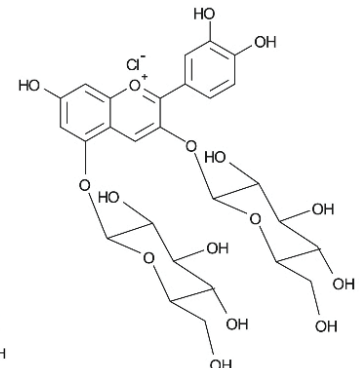
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: UV-Vis, 525 nm

Analytes

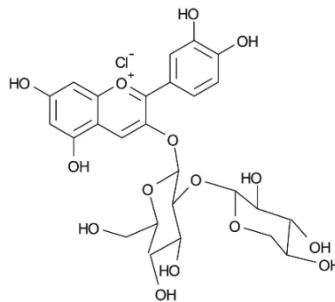
1. Cyanidin-3-sambubioside-5-glucoside
2. Cyanidin-3,5-diglucoside
3. Cyanidin-3-sambubioside
4. Cyanidin-3-glucoside



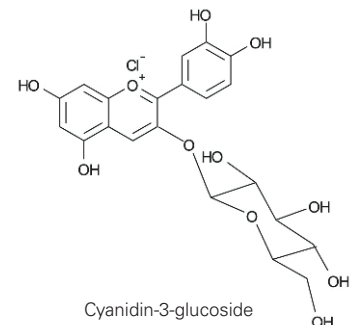
Cyanidin-3-sambubioside-5-glucoside



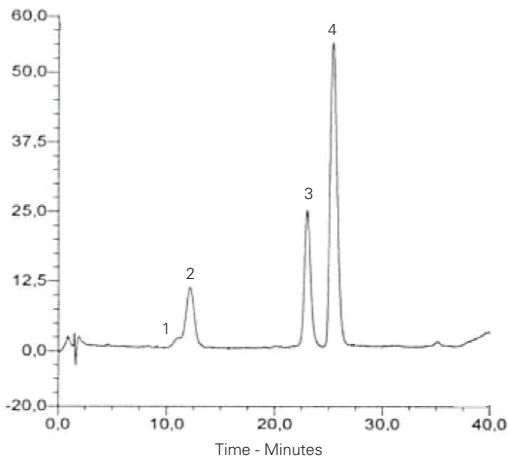
Cyanidin-3,5-diglucoside



Cyanidin-3-sambubioside



Cyanidin-3-glucoside



Reproduced with permission of University of Vila Real, Portugal

Antihistamines

Application #AN1400

Conditions

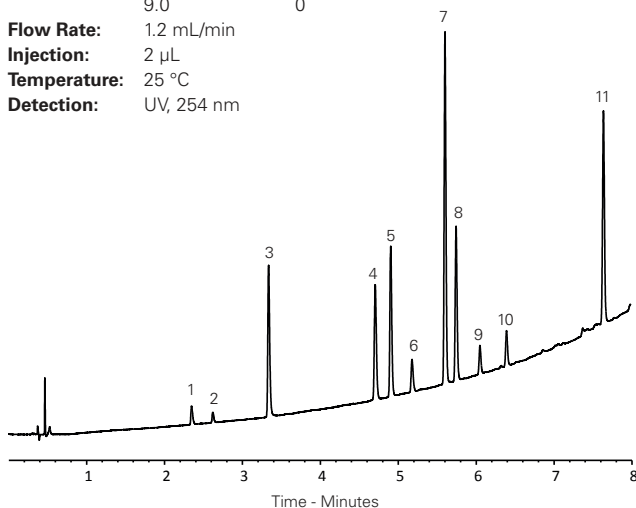
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: CORE-25A-1003U
Mobile Phase: A: 20 mM ammonium formate pH 3.0 in H₂O
 B: 20 mM ammonium formate pH 3.0 in MeOH/H₂O (9:1 v/v)
Gradient:

| 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

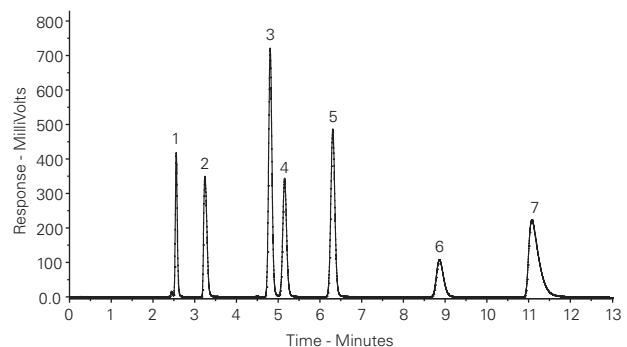
Application #AN3190

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeOH/50 mM KH₂PO₄ (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. Guaiaicol
6. Chlorpheniramine maleate
7. Dextromethorphan



Antihistamines and Expectorants – Mobile Phase Effects

Application #AN3960

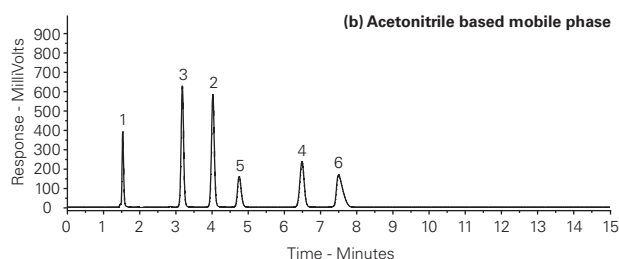
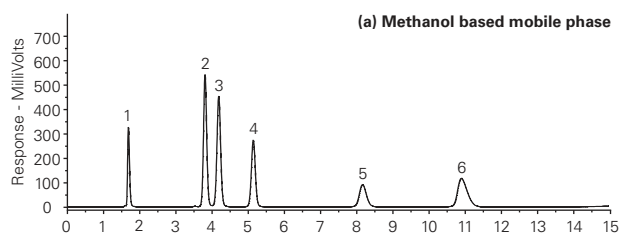
Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: (a) MeOH/50 mM KH₂PO₄ (pH 3.0) (45:55 v/v)
 (b) MeCN/50 mM KH₂PO₄ (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

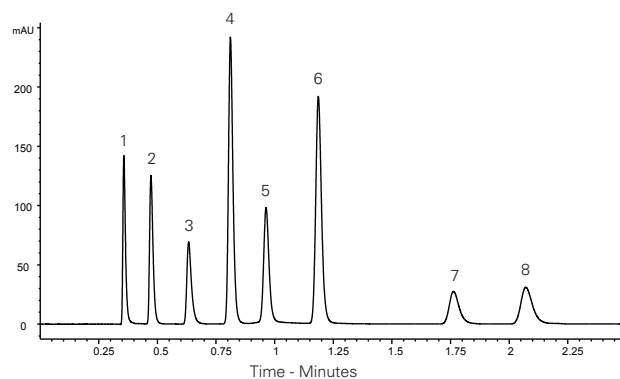
Application #AN4290

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: 30 mM KH₂PO₄ pH 2.7 in H₂O/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 H₂O
 B: 0.1% ammonia in MeCN/H₂O (90:10 v/v)

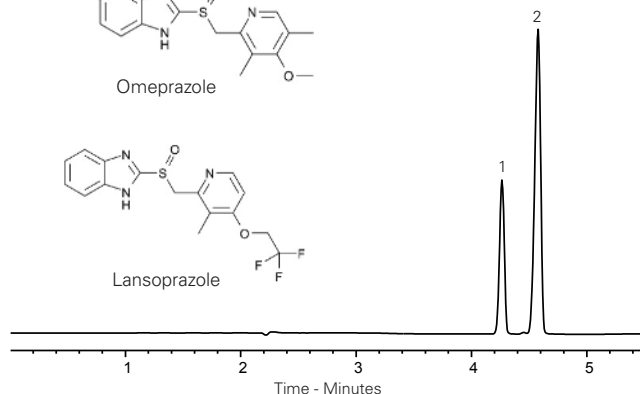
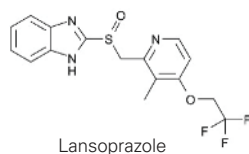
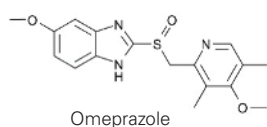
Gradient:

| 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

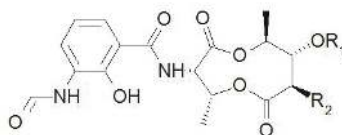
Conditions

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 H₂O
 B: 0.1% (v/v) formic acid in MeCN
Gradient:

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

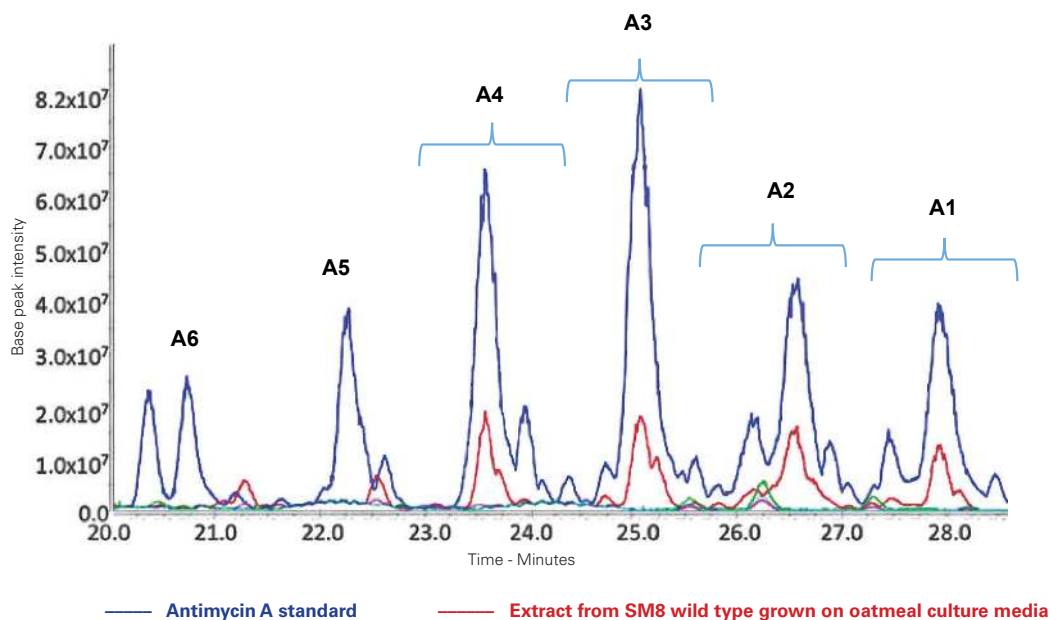
Flow Rate: 0.3 mL/min
Injection: 10 µL
Detection: Thermo Exactive Orbitrap
 High resolution (15,000)
 ESI in positive ion mode
 Spray Voltage: 4.5 kV
 Capillary Temperature: 268 °C
 Capillary Voltage: 30 V

Sample: Antifungal fraction from *Streptomyces* sp.
 SM8 extract from *Haliclona simulans* marine sponge



Antimycin A

| Antimycin | R ₁ | R ₂ |
|-----------|--|---|
| A1a | C=OCH(CH ₃)CH ₂ CH ₃ | (CH ₂) ₅ CH ₃ |
| A1b | C=OCH ₂ CH(CH ₃) ₂ | (CH ₂) ₅ CH ₃ |
| A2a | C=OCH(CH ₃) ₂ | (CH ₂) ₅ CH ₃ |
| A2b | C=OCH ₂ CH ₂ CH ₃ | (CH ₂) ₅ CH ₃ |
| A3a | C=OCH(CH ₃)CH ₂ CH ₃ | (CH ₂) ₅ CH ₃ |
| A3b | C=OCH ₂ CH(CH ₃) ₂ | (CH ₂) ₅ CH ₃ |
| A4a | C=OCH(CH ₃) ₂ | (CH ₂) ₅ CH ₃ |
| A4b | C=OCH ₂ CH ₂ CH ₃ | (CH ₂) ₅ CH ₃ |
| A5 | C=OCH ₂ CH(CH ₃) ₂ | CH ₂ CH ₃ |
| A6 | C=OCH ₂ CH ₂ CH ₃ | CH ₂ CH ₃ |



Vieglmann 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

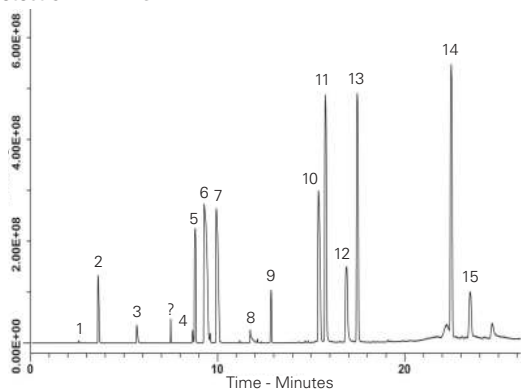
Conditions
Column: ACE Excel 2 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: EXL-1011-1002U
Mobile Phase: A: 10 mM ammonium acetate pH 9.35 with ammonium hydroxide
 B: 10 mM ammonium acetate pH 9.35/MeCN (10:90 v/v)
Gradient:

| 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

- Caffeine
- Ephedrine
- Phentermine
- Phenolphthalein
- Chlordiazepoxide
- Lorcaserin
- Fenfluramine
- Fluoxetine
- Diethylpropion
- Sertraline
- Didesmethylsibutramine
- Rimonabant
- N-Desmethylsibutramine
- Sibutramine
- Orlistat



Reproduced with permission of US FDA

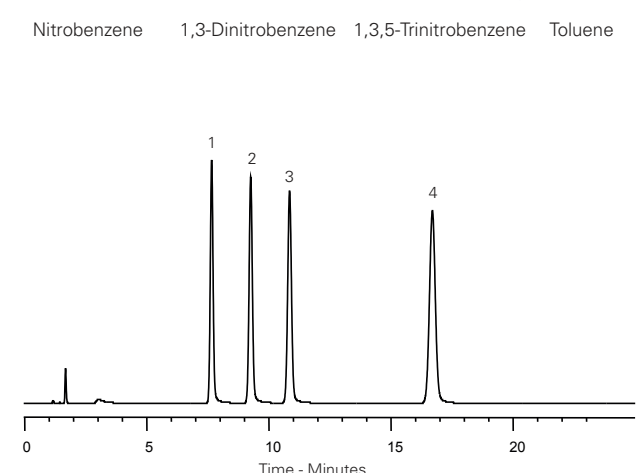
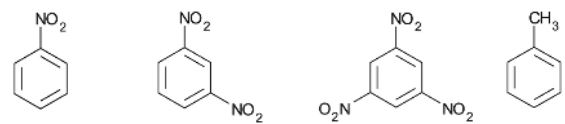
Aromatic Nitrobenzenes

Application #AN2480

Conditions
Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: H₂O/MeOH (50:50 v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: UV, 210 nm

Analytes

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

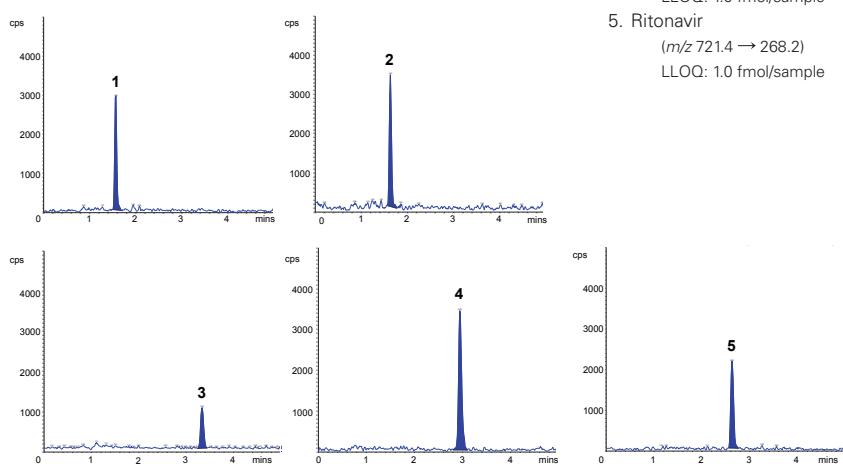
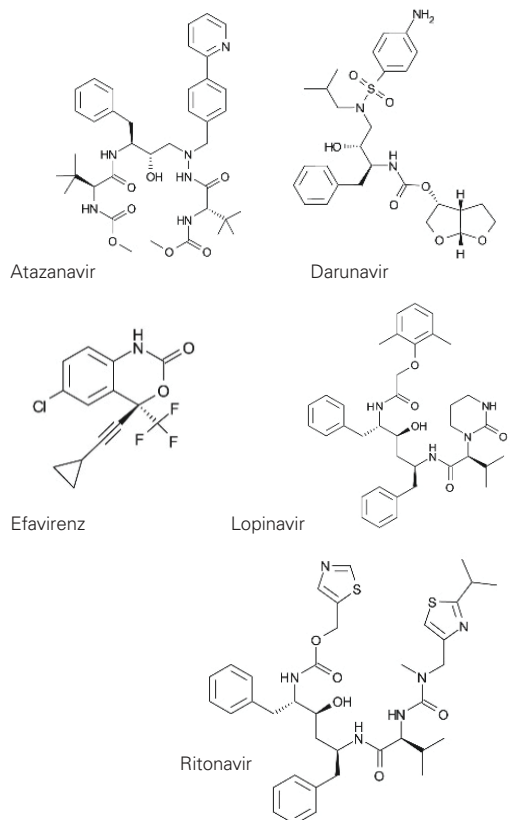


Antiretrovirals in Human Mononuclear Cell Extracts by LC-MS/MS

Application #AN3470

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

- Analytes**
- Atazanavir
(*m/z* 705.4 → 168.2)
LLOQ: 0.04 fmol/sample
 - Darunavir
(*m/z* 548.3 → 392.3)
LLOQ: 1.0 fmol/sample
 - Efavirenz
(*m/z* 313.9 → 244.0)
LLOQ: 4.0 fmol/sample
 - Lopinavir
(*m/z* 629.4 → 447.3)
LLOQ: 1.0 fmol/sample
 - Ritonavir
(*m/z* 721.4 → 268.2)
LLOQ: 1.0 fmol/sample



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 H₂O
 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:

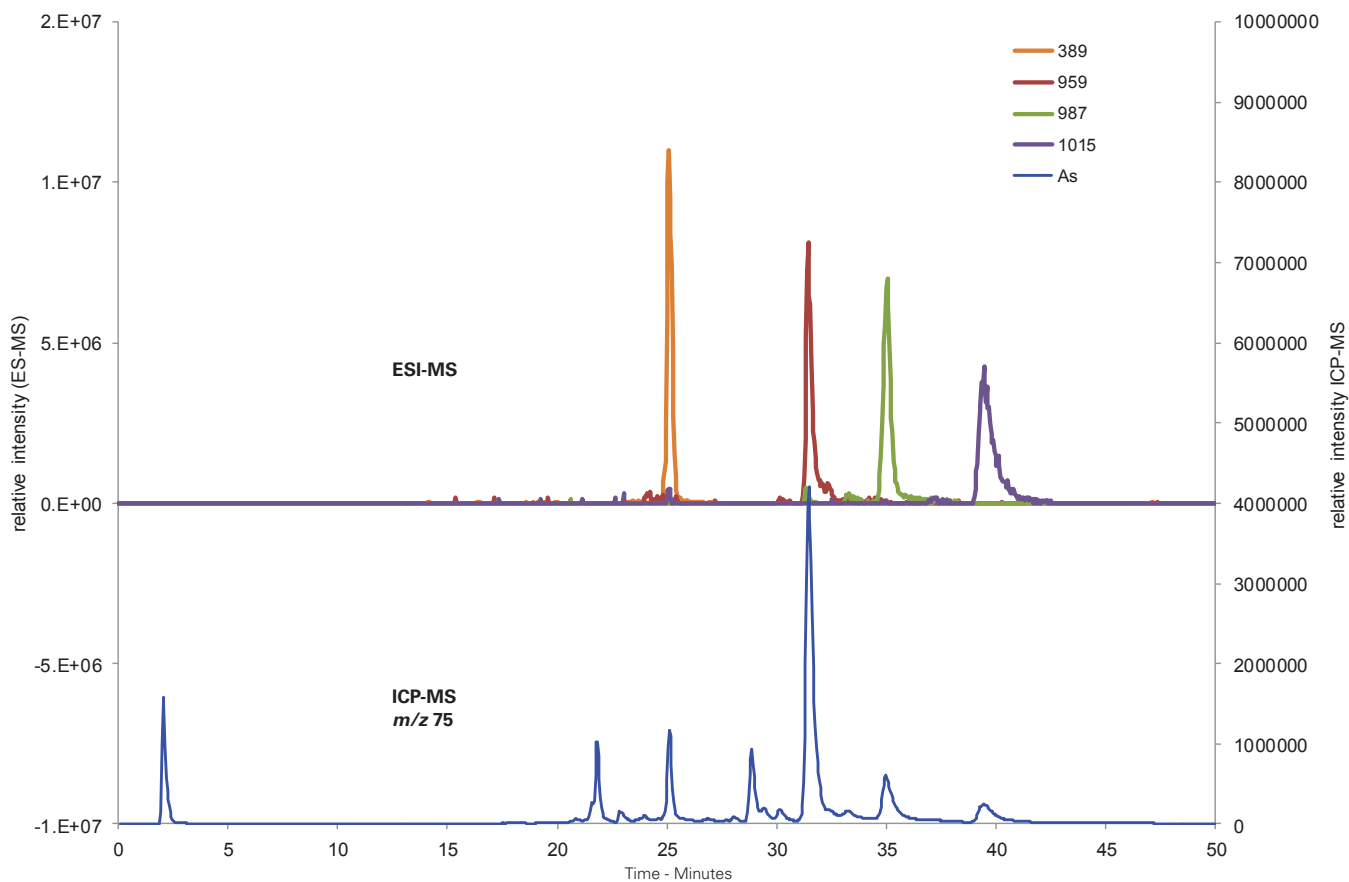
m/z 389 [M + H]⁺ for C₂₁H₄₆AsO

Arsenic-containing phospholipids:

m/z 959 [M + H]⁺ for C₄₅H₈₉AsO₁₄P (C16:0/C16:0)

m/z 987 [M + H]⁺ for C₄₇H₉₃AsO₁₄P (C18:0/C16:0)

m/z 1015 [M + H]⁺ for C₄₉H₉₇AsO₁₄P (C20:0/C16:0)



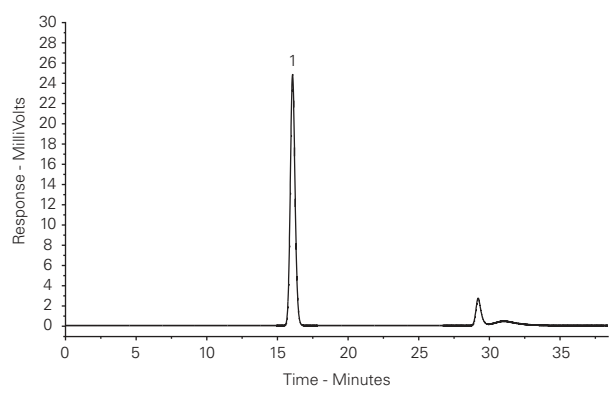
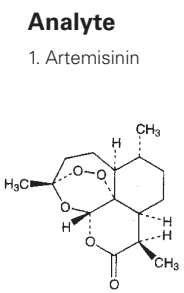
Reproduced with permission of Trace Element Speciation Laboratory, University of Aberdeen, UK

Artemisinin Application #AN3140

Conditions
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: H₂O
 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



Reproduced with permission of Neem Biotech, Cardiff, UK

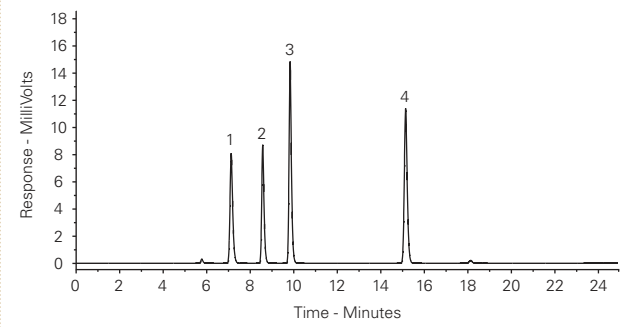
Artificial Food Colours Application #AN2960

Conditions
Column: ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-111-1046
Mobile Phase: A: 3.1 mM TBAB¹ and 5 mM KH₂PO₄ in H₂O
 B: 5 mM KH₂PO₄ 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
¹Tetrabutylammonium bromide

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



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

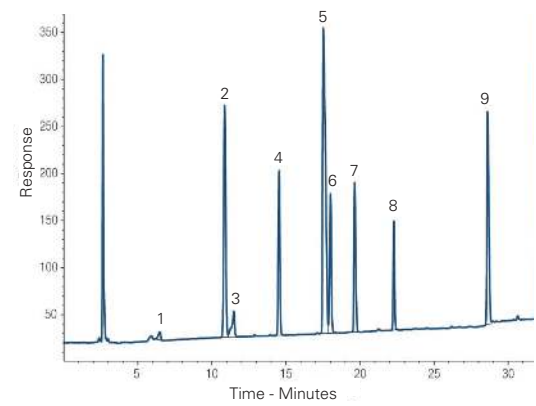
Artificial Sweeteners Global Method Application #AN1980

Conditions
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: H₂O
 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

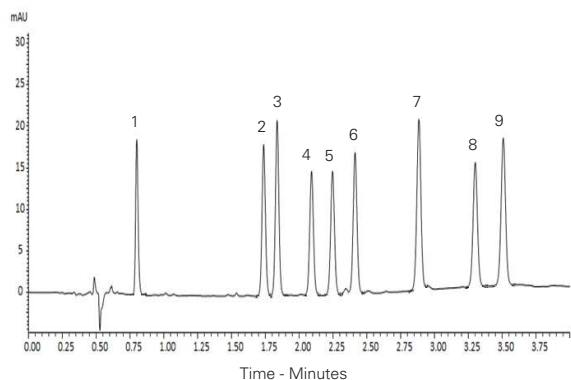
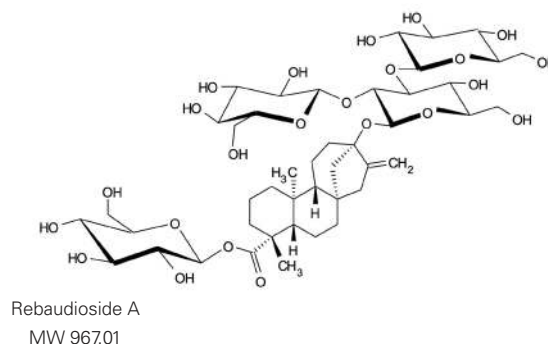
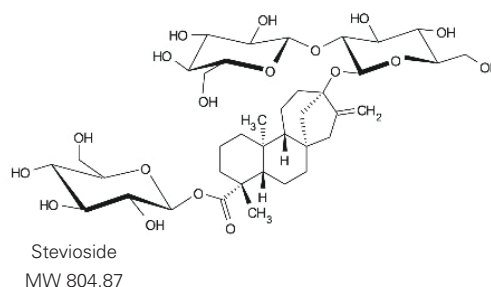
Column: ACE Excel 2 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: EXL-1011-1502U
Mobile Phase: A: 10 mM sodium dihydrogen phosphate pH 2.8 in H₂O
 B: 10 mM sodium dihydrogen phosphate pH 2.8 in H₂O/MeCN (20:80 v/v)
Gradient:

| 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



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

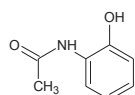
Column: ACE Excel 3 CN-ES
 ACE Excel 3 C18
 ACE Excel 3 CN
Dimensions: 50 x 2.1 mm
Part Numbers: EXL-1113-0502U,
 EXL-111-0502U,
 EXL-114-0502U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.00 | 5 |
| 3.75 | 38 |
| 5.00 | 38 |

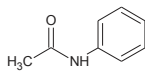
Flow Rate: 0.6 mL/min
Temperature: 40 °C
Detection: UV, 240 nm

Analytes

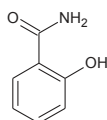
1. 2-Acetamidophenol
2. Acetanilide
3. Salicylamide
4. Aspirin
5. Phenacetin
6. Salicylic acid



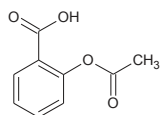
2-Acetamidophenol



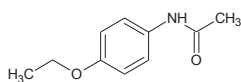
Acetanilide



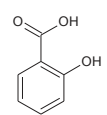
Salicylamide



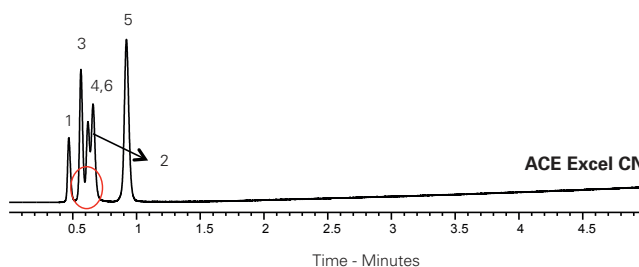
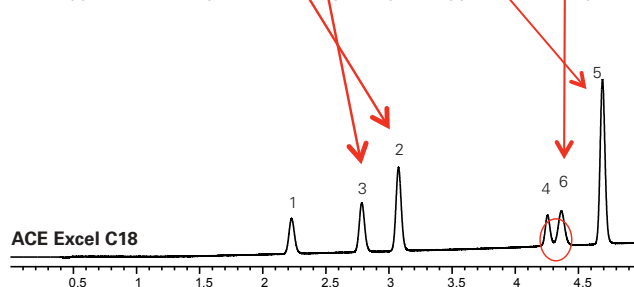
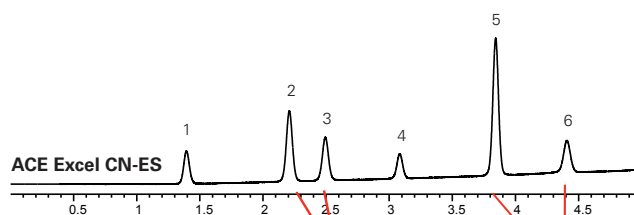
Aspirin



Phenacetin



Salicylic acid



Aspirin and Related Substances (II)

Application #AN2280

Conditions

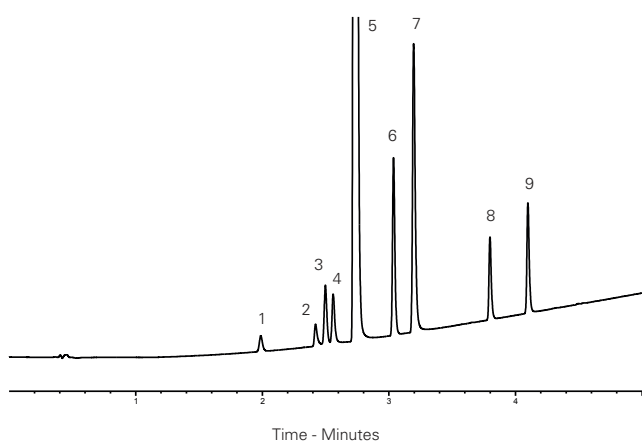
Column: ACE Excel 1.7 CN-ES
Dimensions: 50 x 3.0 mm
Part Number: EXL-1713-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| 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

- 2-Acetamidophenol
- 4-Hydroxyisophthalic acid
- Acetanilide
- Salicylamide
- Aspirin
- Phenacetin
- Salicylic acid
- Acetylsalicylsalicylic acid
- Salsalate



Avenacins

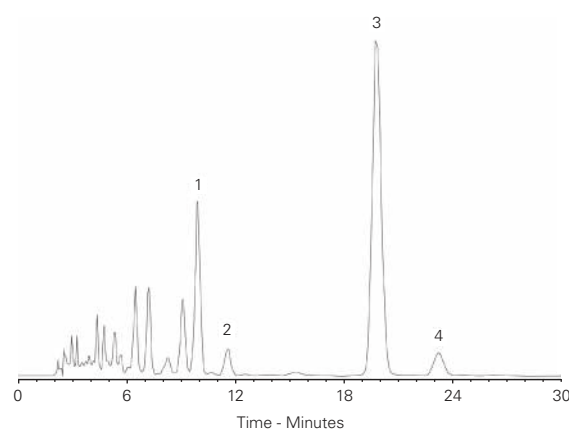
Application #AN2740

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: H₂O/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

- Avenacin A-2
- Avenacin B-2
- Avenacin A-1
- Avenacin B-1



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

β-Antagonists and Diuretics

Application #AN1410

Conditions

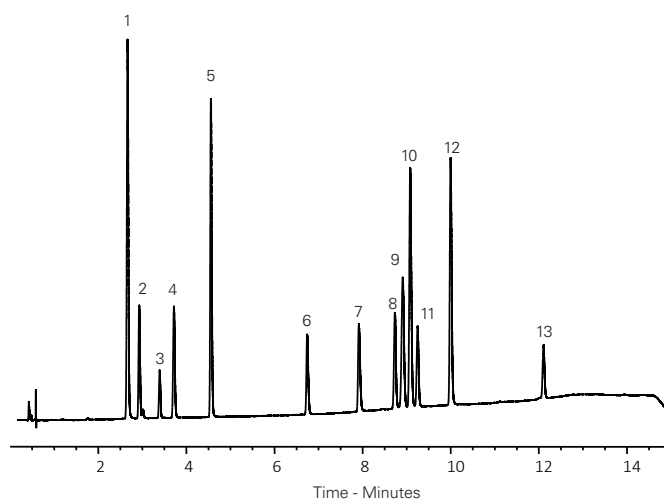
Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-111-1002
Mobile Phase: A: 20 mM KH₂PO₄, pH 2.7
 B: 20 mM KH₂PO₄, pH 2.7
 in MeCN/H₂O (65:35 v/v)
Gradient:

| 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

- Hydrochlorothiazide
- Sotalol
- Amiloride
- Atenolol
- Pindolol
- Metoprolol
- Oxprenolol
- Furosemide
- Indapamide
- Propranolol
- Bendroflumethiazide
- Carvedilol
- Spironolactone





β-Blockers at High pH Application #AN1420

Conditions

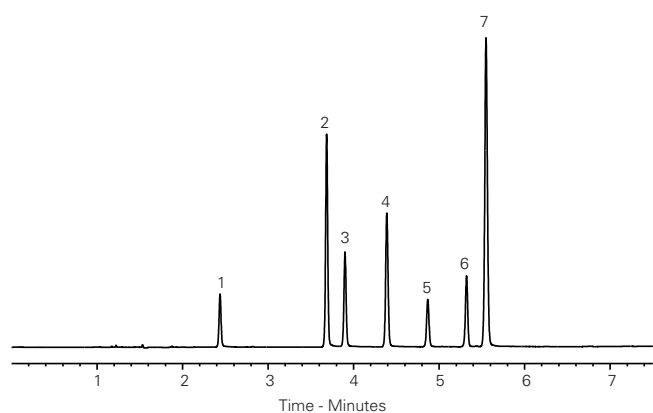
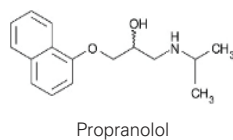
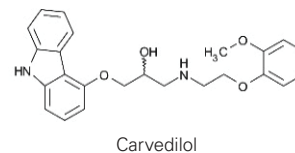
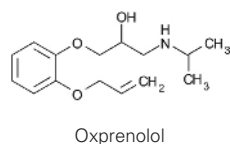
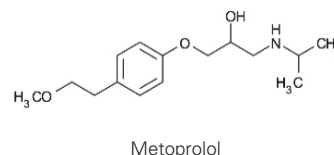
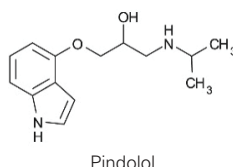
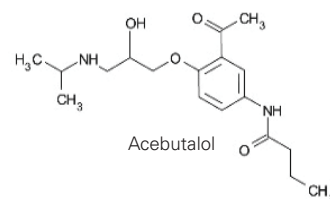
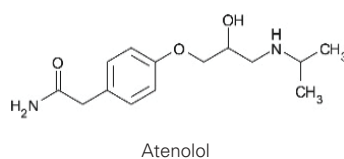
Column: ACE Excel 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 0.1% ammonia in H₂O
 B: 0.1% ammonia in MeCN
Gradient:

| 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



β-Blockers at High pH – Fast Analysis Application #AN2160

Conditions

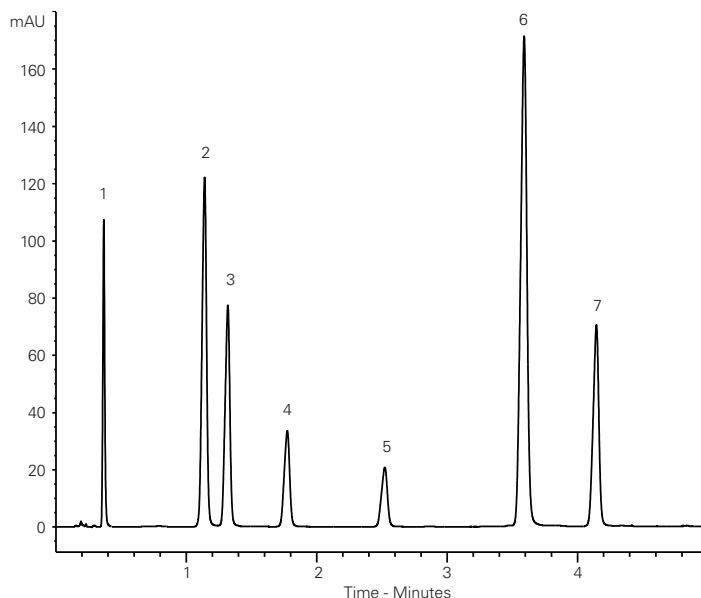
Column: ACE Excel 1.7 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: EXL-1711-0503U
Mobile Phase: A: 0.1% ammonia in H₂O
 B: 0.1% ammonia in MeCN
Gradient:

| 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

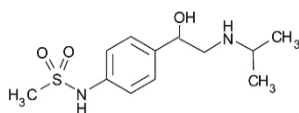
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 2 mM ammonium acetate + 0.1% formic acid in H₂O
 B: 2 mM ammonium acetate + 0.1% formic acid in MeOH
Gradient:

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

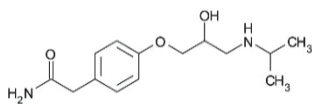
Flow Rate: 0.4 mL/min
Injection: 10 μL
Temperature: 40 °C
Detection: MS/MS ESI in positive ion mode
Sample: 2.5 pg/μL

Analytes

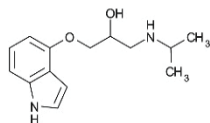
- Sotalol (m/z 272.9 → 212.8)
- Atenolol (m/z 267.0 → 189.8)
- Pindolol (m/z 248.9 → 115.8)
- Nadolol diastereomers (m/z 310.0 → 253.9)
- Metoprolol (m/z 268.0 → 115.8)
- Labetalol (m/z 329.1 → 161.8)
- Propranolol (m/z 260.0 → 115.7)
- Alprenolol (m/z 250.0 → 115.8)



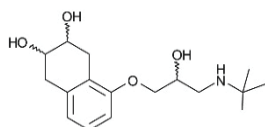
Sotalol



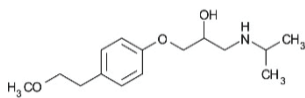
Atenolol



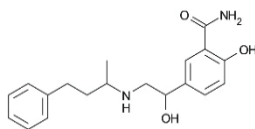
Pindolol



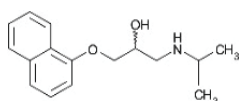
Nadolol diastereomers



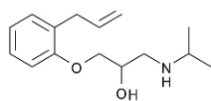
Metoprolol



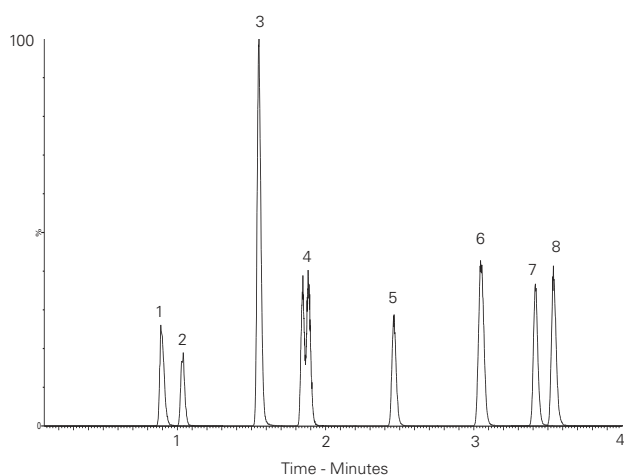
Labetalol



Propranolol



Alprenolol



Reproduced with permission of Biotage GB Ltd, UK

β-Blockers

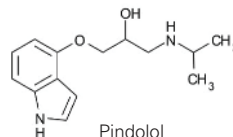
Application #AN3160

Conditions

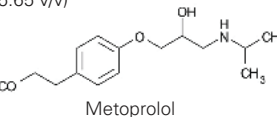
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM 1-methylpiperidine pH 11/MeOH (35:65 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 215 nm

Analytes

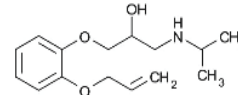
- Pindolol
- Metoprolol
- Oxprenolol
- Propranolol



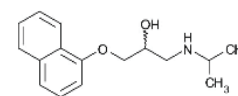
Pindolol



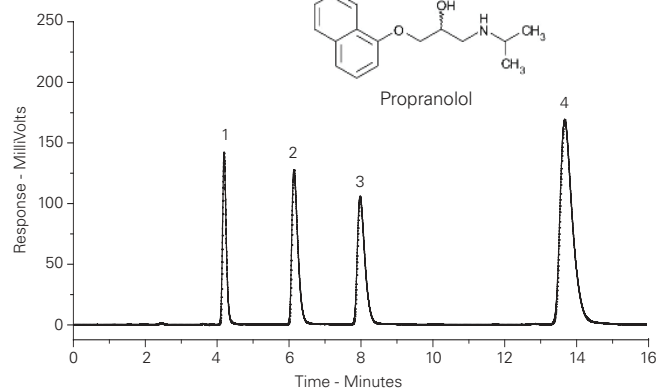
Metoprolol



Oxprenolol



Propranolol

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

Application #AN3170

Conditions

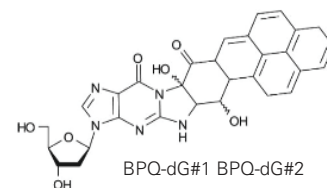
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 25 |
| 8 | 55 |

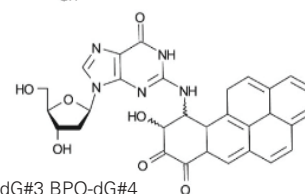
Flow Rate: 1 mL/min
Injection: 5 μL
Temperature: 35 °C
Detection: UV, 285 nm

Analytes

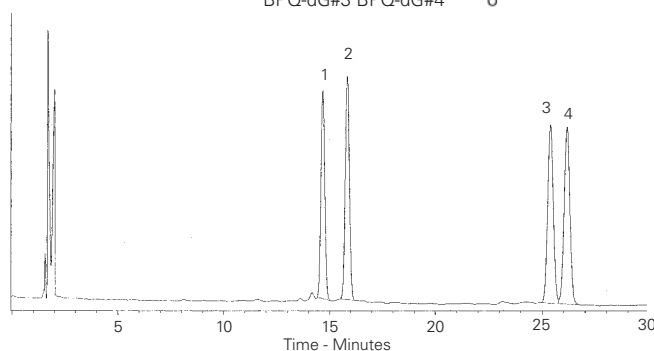
- BPQ-dG#1
- BPQ-dG#2
- BPQ-dG#3
- BPQ-dG#4



BPQ-dG#1 BPQ-dG#2



BPQ-dG#3 BPQ-dG#4

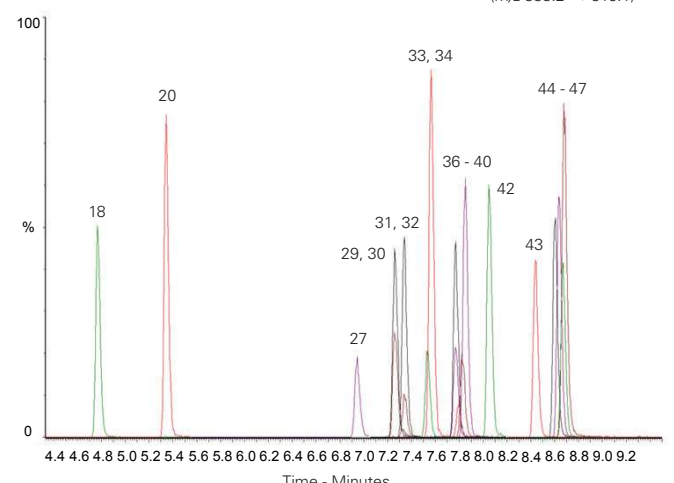


Reproduced with permission of Institute of Cancer Research, Sutton, Surrey, UK



Benzodiazepines from Drugs of Abuse Screen (#AN2190)
Application #AN2370

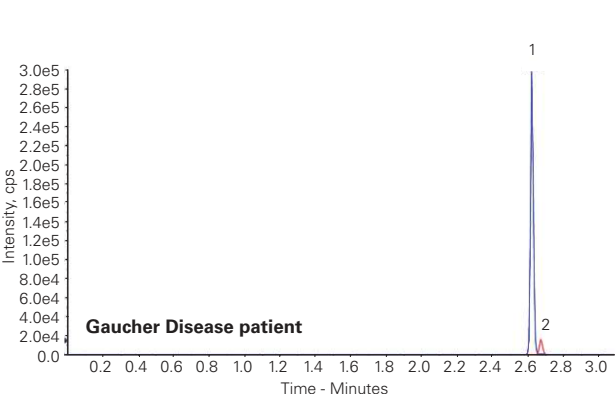
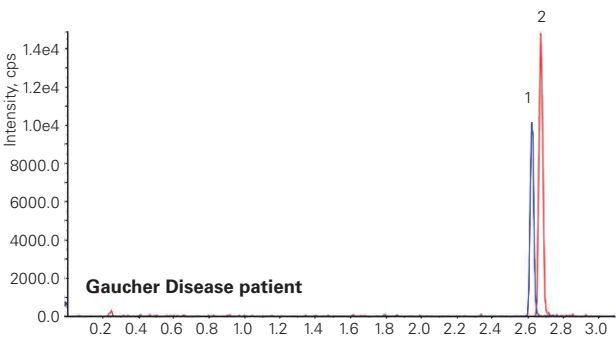
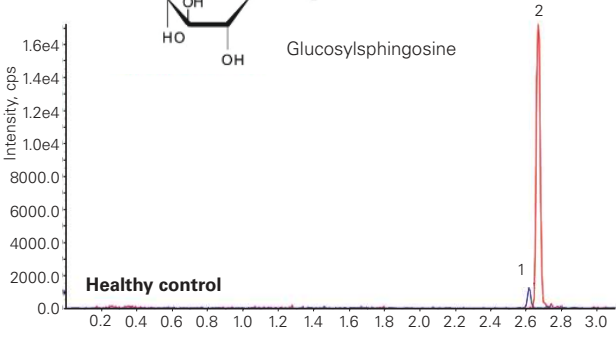
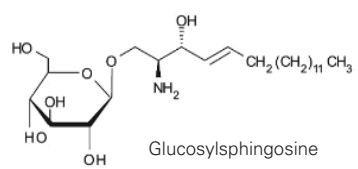
| Conditions | | Analytes |
|----------------------|---|---|
| Column: | ACE Excel 1.7 C18 | 18. 7-Amino-clonazepam (m/z 286.2 → 121.0) |
| Dimensions: | 100 x 2.1 mm | 20. 7-Amino-flunitrazepam (m/z 284.2 → 135.0) |
| Part Number: | EXL-171-1002U | 27. Bromazepam (m/z 316.1 → 182.1) |
| Mobile Phase: | A: 5 mM ammonium acetate in H ₂ O B: 5 mM ammonium acetate in MeOH | 29. Clonazepam (m/z 316.1 → 270.1) |
| Gradient: | Time (mins) %B | 30. Nitrazepam (m/z 282.2 → 236.1) |
| | 0.0 10 | 31. α-Hydroxytriazolam (m/z 359.1 → 331.1) |
| | 10.0 90 | 32. Flunitrazepam (m/z 314.2 → 268.2) |
| | 11.9 90 | 33. α-Hydroxyalprazolam (m/z 325.2 → 297.1) |
| | 13.4 10 | 34. Estazolam (m/z 295.2 → 267.2) |
| | 15.5 10 | 36. Triazolam (m/z 343.0 → 308.1) |
| Flow Rate: | 0.3 mL/min | 37. 2-Hydroxyethylflurazepam (m/z 333.2 → 109.0) |
| Injection: | 10 µL | 38. Lorazepam (m/z 321.1 → 275.1) |
| Temperature: | 40 °C | 39. Oxazepam (m/z 287.2 → 241.0) |
| Detection: | MS Quattro Premier XE triple quad MRM, positive and negative ESI mode Desolvation temperature: 450 °C IonSource temperature: 150 °C Collision gas pressure: 3.5 x 10 ⁻³ mbar | 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 | | Analytes |
|----------------------|--|---|
| Column: | ACE 3 C8 | 1. Glucosylsphingosine (m/z 462 → 282) |
| Dimensions: | 50 x 2.1 mm | 2. Lyso-Gb2 (IS) (m/z 624 → 282) |
| Part Number: | ACE-112-0502 | |
| Mobile Phase: | A: 50 mM formic acid in H ₂ O 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 | |



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

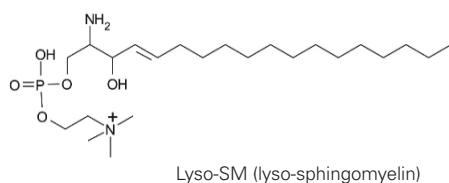
Column: ACE 3 C8
Dimensions: 50 x 2.1 mm
Part Number: ACE-112-0502
Mobile Phase: A: 50 mM formic acid in H₂O
 B: 50 mM formic acid in MeCN/acetone (1:1 v/v)
Gradient:

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

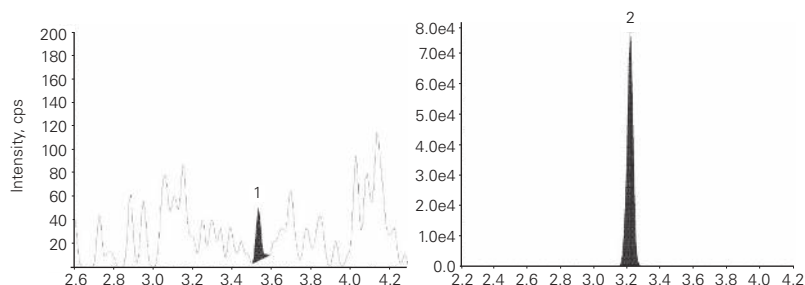
Flow Rate: 0.9 mL/min
Injection: 5 µL
Temperature: 60 °C
Detection: API 4000 triple quad MS
 ESI in positive ion mode
 Temperature: 500 °C

Analytes

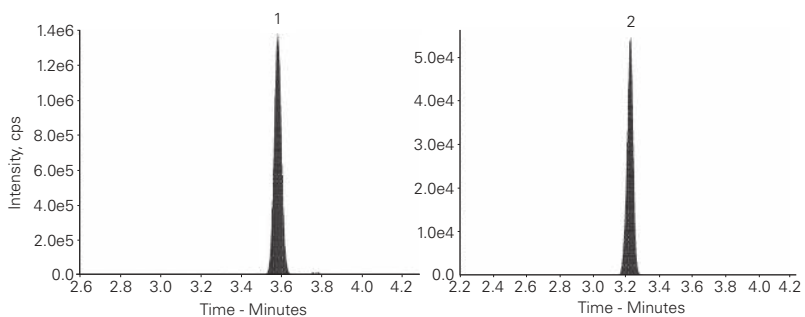
1. Lyso-SM-509
(*m/z* 509 → 184)
2. Lyso-Gb2 (IS)
(*m/z* 624 → 282)



Human Control Plasma



Niemann-Pick Patient Sample



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

Biomarker Profiling

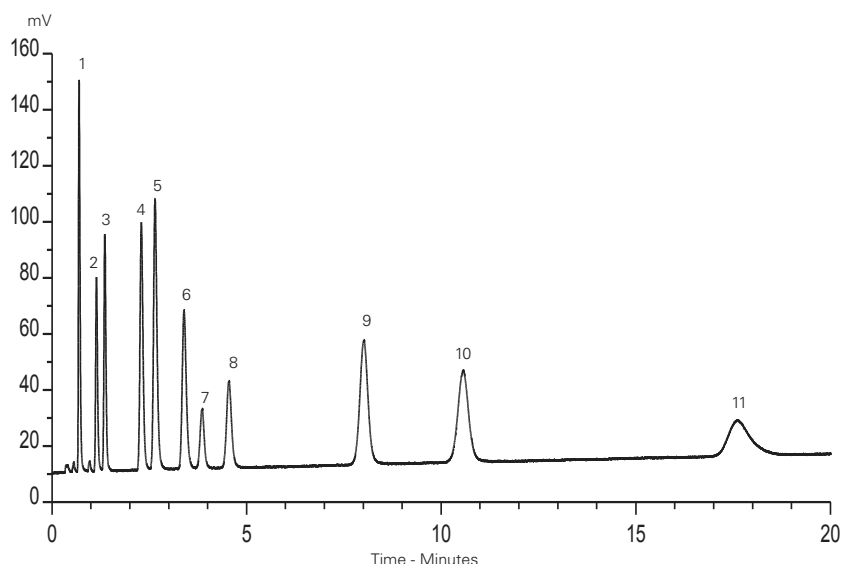
Application #AN1990

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 bisulfate + 84 mM KH₂PO₄, pH 6 with KOH
 B: 7% methanol, 2.1 mM tetrabutylammonium bisulfate + 8.4 mM KH₂PO₄, pH 6 with KOH
 A/B: (90:10 v/v)
Flow Rate: 0.4 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: UV, 260 nm

Analytes

1. Deoxyuridine
2. Deoxyguanosine
3. Deoxythymidine
4. Adenosine
5. Deoxyadenosine
6. 2-Fluoro-2'-fluoroadenine arabinoside
7. 2-Fluoro-deoxyadenosine
8. 2-Fluoro-adenosine
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

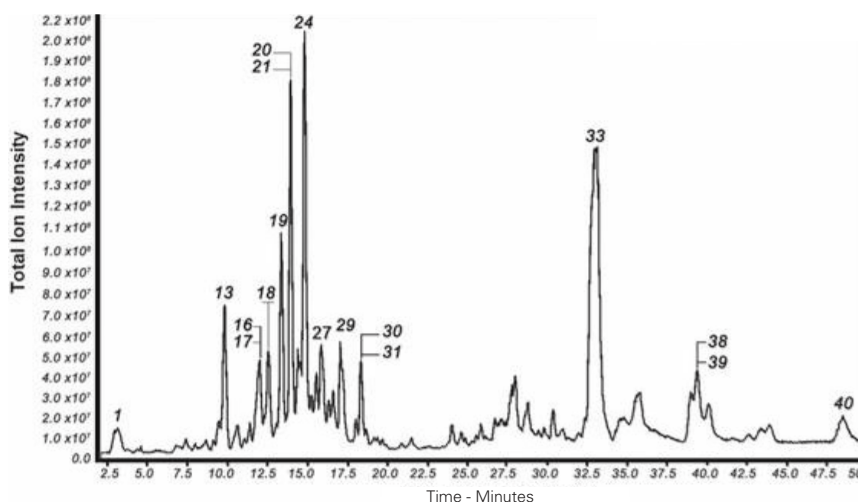
Column: ACE 5 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-121-1046
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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



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

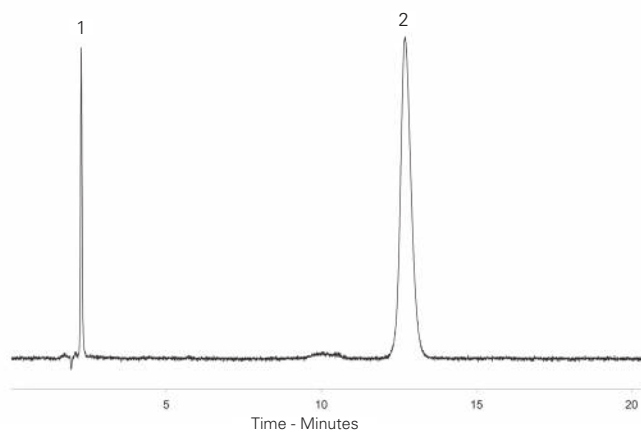
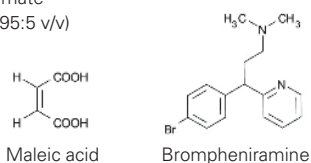
Application #AN3150

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 H₂O/MeOH (95:5 v/v)
Flow Rate: 1.0 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV, 265 nm

Analytes

- Maleic acid
- Brompheniramine



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

BSA Tryptic Digest Profiling

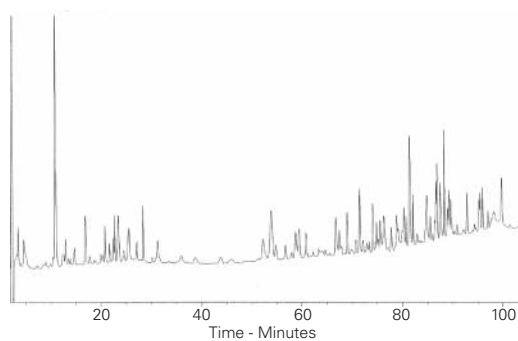
Application #AN2000

Conditions

Column: ACE 5 C18-300
Dimensions: 150 x 4.6 mm
Part Number: ACE-221-1546
Mobile Phase: A: 1% TFA in H₂O
 B: 1% TFA in MeCN/H₂O (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 H₂O
 B: 0.1% TFA in H₂O/MeCN (10:90 v/v)

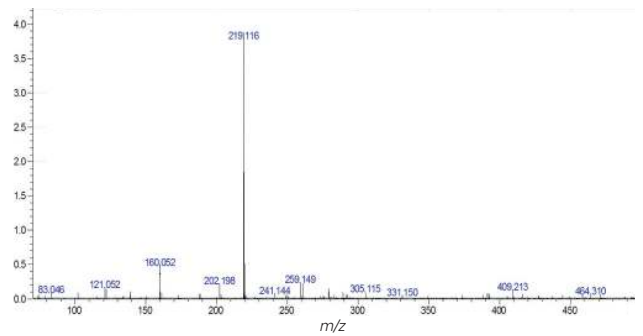
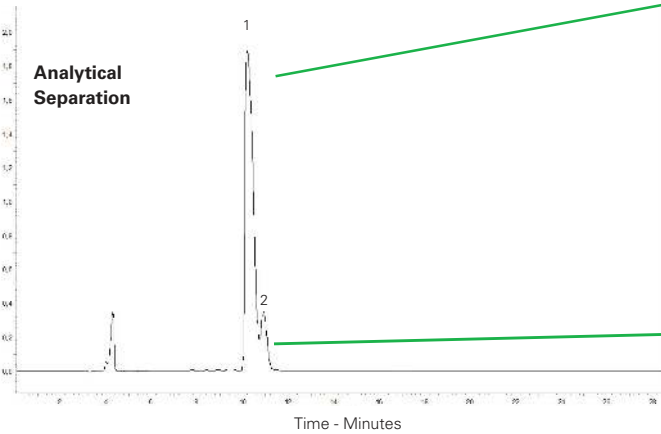
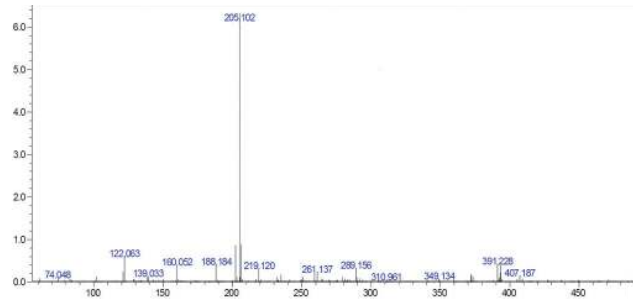
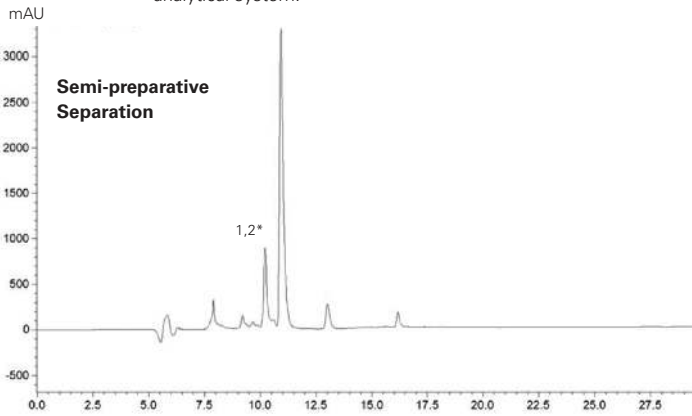
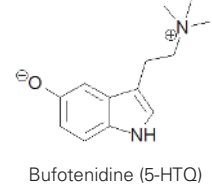
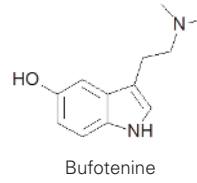
| Gradient: | Semi-Preparative | | Analytical | |
|-----------|------------------|----|-------------|----|
| | Time (mins) | %B | Time (mins) | %B |
| | 0 | 10 | 0 | 13 |
| | 35 | 70 | 15 | 15 |

Flow Rate: 1.7 mL/min (semi-preparative) and 1.1 mL/min (analytical)
Temperature: 4 °C
Detection: UV, 214 nm

Sample: MS positive ESI mode for peak identification
 Aqueous extract from liquid-liquid partition of toad skin secretion
 Fraction* from semi-preparative separation injected into analytical system.

Analytes

1. Bufotenine ((M+H)⁺ m/z 205)
2. Bufotenidine (5-HTQ) ((M+H)⁺ m/z 219)



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



Caffeine and Metabolites

Application #AN2010

Conditions

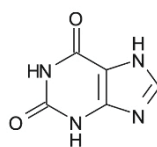
Column: ACE Excel 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 20 mM ammonium acetate pH 7.0 in H₂O
 B: 20 mM ammonium acetate pH 7.0 in MeCN/H₂O (90:10 v/v)
Gradient:

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

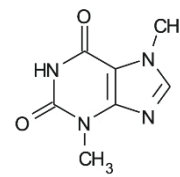
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: 60 °C
Detection: UV, 273 nm

Analytes

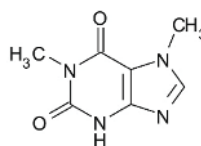
1. Xanthine
2. Theobromine
3. Paraxanthine
4. Theophylline
5. Caffeine



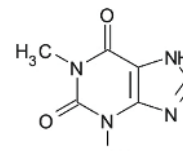
Xanthine



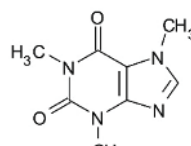
Theobromine



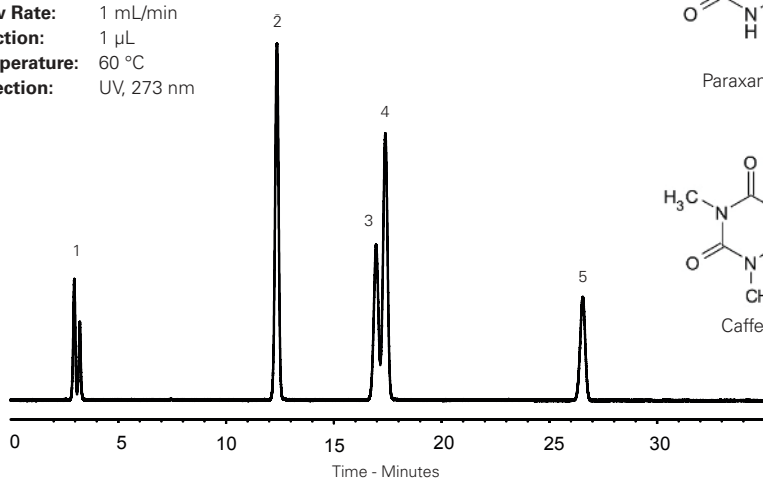
Paraxanthine



Theophylline



Caffeine



Caffeoylquinic and Dicafeoylquinic Acids

Application #AN3520

Conditions

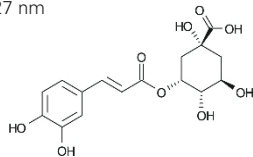
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 4.6 mm
Part Number: CORE-25A-1046U
Mobile Phase: A: 0.2% phosphoric acid in H₂O
 B: MeCN
Gradient:

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

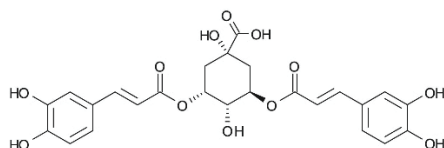
Flow Rate: 0.8 mL/min
Temperature: 35 °C
Detection: UV-Vis, 327 nm

Analytes

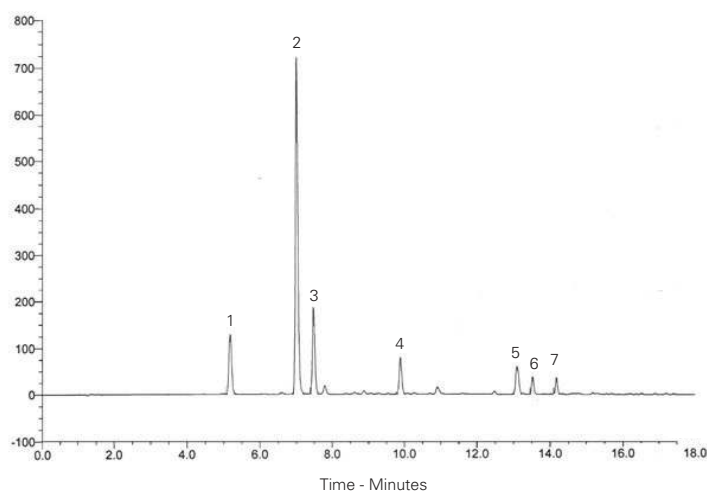
1. 3-Caffeoylquinic acid (chlorogenic acid)
2. 5-Caffeoylquinic acid (neochlorogenic acid)
3. 4-Caffeoylquinic acid (cryptochlorogenic acid)
4. Feruloylquinic acid
5. 3,4-Dicafeoylquinic acid (isochlorogenic acid B)
6. 3,5-Dicafeoylquinic acid (isochlorogenic acid A)
7. 4,5-Dicafeoylquinic acid (isochlorogenic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



5-Caffeoylquinic acid (neochlorogenic acid)



3,5-Dicafeoylquinic acid (isochlorogenic acid A)



Cannabinoids (Synthetic) by LC-MS/MS

Application #AN2540

Conditions

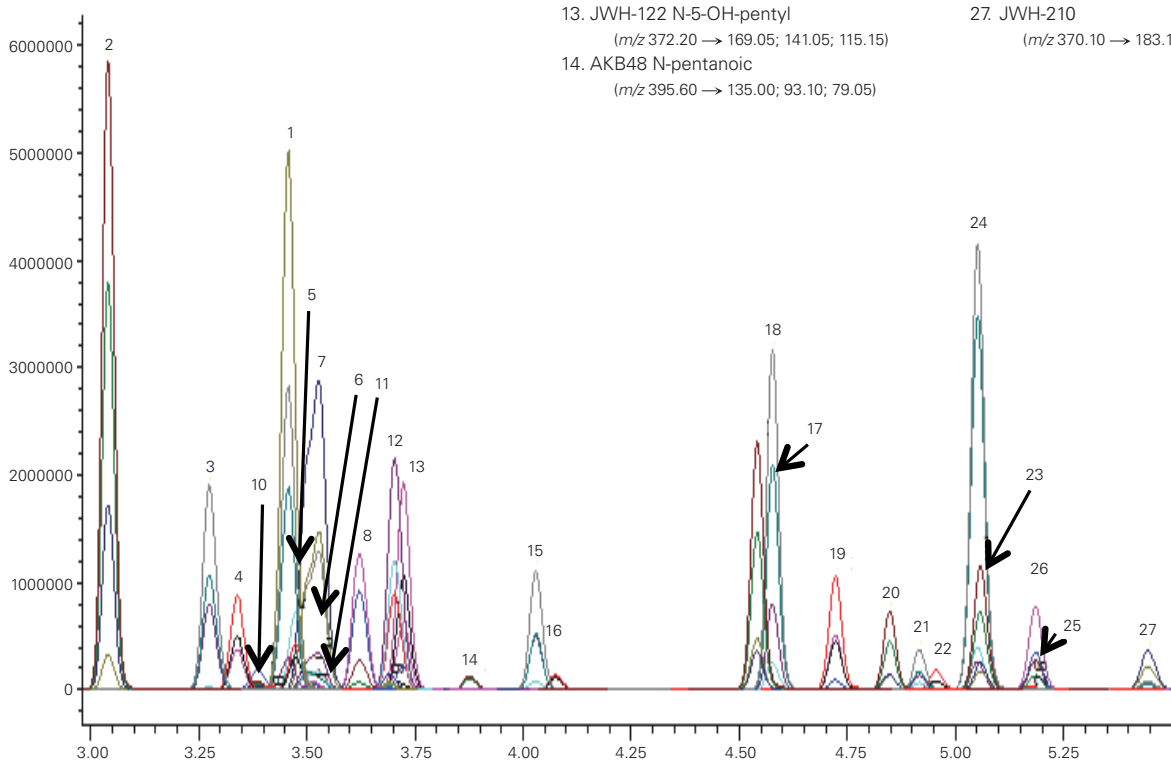
Column: ACE Excel 3 C18-AR
Dimensions: 100 x 3.0 mm
Part Number: EXL-119-1003U
Mobile Phase: A: 15 mM ammonium formate pH 4.0 in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

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

Analytes

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



Reproduced with permission of ISZKI (Institute of Toxicology), Hungary



Cannabinoids in Rat Plasma

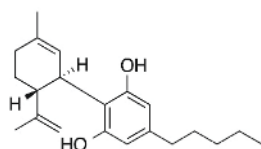
Application #AN2310

Conditions

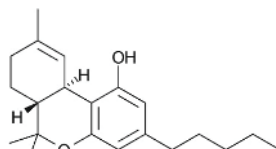
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: H₂O/MeCN (38:62 v/v)
Flow Rate: 1 mL/min
Injection: 30 µL
Temperature: 55 °C
Detection: UV, 220 nm

Analytes

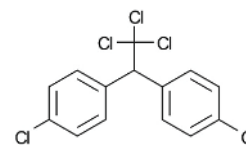
1. Cannabidiol (CBD)
2. Δ⁹-Tetrahydrocannabinol (THC)
3. 4,4-Dichlorodiphenyltrichloroethane (DDT) (IS)



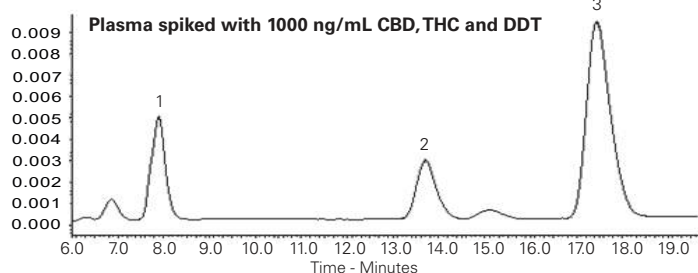
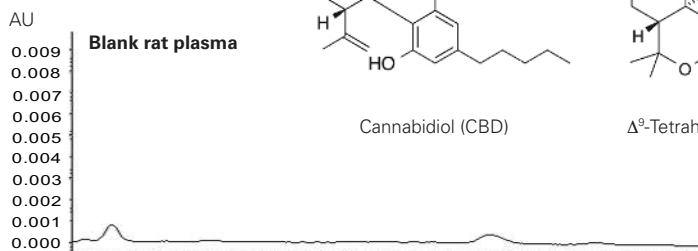
Cannabidiol (CBD)



Δ⁹-Tetrahydrocannabinol (THC)



4,4-Dichlorodiphenyltrichloroethane (DDT) (IS)



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



Reproduced with permission of School of Pharmacy, Centre for Biomolecular Sciences, The University of Nottingham, UK

Carglumic Acid in Human Plasma by LC-MS/MS

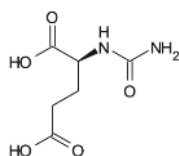
Application #AN3750

Conditions

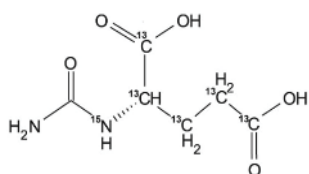
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: MeCN/MeOH/0.1% acetic acid pH 3.2 (40:40:20 v/v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: MDS Sciex API-4000 triple quad MS
 Negative ion mode ESI
 Ion source temperature: 500 °C
 Ion spray voltage: -4500 V
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

Analytes

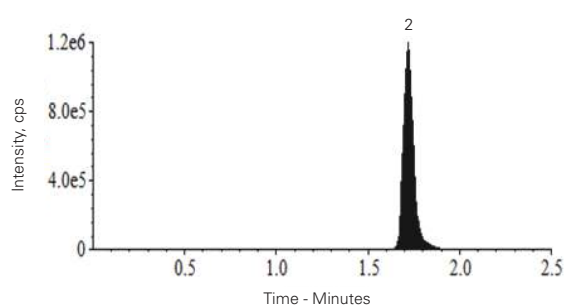
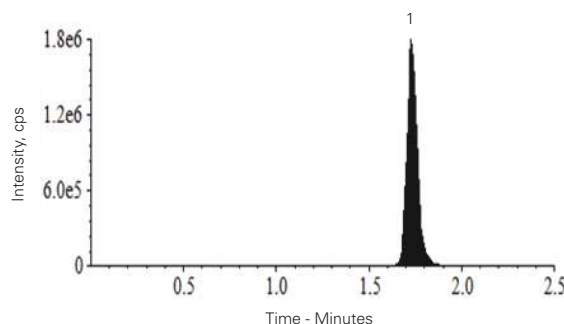
1. Carglumic acid
(*m/z* 189 → 146)
(LLOQ 6.0 ng/mL)
2. Carglumic acid-¹³C ¹⁵N (I.S.)
(*m/z* 195 → 152)



Carglumic acid



Carglumic acid-¹³C ¹⁵N (I.S.)



Reproduced with permission of Chemistry Department, School of Sciences, Gujarat University, India

Catechins

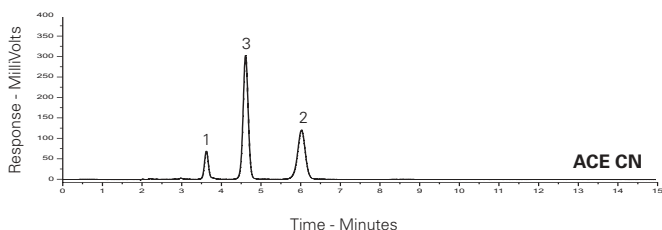
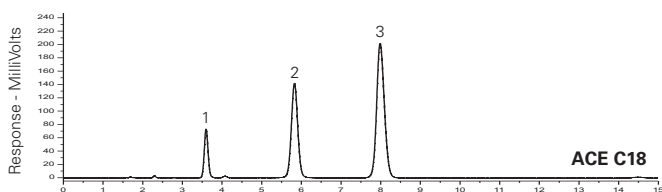
Application #AN3950

Conditions

Column: ACE 5 C18, ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546, ACE-124-1546
Mobile Phase: MeOH/0.1% formic acid in H₂O (25:75 v/v)
Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: UV, 280 nm

Analytes

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



Catecholamine Analysis (I)

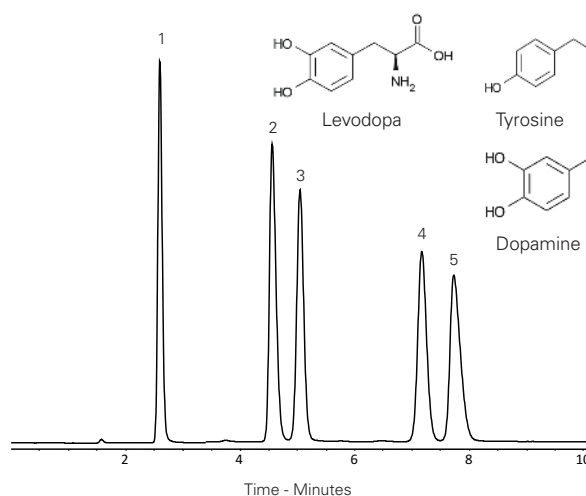
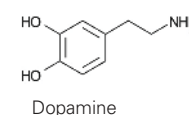
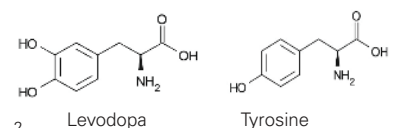
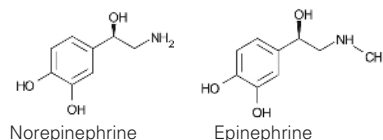
Application #AN2020

Conditions

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

Analytes

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



Catecholamine Analysis (II)

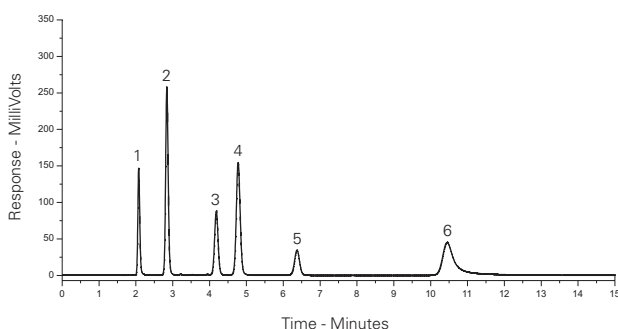
Application #AN3910

Conditions

Column: ACE 5 AQ
Dimensions: 150 x 4.6 mm
Part Number: ACE-126-1546
Mobile Phase: 50 mM KH₂PO₄ pH 3.0 in H₂O
Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: UV, 210 nm

Analytes

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



Catecholamines by LC-MS/MS

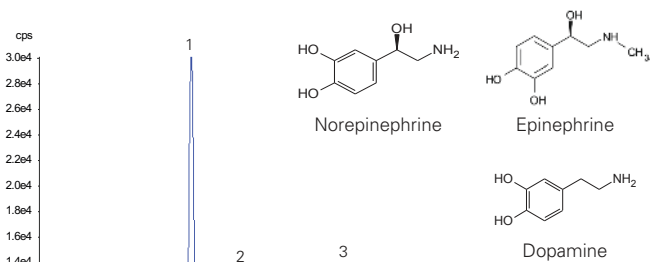
Application #AN2320

Conditions

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

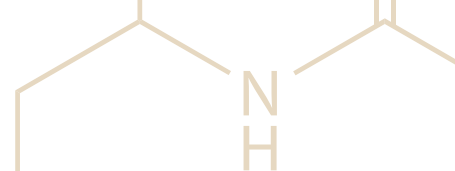
Analytes

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



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

Reproduced with permission of Biotage GB Ltd, UK



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

Application #AN4040

Conditions

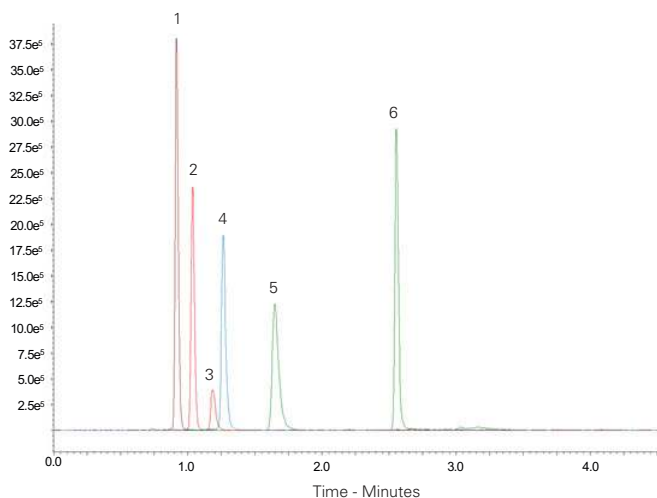
Column: ACE UltraCore 2.5 SuperPhenylHexyl
Dimensions: 100 x 2.1 mm
Part Number: CORE-25B-1002U
Mobile Phase: A: 2 mM ammonium formate + 0.05% formic acid in H₂O
 B: 2 mM ammonium formate + 0.05% formic acid in MeOH
Gradient:

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

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

Analytes

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



Reproduced with permission of Shimadzu, France

Catecholamines and Metanephrines Separation (Gradient)

Application #AN1480

Conditions

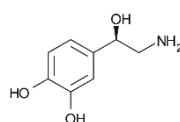
Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: A: 20 mM ammonium formate pH 3.0 in H₂O
 B: 20 mM ammonium formate pH 3.0 in MeOH/H₂O (90:10 v/v)
Gradient:

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

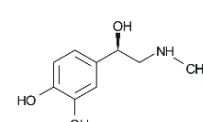
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 260 nm

Analytes

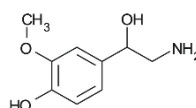
1. Norepinephrine
2. Epinephrine
3. Normetanephrine
4. Dopamine
5. Metanephrine



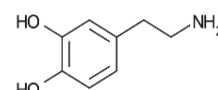
Norepinephrine



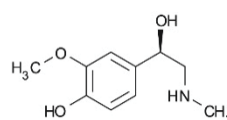
Epinephrine



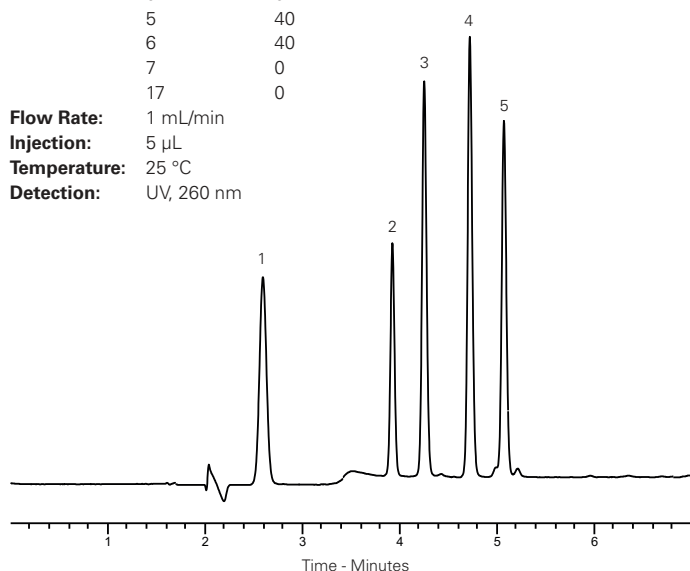
Normetanephrine



Dopamine



Metanephrine



Catecholamines and Metanephrines Separation (Isocratic)

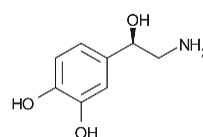
Application #AN1490

Conditions

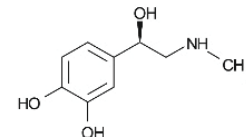
Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: 20 mM ammonium formate pH 3.0 in H₂O
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 260 nm

Analytes

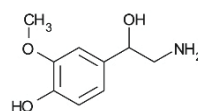
1. Norepinephrine
2. Epinephrine
3. Normetanephrine
4. Dopamine
5. Metanephrine



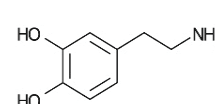
Norepinephrine



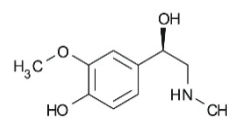
Epinephrine



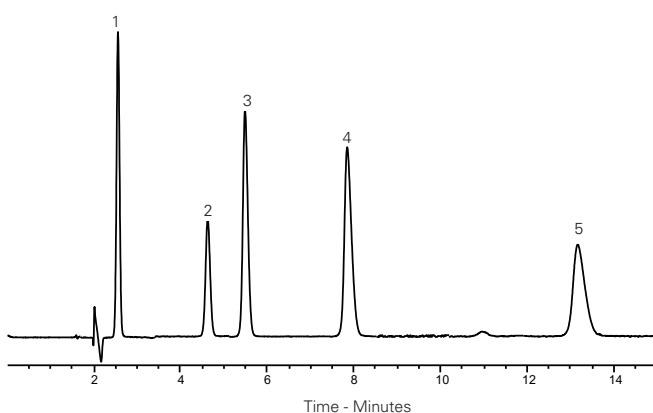
Normetanephrine



Dopamine



Metanephrine



Catecholamines from Plasma

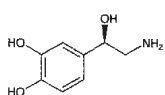
Application #AN3210

Conditions

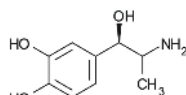
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 50 mM sodium acetate
 pH 7.0/MeCN/MeOH (50:35:15 v/v/v)
Flow Rate: 0.9 mL/min
Temperature: Ambient
Detection: Fluorescence – λ_{Ex} 350 nm, λ_{Em} 480 nm
Sample: Ion pair extraction using diphenyl-borate-ethanolamine.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

Analytes

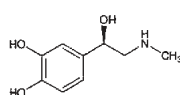
1. Noradrenaline (Norepinephrine)
2. 3,4-Dihydroxynorephedrine (l.S.)
3. Adrenaline (Epinephrine)



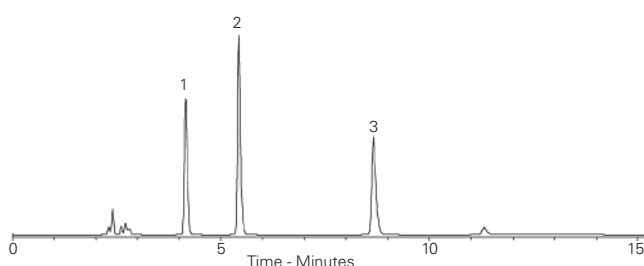
Noradrenaline



3,4-Dihydroxynorephedrine (l.S.)



Adrenaline



Reproduced with permission of MAS University Hospital, Malmo, Sweden

Catecholamines from Urine

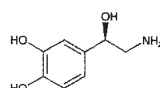
Application #AN3200

Conditions

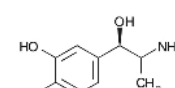
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 50 mM sodium acetate
 pH 7.0/MeCN/MeOH
 (50:35:15 v/v/v)
Flow Rate: 0.9 mL/min
Temperature: Ambient
Detection: Fluorescence – λ_{Ex} 350 nm, λ_{Em} 480 nm
Sample: Ion pair extraction using diphenyl-borate-ethanolamine.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

Analytes

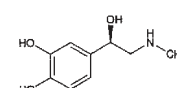
1. Noradrenaline (Norepinephrine)
2. 3,4-Dihydroxynorephedrine (l.S.)
3. Adrenaline (Epinephrine)
4. Dopamine



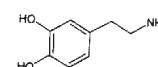
Noradrenaline



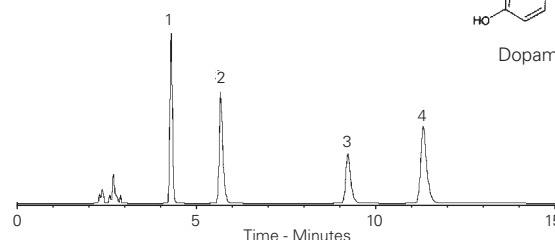
3,4-Dihydroxynorephedrine (l.S.)



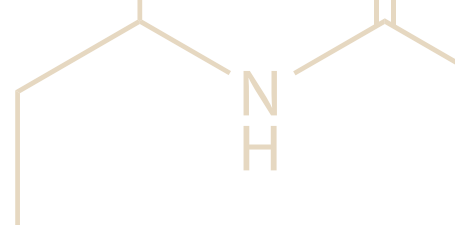
Adrenaline



Dopamine



Reproduced with permission of MAS University Hospital, Malmo, Sweden



Catechols Mixture Separations (I) and (II)

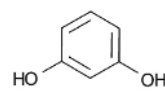
Application #AN1430 and #AN1440

Conditions

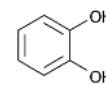
Column: (I) ACE Excel 3 CN-ES (II) ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: (I) EXL-1113-1546U (II) EXL-1112-1546U
Mobile Phase: (I) 20 mM H₃PO₄ in MeCN/H₂O (25:75 v/v)
 (II) 20 mM H₃PO₄ in MeCN/H₂O (10:90 v/v)
Flow Rate: 1.5 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 270 nm

Analytes

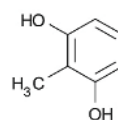
1. Resorcinol
2. Catechol
3. 2-Methylresorcinol
4. 4-Methylcatechol
5. 3-Methylcatechol
6. 4-Nitrocatechol



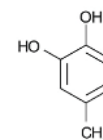
Resorcinol



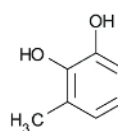
Catechol



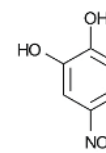
2-Methylresorcinol



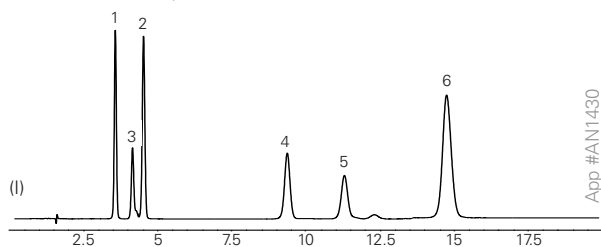
4-Methylcatechol



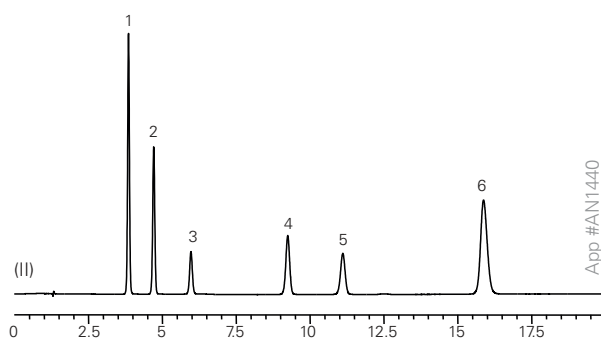
3-Methylcatechol



4-Nitrocatechol



App #AN1430



App #AN1440

Cathinone Psychoactive Substances by LC-UV and LC-Amperometry

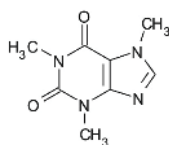
Application #AN3500

Conditions

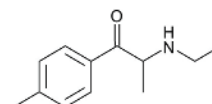
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: 10 mM ammonium acetate-100 mM KCl pH 4.3/MeOH (70:30 v/v)
Flow Rate: 0.8 mL/min
Injection: 10 µL
Temperature: 22 °C
Detection: UV, 264 nm
 Amperometric Potential +1.4 V

Analytes

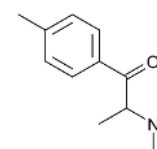
1. Caffeine
2. 4-Methylmethcathinone (4-MMC, mephedrone)
3. 4-Methylethcathinone (4-MEC)



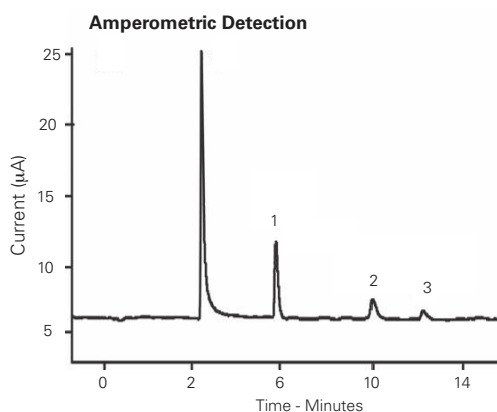
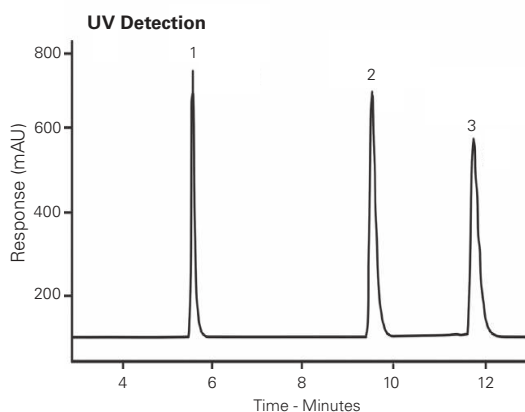
Caffeine



4-Methylethcathinone (4-MEC)



4-Methylmethcathinone (4-MMC, mephedrone)



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

Cefquinome by LC-MS

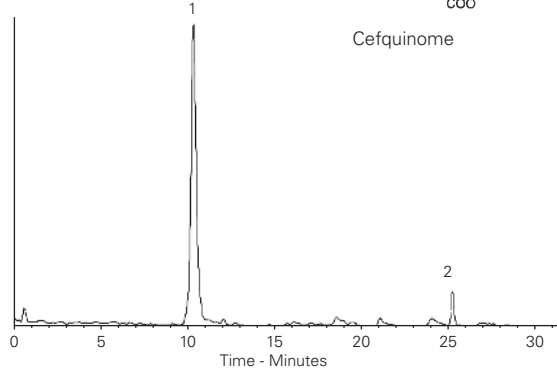
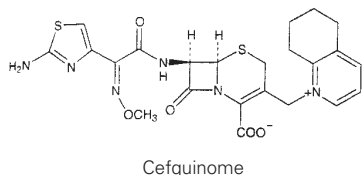
Application #AN3130

Conditions
Column: ACE 5 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-121-1502
Mobile Phase: A: 2 mM formic acid in H₂O
 B: 2 mM formic acid in MeCN
Gradient:

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

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

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



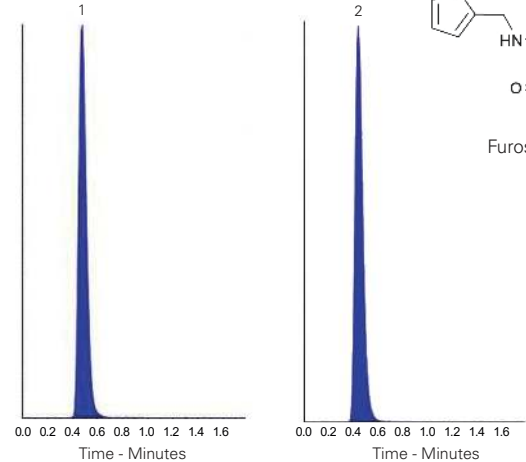
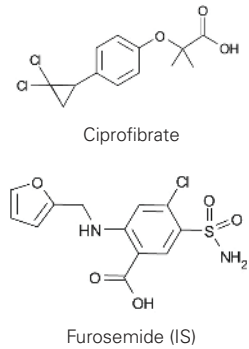
Reproduced with permission of Department of Soil Science, University of Reading, UK

Ciprofibrate from Human Plasma by LC-MS/MS

Application #AN2670

Conditions
Column: ACE 5 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-121-0546
Mobile Phase: 0.001% ammonia in MeOH/ MeCN/H₂O (70:20:10 v/v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: API 3200 triple quad MS
 ESI in negative ion mode
 Ion source temperature: 550 °C
 Ion spray voltage: 4500 V

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



Reproduced with permission of Indukaka Ipcowala College of Pharmacy, New Vallabh Vidyanagar, Gujarat, India

Chloramphenicol in Milk by LC-MS/MS

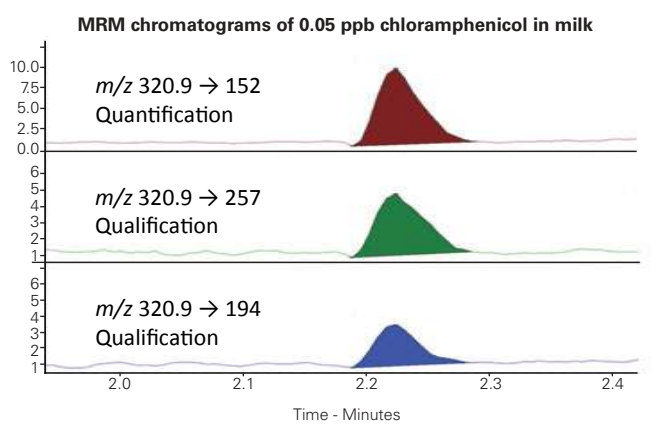
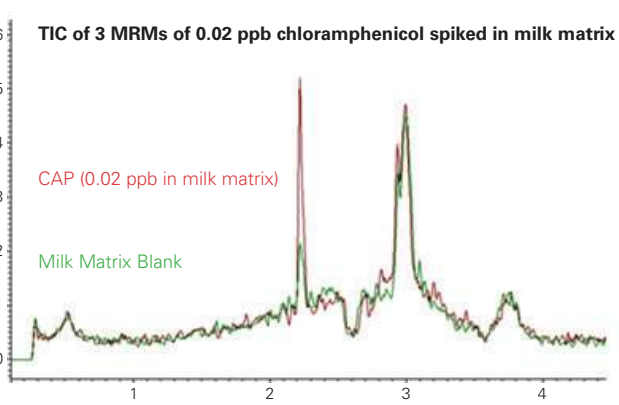
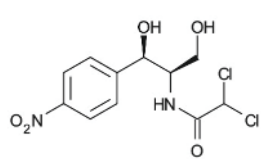
Application #AN2030

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

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

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

Analyte
 1. Chloramphenicol



Reproduced with permission of Bruker UK Ltd



Chocolate Analysis

Application #AN2040

Conditions

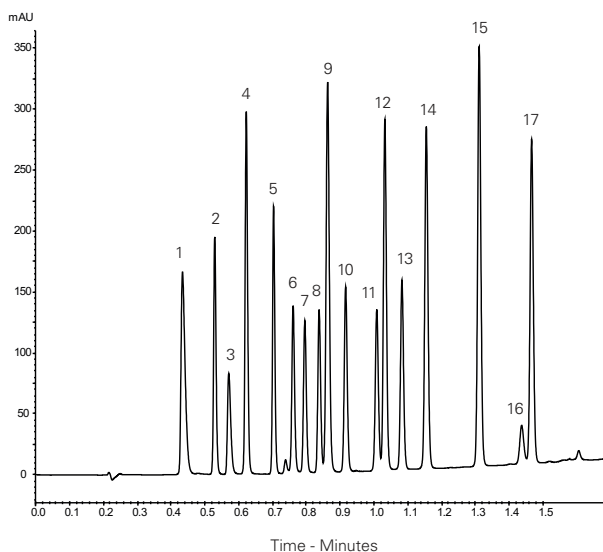
Column: ACE Excel 2 C18-Amide
Dimensions: 100 x 2.1 mm
Part Number: EXL-1012-1002U
Mobile Phase: A: 10 mM ammonium formate pH 2.8 in H₂O
 B: 10 mM ammonium formate pH 2.8 in MeCN/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 5 |
| 1.5 | 85 |

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

Analytes

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



Reproduced with permission of Shimadzu Europa GmbH. Analysed on Shimadzu Nexera X2.

Clenbuterol in Equine Plasma by LC-MS/MS

Application #AN2050

Conditions

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

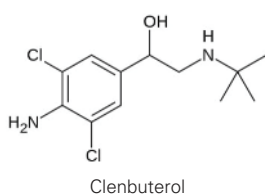
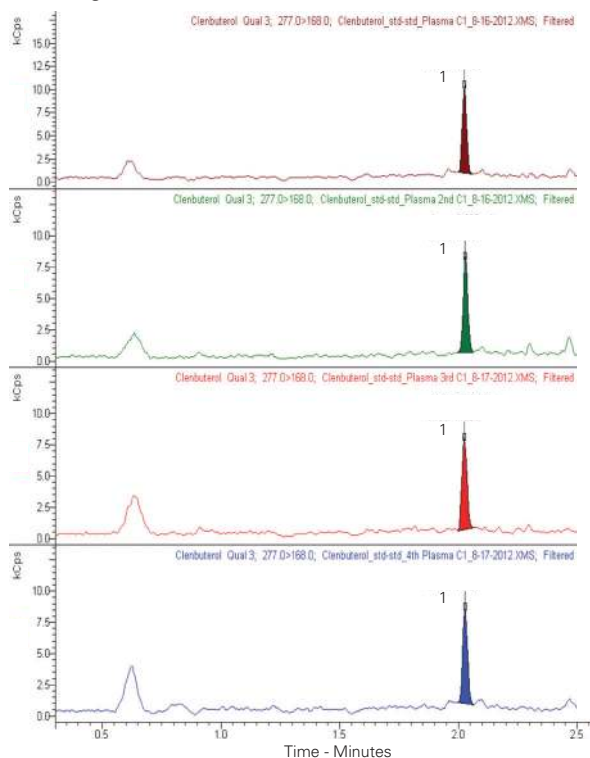
| Time (mins) | %B |
|-------------|----|
| 0.0 | 10 |
| 0.3 | 10 |
| 2.5 | 95 |
| 2.8 | 10 |
| 4.5 | 10 |

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

Analyte

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

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



Reproduced with permission of Bruker UK Ltd (Bruker Application Note #704055)

Clonidine Hydrochloride Oral Solution
Containing Preservatives

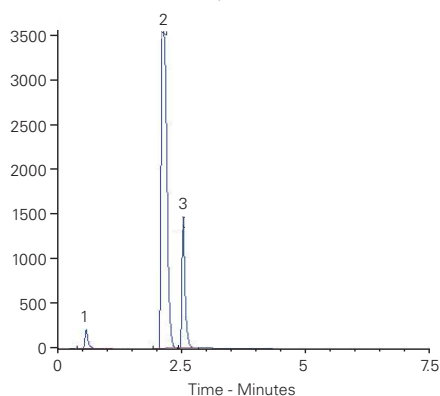
Application #AN2060

Conditions

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

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

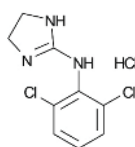
Flow Rate: 2 mL/min
Injection: 100 µL
Temperature: 20 °C
Detection: UV, 220 nm



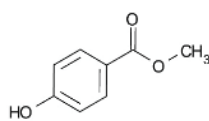
Reproduced with permission of Guy's Hospital, London, UK

Analytes

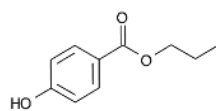
1. Clonidine HCl
(10 µg/mL)
2. Methyl paraben
(1.5 g/mL)
3. Propyl paraben
(1.5 g/mL)



Clonidine HCl



Methyl paraben



Propyl paraben

Clopidogrel and Photodegradation Products

Application #AN3110

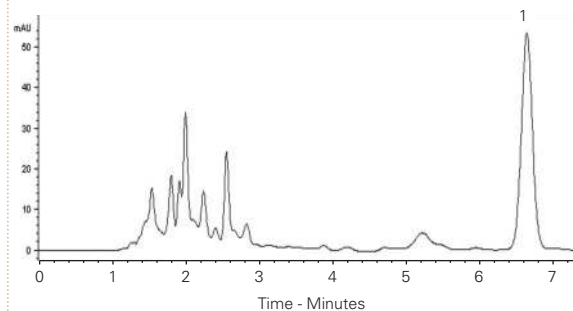
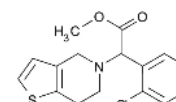
Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeOH/aqueous TEA
 (pH 5.3 with H₃PO₄) (75:25 v/v)

Flow Rate: 1.2 mL/min
Injection: 20 µL
Temperature: 25 °C
Detection: UV, 220 nm
Sample: Exposed to UV light for 3.5 hours

Analyte

1. Clopidogrel



Reproduced with permission of Brazilian Pharmacopoeia



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

email: info@ace-hplc.com



Coffee Metabolite Profiling by LC-MS

Application #AN2590

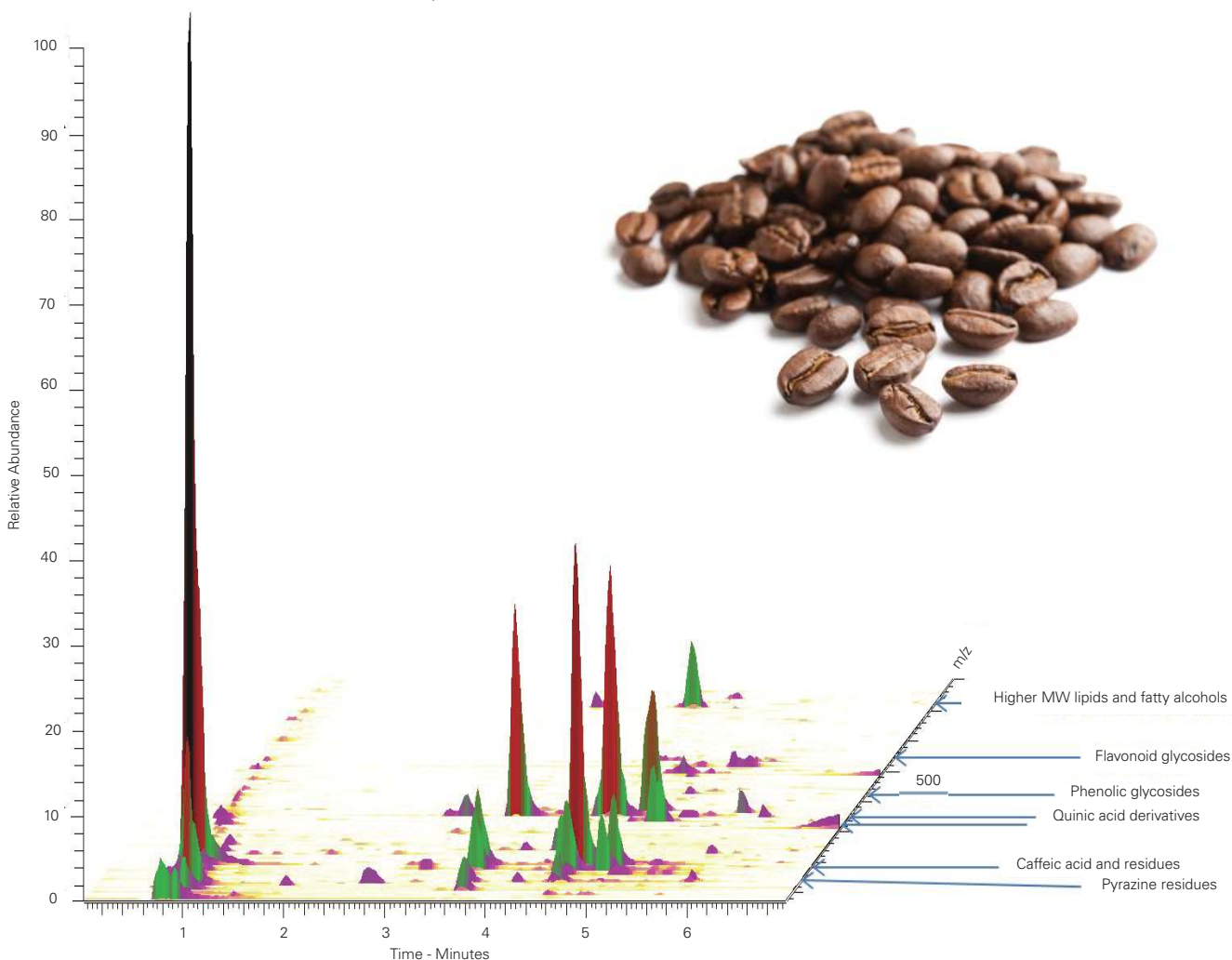
Conditions

Column: ACE Excel 1.7 C18-Amide
Dimensions: 100 x 2.1 mm
Part Number: EXL-1712-1002U
Mobile Phase: A: 0.01% formic acid in H₂O
 B: 0.01% formic acid in MeCN
Gradient:

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

Flow Rate: 0.5 mL/min
Detection: Exacte accurate mass MS system
 ESI in negative ion mode

Analytes between *m/z* 70-800 monitored
Sample: Metabolites from coffee extracted into cold water by vortexing for 20 mins. Samples filtered prior to injection onto column and modular Accela LC system.



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

Cold Medicine Analytes (I) and (II)

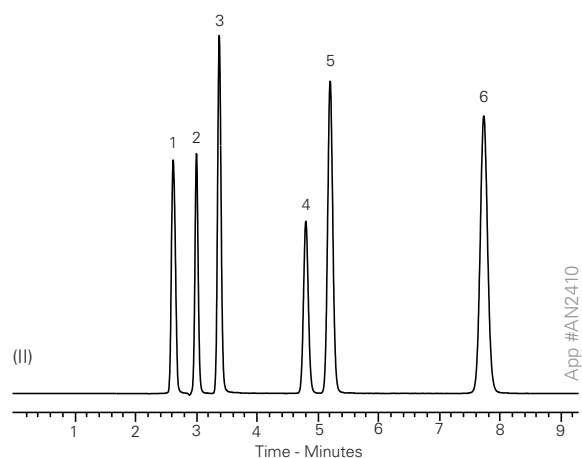
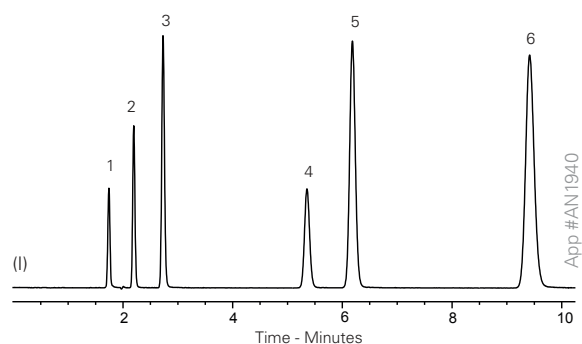
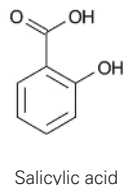
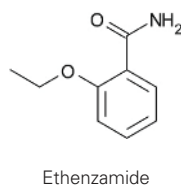
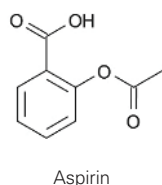
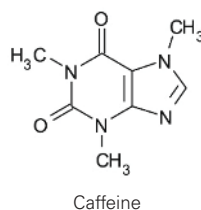
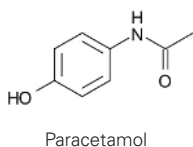
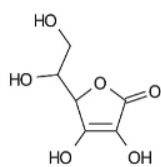
Application #AN1940 and #AN2410

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: (I) 20 mM phosphoric acid in MeOH/H₂O (25:75 v/v)
 (II) 0.1% formic acid in MeOH/H₂O (55:45 v/v)
Flow Rate: (I) 1.5 mL/min (II) 1.0 mL/min
Injection: 5 µL
Temperature: (I) 40 °C (II) 25 °C
Detection: (I) UV, 280 nm (II) UV, 275 nm

Analytes

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



Corticosteroids by LC-MS/MS

Application #AN1030

Conditions

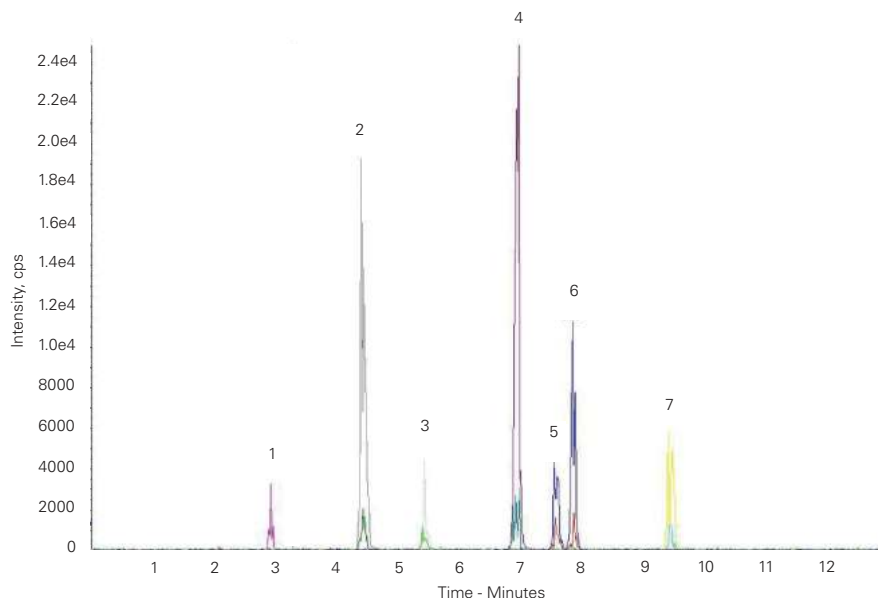
Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H₂O
 B: MeCN/0.1% formic acid in H₂O (90:10 v/v)
Gradient:

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

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

Analytes

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



Reproduced with permission of Laboratorio Salud Publica de Burgos, Spain



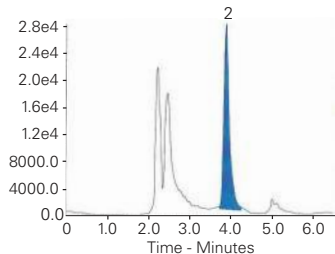
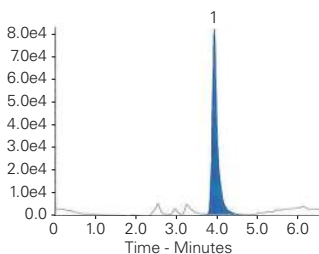
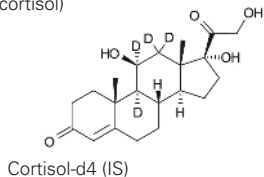
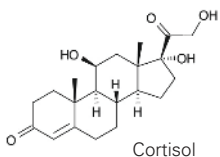
Cortisol in Urine by LC-MS/MS
Application #AN2680

Conditions

Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: 4 mM ammonium acetate in H₂O/0.2% (v/v) formic acid in MeOH (71.5:28.5 v/v)
Flow Rate: 0.7 mL/min
Injection: 50 µL
Temperature: 50 °C
Detection: Applied Biosystems 5000 MS/MS APCI in positive ion mode
Sample: BioRad Liquichek Urine Quality Control standard (16 nmol/L cortisol)

Analytes

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



Reproduced with permission of Department of Pathology and Laboratory Medicine, Heartlands Hospital, Birmingham, UK

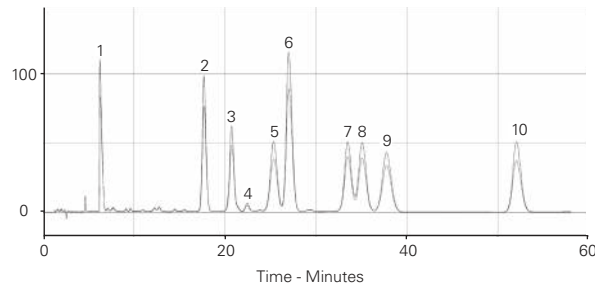
Cyclosporin Mixture
Application #AN3270

Conditions

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

Analytes

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



Reproduced with permission of Camurus AB, Lund, Sweden

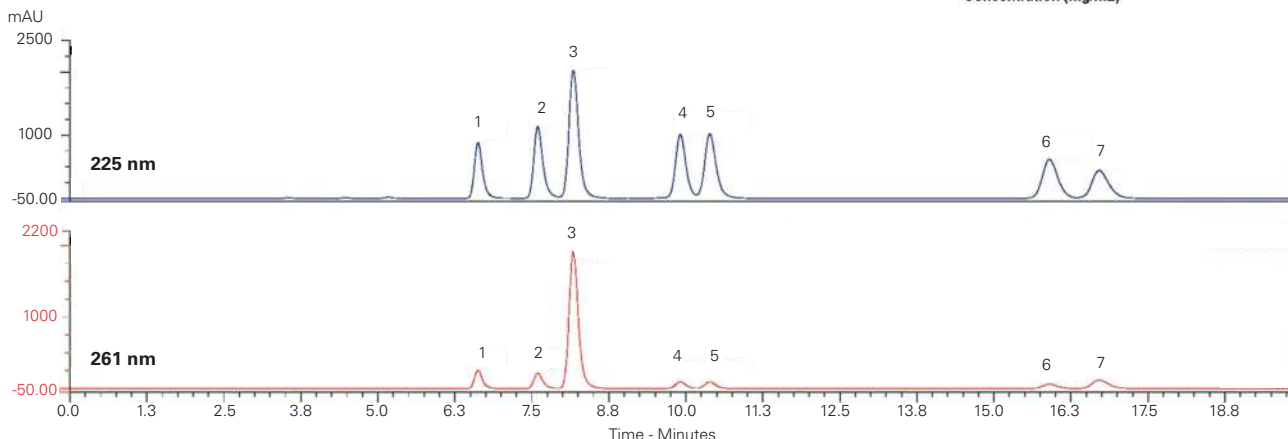
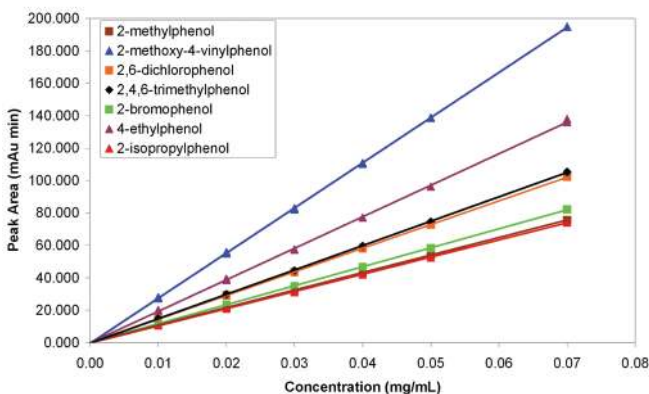
Cyclodextrin-Encapsulated Flavour Compounds in Beer
Application #AN2300

Conditions

Column: ACE 3 C18
Dimensions: 150 x 4.0 mm
Part Number: ACE-111-1504
Mobile Phase: 0.1% phosphoric acid in MeOH/H₂O (53:47 v/v)
Flow Rate: 0.5 mL/min
Injection: 20 µL
Temperature: 35 °C
Detection: UV, 225 nm and 261 nm

Analytes

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



Reproduced with permission of FlavorActiV Ltd, UK

Cytarabine Analogues by Ion-Pairing LC-MS/MS

Application #AN2070

Conditions

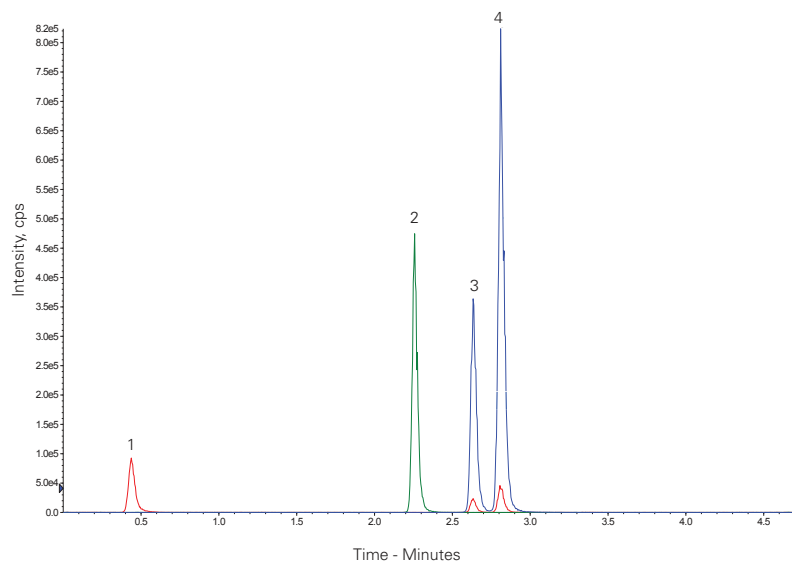
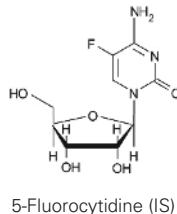
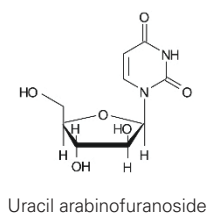
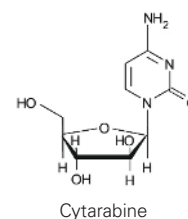
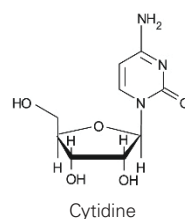
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: 0.1% perfluoropentanoic acid + 0.1% formic acid in H₂O
 B: 0.1% perfluoropentanoic acid + 0.1% formic acid in MeCN
Gradient:

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

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

Analytes

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



Reproduced with permission of Agilux Laboratories, USA

Cytotoxic Agents by UHPLC-MS/MS

Application #AN1070

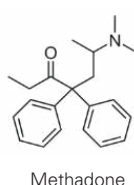
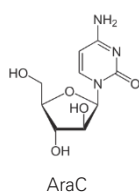
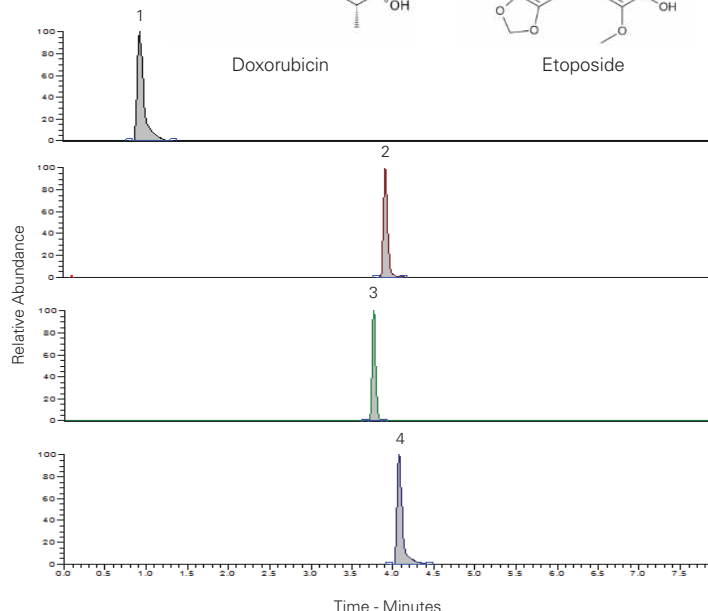
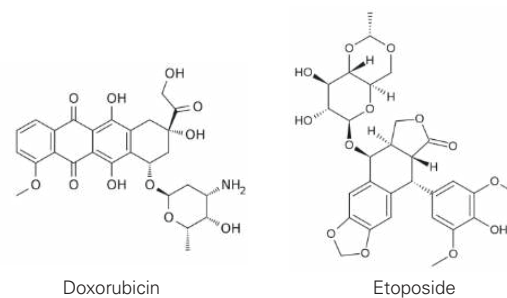
Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

Analytes

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



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



Decarboxylation of Sirohaem by Sirohaem Decarboxylase

Application #AN3830

Conditions

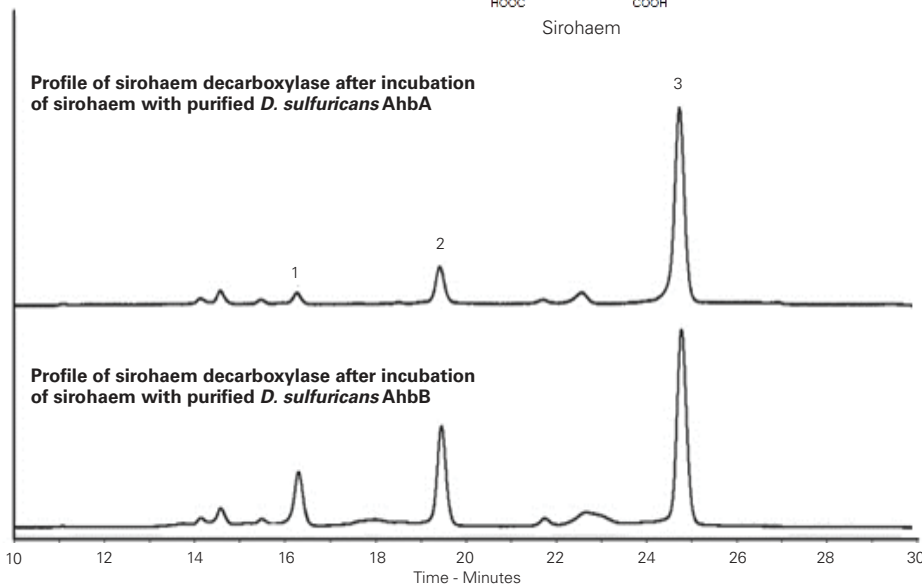
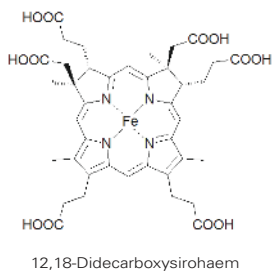
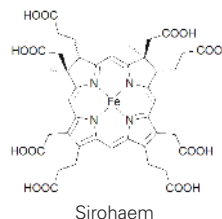
Column: ACE 5 AQ
Dimensions: 150 x 2.1 mm
Part Number: ACE-126-1502
Mobile Phase: A: 0.1% TFA in H₂O
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 5 |
| 6 | 20 |
| 25 | 30 |
| 35 | 100 |
| 40 | 100 |

Flow Rate: 0.2 mL/min
Detection: DAD, 380 nm

Analytes

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



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

Defensins (Human) in Saliva Matrix

Application #AN1270

Conditions

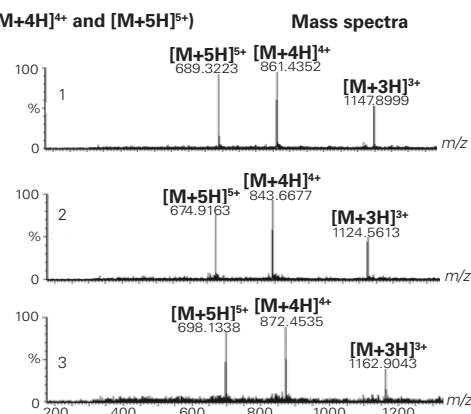
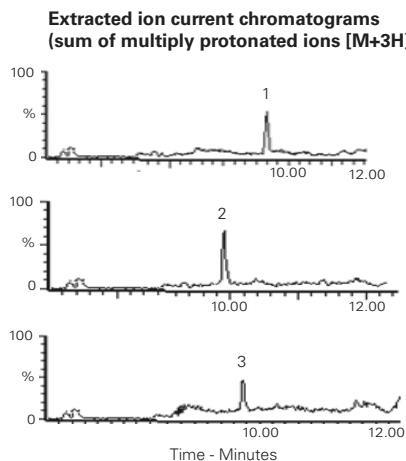
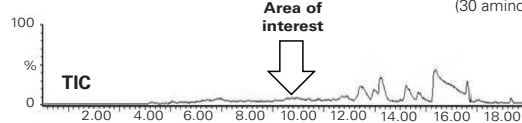
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

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

Defensin Human Neutrophil Peptides

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



Dermorphin in Equine Urine by LC-MS/MS Application #AN1040

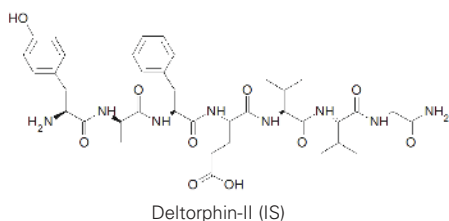
Conditions

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

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

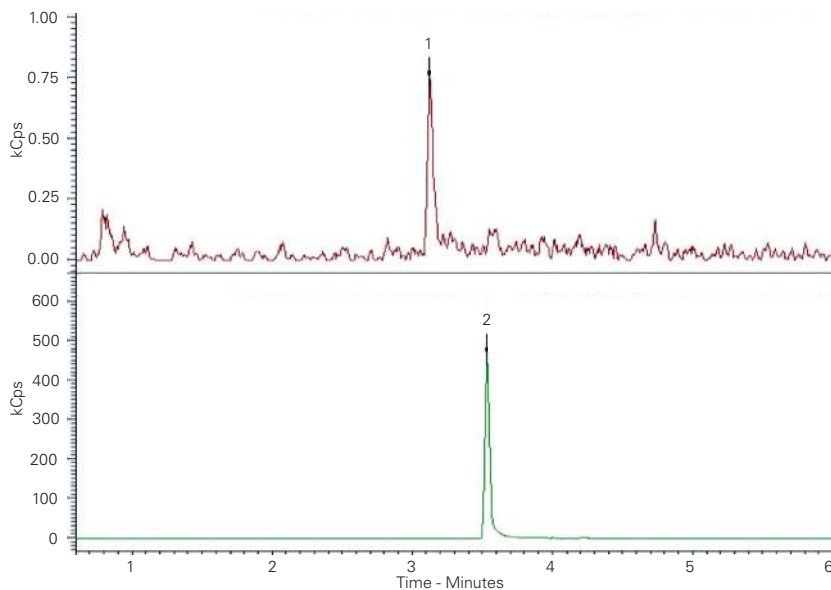
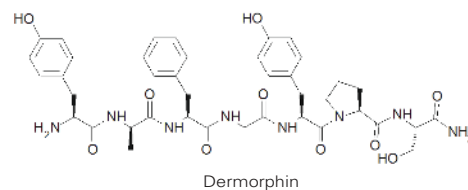
Flow Rate: 0.4 mL/min
Injection: 40 µL
Detection: Bruker EVOQ Elite triple quad MS
 VIP heated-ESI temperature: 350 °C
 Cone gas temperature: 250 °C
 Spray voltage: +4000 V

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



Analytes

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



Reproduced with permission of Bruker UK Ltd (Bruker Application Note #704423)

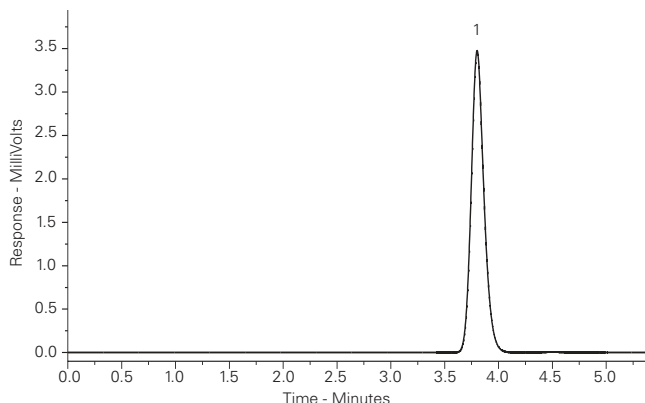
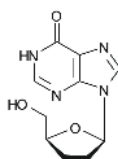
Didanosine Application #AN3590

Conditions

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

Analyte

- Didanosine



Reproduced with permission of Aptuit Ltd, Edinburgh, UK

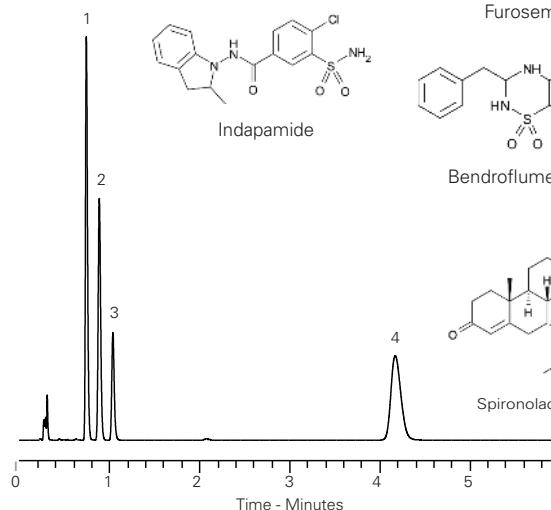
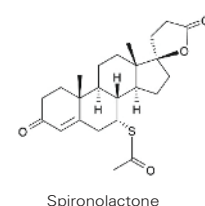
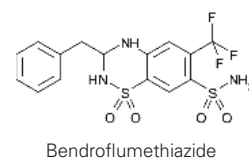
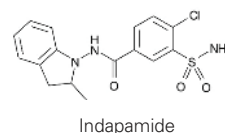
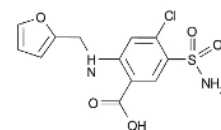
Diuretics (Isocratic) Application #AN2140

Conditions

Column: ACE Excel 2 C18-PFP
Dimensions: 50 x 3.0 mm
Part Number: EXL-1010-0503U
Mobile Phase: 10 mM ammonium formate
 pH 3.0 in MeOH/H₂O (45:55 v/v)
Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: UV, 254 nm

Analytes

- Furosemide
- Indapamide
- Bendroflumethiazide
- Spirolactone





Diuretics Application #AN1450

Conditions

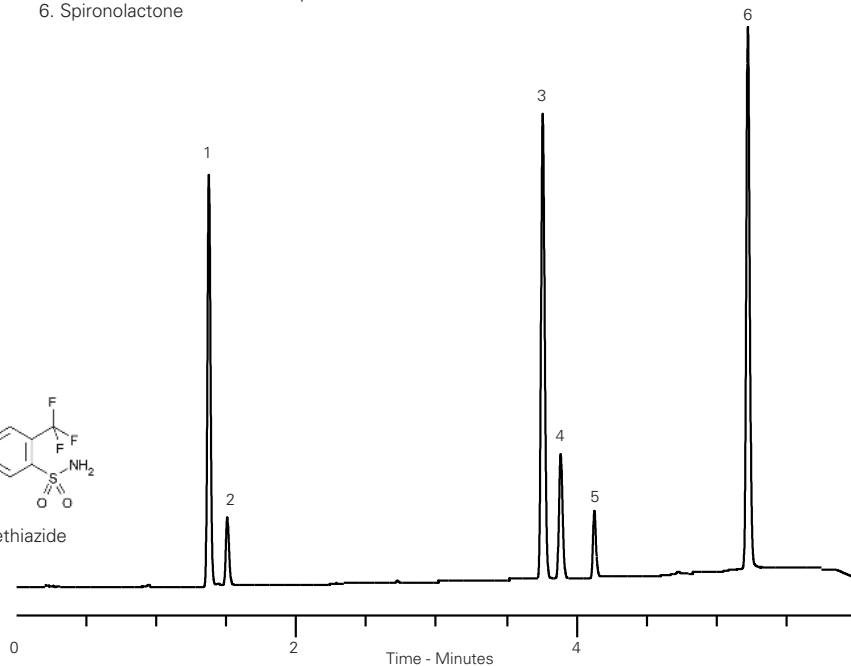
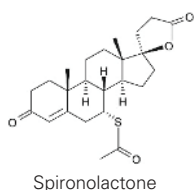
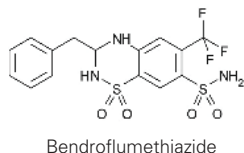
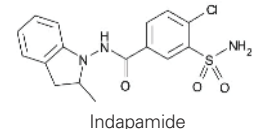
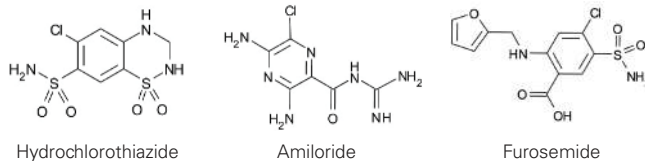
Column: ACE Excel 2 C18-PFP
Dimensions: 50 x 3.0 mm
Part Number: EXL-1010-0503U
Mobile Phase: A: 10 mM ammonium formate pH 3.0 in H₂O
 B: 10 mM ammonium formate pH 3.0 in MeOH/H₂O (9:1 v/v)
Gradient:

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

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

Analytes

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



DOTATATE and Octreotide

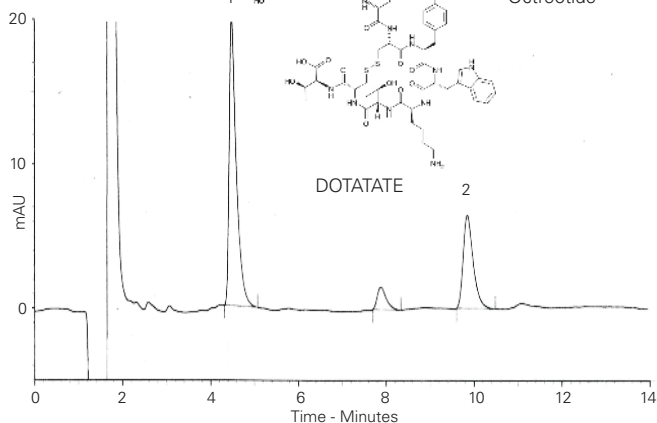
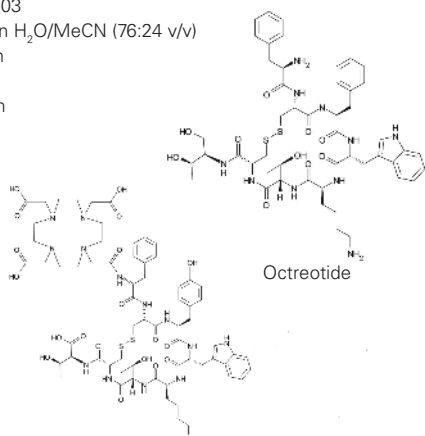
Application #AN2730

Conditions

Column: ACE 3 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-111-1503
Mobile Phase: 0.1% TFA in H₂O/MeCN (76:24 v/v)
Flow Rate: 0.6 mL/min
Injection: 20 µL
Detection: UV, 220 nm

Analytes

1. DOTATATE
2. Octreotide



⁶⁸Ga-DOTATATE QC Analysis by Radiometric Detection

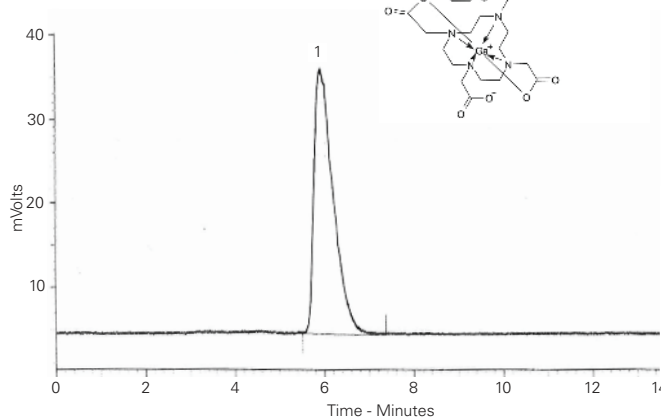
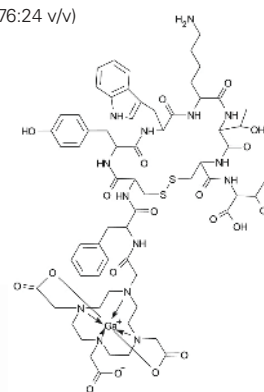
Application #AN2720

Conditions

Column: ACE 3 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-111-1503
Mobile Phase: 0.1% TFA in H₂O/MeCN (76:24 v/v)
Flow Rate: 0.6 mL/min
Injection: 20 µL
Detection: Radiometric

Analyte

1. ⁶⁸Ga-DOTATATE



⁶⁸Ga-DOTATATE PET Tracer by LC-MS/MS

Application #AN2710

Conditions

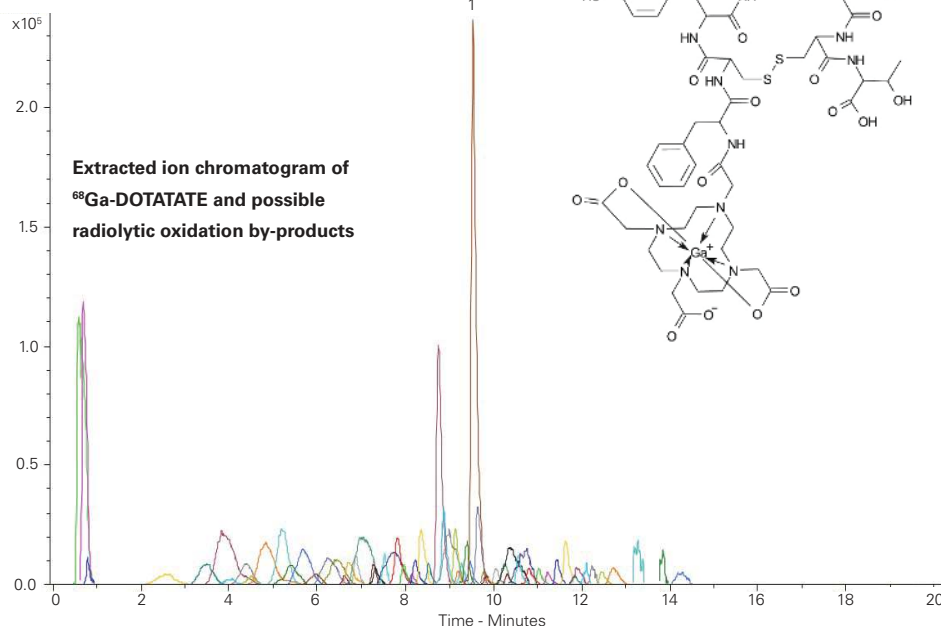
Column: ACE 3 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-111-0546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

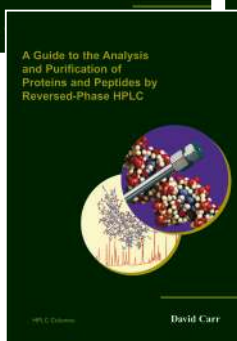
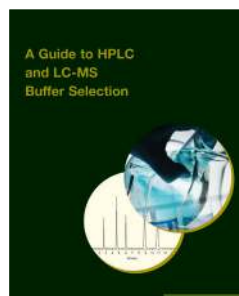
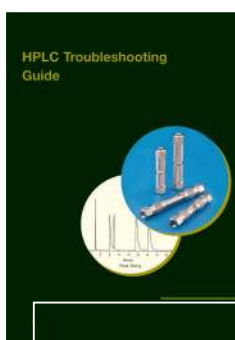
Flow Rate: 1 mL/min
Injection: 10 µL
Detection: Bruker ESI-Q-TOF
 ESI positive ion mode

Analyte

1. ⁶⁸Ga-DOTATATE



Reproduced with permission of Centre of Radiopharmaceutical Science, University Hospital Zurich, Switzerland



FREE HPLC Technical Guides

- HPLC Column Comparison Guide
- HPLC Protein and Peptide Guide
- HPLC & LC-MS Buffer Selection Guide
- HPLC Troubleshooting Guide

To receive your FREE copies of these guides or the latest ACE HPLC Columns Catalogue contact your local distributor or

email: info@ace-hplc.com



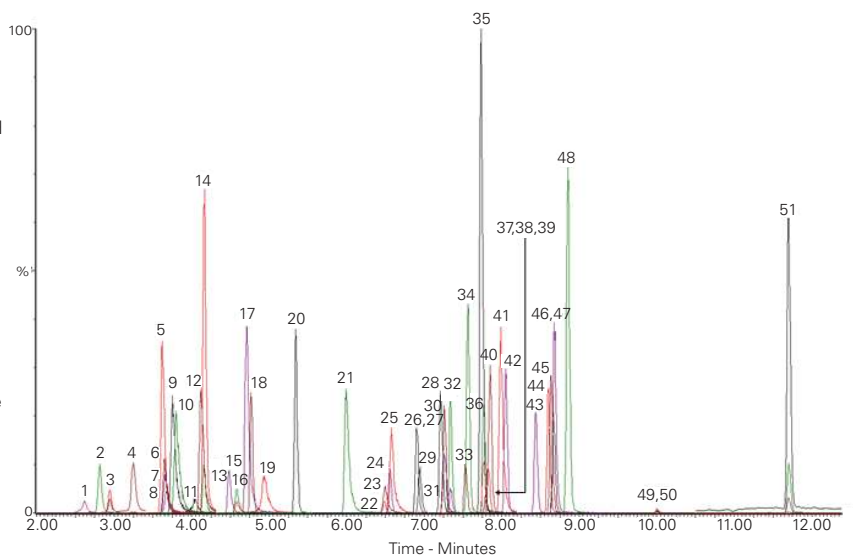
Drugs of Abuse Screen by UHPLC-MS/MS Application #AN2190

Conditions

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

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

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



Reproduced with permission of Biotage GB Ltd, UK

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

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

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

Page 1 of 3

Application #AN4140

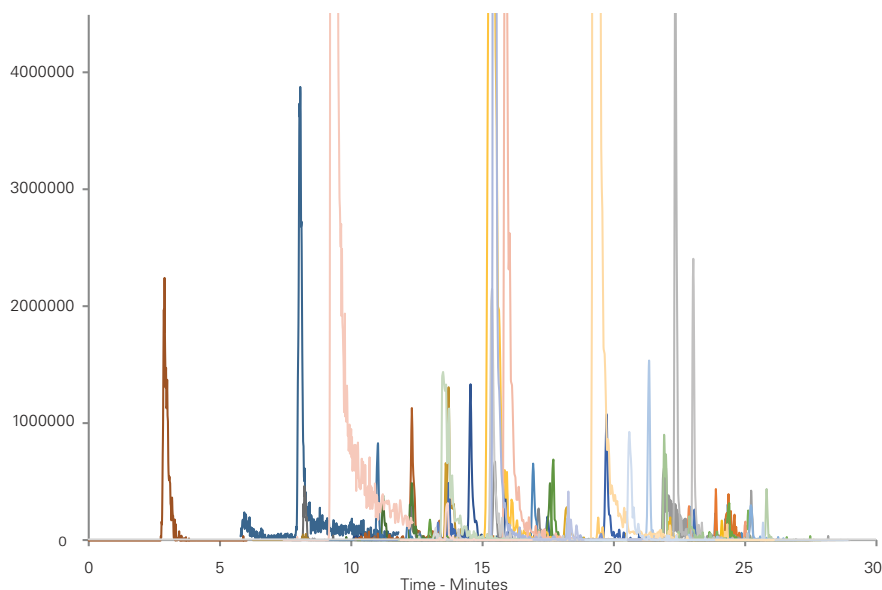
Conditions

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

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

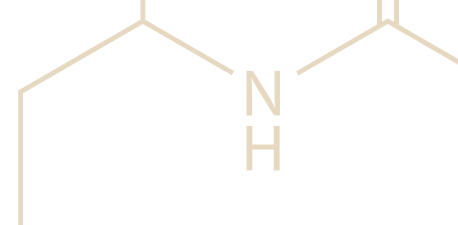
Flow Rate: 0.3 mL/min
Injection: 10 µL
Temperature: 37 °C
Detection: Thermo Quantum Ultra MS
 ESI in positive ion mode

Analytes in blue are included in
 Extracted Ion Chromatogram



Reproduced with permission of Toxicology, Clinical Chemistry, Wansbeck General Hospital, Northumberland, UK

| Analyte | R _t (Mins) | MRM Transitions (m/z) | Analyte | R _t (Mins) | MRM Transitions (m/z) |
|------------------------------|-----------------------|-----------------------|-----------------------------|-----------------------|-----------------------|
| 6-Acetylcodeine | 16.9 | 342.2 > 165.1 | Buphedrone | 14.2 | 178.2 > 160.1 |
| Alfentanil | 21.1 | 417.4 > 197.2 | Buphedrone ephedrine | 13.5 | 180.4 > 162.2 |
| Alprazolam | 23.3 | 309.11 > 205.1 | Bupivacaine | 19.5 | 289.2 > 84.2 |
| Aminoclonazepam | 13.9 | 286.2 > 222.3 | Buprenorphine glucuronide | 18.1 | 644.4 > 468.4 |
| Aminodesmethylflunitrazepam | 20.0 | 270.1 > 121.1 | Bupropion | 19.5 | 240.1 > 131.1 |
| Aminoflunitrazepam | 16.2 | 284.1 > 135.1 | Butylone | 14.7 | 222.1 > 131.1 |
| Aminonitrazepam | 10.9 | 252.1 > 94.1 | Caffeine | 13.1 | 195.1 > 110.1 |
| Aminorex | 12.2 | 163 > 120.1 | Camfetamine | 18.7 | 202.2 > 67.1 |
| Amiodarone | 31.3 | 646.2 > 100 | Carbamazepine | 21.5 | 237.1 > 192.2 |
| Amisulpride | 16.2 | 370.1 > 242 | Carbamazepine 10,11-Epoxide | 18.6 | 253.2 > 180.1 |
| Amitriptyline | 24.4 | 278.2 > 91.1 | Cathine | 20.0 | 134.2 > 91.1 |
| Amlodipine | 25.3 | 409.3 > 238.2 | Cathinone | 9.5 | 150.2 > 117.1 |
| Amlodipine met | 22.9 | 407 > 318 | 2C-B-FLY | 20.1 | 286 > 269.1 |
| Amphetamine | 11.6 | 136.1 > 65.2 | Chlordiazepoxide | 19.5 | 300.1 > 227.1 |
| Amphetamine-d6 | 11.6 | 142.2 > 67.2 | Chloroquine | 18.5 | 320.1 > 142.1 |
| Anhydroecgonine methyl ester | 9.8 | 182.2 > 91.1 | Chlorpheniramine | 20.4 | 275.1 > 167.2 |
| Aripiprazole | 25.5 | 448.1 > 285.1 | Chlorpromazine | 25.9 | 319.2 > 58.1 |
| Atenolol | 10.7 | 267.1 > 145.1 | Citalopram | 22.2 | 325.1 > 246.1 |
| Atomoxetine | 23.1 | 256.2 > 44.1 | Clobazam | 22.8 | 301.1 > 259.2 |
| Atomoxetine metabolite | 22.5 | 242.2 > 44.1 | Clomethiazole | 17.3 | 161.9 > 113 |
| Benzedrone | 21.7 | 254 > 65.1 | Clomipramine | 27.0 | 315.1 > 86.1 |
| Benzoylecgonine | 15.6 | 290.1 > 77.2 | Clonazepam | 23.1 | 316.1 > 214.2 |
| Benzoylecgonine-d3 | 15.6 | 293.2 > 77.2 | Clonidine | 13.2 | 230 > 44.2 |
| Benzylpiperazine | 5.1 | 177.2 > 65.1 | Clozapine | 21.7 | 327.1 > 192.1 |
| Bisoprolol | 19.9 | 326.3 > 116.1 | Cocaethylene | 19.5 | 318.2 > 82.2 |
| Bromazepam | 20.4 | 316 > 182.1 | Cocaine | 18.0 | 304.2 > 82.2 |



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

Page 2 of 3

Application #AN4140

| Analyte | R _t (Mins) | MRM Transitions (m/z) | Analyte | R _t (Mins) | MRM Transitions (m/z) |
|-------------------------------|-----------------------|-----------------------|--------------------------|-----------------------|-----------------------|
| Codeine | 11.9 | 300.2 > 153.2 | 4-Fluoromethcathinone | 20.0 | 182 > 148.1 |
| Cotinine | 2.5 | 177.1 > 80.1 | Fluoxetine | 25.3 | 310.1 > 44.2 |
| Creatinine | 1.3 | 114 > 44 | Fluphenazine | 28.1 | 438.3 > 143.1 |
| Cyclizine | 22.5 | 267.1 > 167.1 | Flurazepam | 21.6 | 388 > 315 |
| D2PM (Diphenylprolinol) | 7.3 | 254.1 > 130.1 | Fluvoxamine | 26.0 | 319.1 > 71 |
| Dehydroaripiprazole | 25.3 | 446.1 > 285.1 | Gabapentin | 10.5 | 172.1 > 67.2 |
| Desipramine | 24.3 | 267.1 > 72.2 | Glibenclamide | 28.2 | 494.1 > 168.9 |
| N-Desmethyloclozapine | 21.0 | 313 > 192.1 | Gliclazide | 24.6 | 324.1 > 110 |
| Desmethylcitalopram | 22.4 | 311.1 > 109.1 | Glimepiride | 28.4 | 491.1 > 126 |
| Desmethylflunitrazepam | 22.5 | 300.1 > 254.2 | Glipizide | 24.5 | 446.1 > 286 |
| Desmethylfluoxetine | 25.4 | 296.2 > 134.1 | Haloperidol | 23.1 | 376.1 > 95.1 |
| N-Desmethylnortazepam | 16.1 | 252.1 > 195.1 | Hippuric acid | 10.9 | 180 > 77 |
| Desmethylolanzapine | 12.6 | 299.1 > 198.1 | Hydrocodone | 13.1 | 300.1 > 199.1 |
| N-Desmethyltramadol | 16.7 | 250.1 > 44.2 | Hydromorphone | 10.4 | 286.2 > 185.1 |
| O-Desmethyltramadol | 12.8 | 250.1 > 58.2 | Hydroxyalprazolam | 22.4 | 325.1 > 216.1 |
| Desmethylvenlafaxine | 15.5 | 264.3 > 58.1 | 4-Hydroxyamphetamine | 5.4 | 152.1 > 107.1 |
| N-Desmethylzopiclone | 20.0 | 375.1 > 245.1 | Hydroxybupropion | 18.5 | 253.1 > 130.1 |
| Desomorphine | 13.1 | 272.1 > 152.1 | 4-Hydroxymethamphetamine | 20.0 | 166.1 > 107.1 |
| Desoxypropidol | 20.5 | 252.1 > 91.1 | 8-Hydroxymirtazapine | 15.6 | 282.1 > 211 |
| Dextromethorphan | 20.0 | 272.2 > 171.1 | 7-Hydroxymirtazapine | 18.2 | 415.3 > 175.1 |
| Diamorphine | 16.9 | 370.1 > 165.1 | 3-Hydroxyphenazepam | 23.3 | 366.9 > 320.8 |
| Diazepam | 25.5 | 285.1 > 154.1 | 7-Hydroxyquetiapine | 15.3 | 400.3 > 208.1 |
| Didesmethylcitalopram | 22.2 | 297 > 262.1 | 9-Hydroxyrisperidone | 19.5 | 427.2 > 69.1 |
| Digoxin | 24.2 | 781.2 > 97 | Imipramine | 24.2 | 281.1 > 86.2 |
| Dihydrocodeine | 11.7 | 302.2 > 128.1 | 5-Iodo-2-aminoindane | 18.4 | 260.1 > 115.1 |
| Diltiazem | 22.7 | 415.1 > 178.1 | Ketamine | 15.4 | 238.1 > 125.1 |
| Dimethocaine | 16.3 | 279.3 > 92.1 | Lamotrigine | 16.8 | 256.1 > 211.1 |
| Dinitrophenol | 18.4 | 183 > 109 | Levamisole | 13.3 | 205.1 > 91.1 |
| Diphenhydramine | 21.2 | 256.1 > 167.1 | Levetiracetam | 8.9 | 171.2 > 126.1 |
| Dipipanone | 25.0 | 350.2 > 265.2 | Lidocaine | 14.8 | 235.1 > 86.2 |
| Donepezil | 22.2 | 380.1 > 91 | Lorazepam | 22.8 | 321 > 229.1 |
| Dothiepin | 23.7 | 296.2 > 202.2 | Lormetazepam | 23.8 | 335 > 289.1 |
| Ecgonine ethyl ester | 2.5 | 214.1 > 196.1 | LSD | 20.1 | 324.3 > 223.1 |
| Ecgonine methyl ester | 1.0 | 200.1 > 182.1 | MCAT | 5.4 | 164.2 > 130.1 |
| EDDP | 21.4 | 278.2 > 219.2 | mCPP | 17.0 | 197.1 > 118.1 |
| Estazolam | 22.5 | 295.1 > 267.1 | MDA | 13.4 | 180.1 > 133.1 |
| Ethylamphetamine | 14.5 | 164.1 > 91.2 | MDAI | 12.3 | 178.19 > 161.1 |
| Ethylmethcathinone | 15.8 | 192.2 > 131.2 | MDEA | 15.2 | 208.1 > 135.1 |
| Ethylphenidate | 19.2 | 248.1 > 56.2 | MDMA | 14.1 | 194.1 > 135.2 |
| Etizolam | 23.5 | 343.1 > 314.2 | MDPV | 18.1 | 276.1 > 135.1 |
| Fenfluramine | 20.3 | 232.1 > 159.1 | MEGX | 13.4 | 207.1 > 58.1 |
| Fentanyl | 21.4 | 337.2 > 105.1 | MeOPP | 13.3 | 193.2 > 133.1 |
| Flubromazolam | 23.2 | 371.1 > 223.1 | Mephedrone | 14.6 | 178.1 > 144.2 |
| Flunitrazepam | 23.5 | 314.1 > 269.3 | Mescaline | 12.7 | 212.1 > 165.1 |
| 2-Fluoroamphetamine | 13.2 | 154.1 > 83.1 | Metformin | 2.5 | 130 > 60.1 |
| Fluoroamphetamine interferent | 10.6 | 154 > 67.1 | Methadone | 24.0 | 310.2 > 105.1 |
| 3-Fluoromethcathinone | 20.0 | 182.1 > 149.1 | Methadone-d3 | 24.0 | 313.2 > 268.2 |



Drugs of Abuse Screen (250 Analytes) in Urine by LC-MS/MS Page 3 of 3
Application #AN4140

| Analyte | R _t (Mins) | MRM Transitions (m/z) | Analyte | R _t (Mins) | MRM Transitions (m/z) |
|------------------------------|-----------------------|-----------------------|----------------------|-----------------------|-----------------------|
| Methamphetamine | 12.8 | 150.1 > 91.2 | Paracetamol | 7.8 | 152.1 > 65.1 |
| Methaqualone | 22.8 | 251.2 > 91.1 | PCP | 20.5 | 244.3 > 86.2 |
| Methedrone | 13.9 | 194.1 > 146.1 | Pentazocine | 19.5 | 286.3 > 175.2 |
| Methiopropamine | 10.6 | 156.1 > 97 | Pentedrone | 16.0 | 192.2 > 131.1 |
| Methocarbamol | 16.8 | 242.1 > 118.1 | Phenazepam | 24.5 | 350.9 > 206 |
| Methoxetamine | 17.2 | 248.2 > 121.1 | Pheniramine | 15.1 | 241.2 > 196.2 |
| 3-Methoxytyramine | 6.6 | 168 > 91 | Phenytoin | 20.0 | 253.1 > 77 |
| Methylethcathinone | 20.0 | 192.1 > 144.2 | Pholcodine | 9.2 | 399.2 > 114.1 |
| Methylhexanamine | 13.4 | 116.1 > 57.3 | PMA | 13.8 | 149.2 > 91.1 |
| Methylone | 12.7 | 208.1 > 132.1 | PMMA | 14.6 | 180.2 > 121.1 |
| Methylphenidate | 16.5 | 234.1 > 56.2 | Powder 20140730 | 18.7 | 248.3 > 84.2 |
| 5-Methyltryptamine | 16.9 | 175.1 > 143 | Prazepam | 27.0 | 325 > 140 |
| Metoclopramide | 17.2 | 300.1 > 227.1 | Pregabalin | 10.4 | 160.1 > 97.2 |
| Midazolam | 20.9 | 326.1 > 249.1 | Procyclidine | 22.4 | 288.3 > 42 |
| Mirtazapine | 16.6 | 266.1 > 72.2 | Promethazine | 20.0 | 285.1 > 86.2 |
| Mitragynine | 22.6 | 399.3 > 174.1 | Propofol | 23.9 | 179 > 137 |
| Modafinil | 21.1 | 296.1 > 129 | Propofol glucuronide | 20.1 | 372.2 > 148.1 |
| 6-Monoacetylmorphine | 12.9 | 328.1 > 165.1 | Propoxyphene | 23.6 | 340.2 > 58.2 |
| Mono-N-desethylamiodarone | 30.8 | 618.2 > 547.2 | Propranolol | 23.0 | 260.1 > 157.1 |
| Morphine | 7.7 | 286.1 > 152.2 | Quetiapine | 21.7 | 384.1 > 221.1 |
| Morphine glucuronide | 2.7 | 462.2 > 201.1 | Remifentanil | 18.4 | 377.3 > 113.1 |
| Morphine-d3 | 7.7 | 289.2 > 152.2 | Risperidone | 20.4 | 411.1 > 190.8 |
| Naloxone | 20.0 | 328.3 > 212.1 | Ritalinic acid | 14.4 | 220.2 > 56.1 |
| Naphyrone | 23.2 | 282.2 > 141.1 | Sertraline | 25.6 | 306.1 > 159 |
| Nefopam | 19.5 | 254.9 > 166.1 | Sildenafil | 23.6 | 475.4 > 58.1 |
| Nifoxipam | 20.9 | 316.05 > 298.1 | Sildenafil N-oxide | 23.9 | 491.4 > 312.3 |
| Nimetazepam | 23.6 | 296.1 > 250.2 | Sufentanil | 22.9 | 387.3 > 140.2 |
| Nitrazepam | 22.8 | 282.1 > 236.1 | Temazepam | 24.2 | 301.1 > 177.1 |
| Noralfentanil/sufentanil | 19.4 | 277.1 > 245.1 | Temazepam-d5 | 24.1 | 306.1 > 260.2 |
| Norbuprenorphine glucuronide | 15.5 | 590.3 > 414.3 | Tetrazepam | 24.5 | 289.2 > 225.2 |
| Norcyclizine | 21.9 | 253.2 > 167.1 | TFMPP | 7.9 | 231.1 > 118.1 |
| Nordiazepam | 24.4 | 271.1 > 140.1 | Theophylline | 11.2 | 181.1 > 124.1 |
| Nordothiepin | 24.4 | 282.1 > 202.1 | Tramadol | 16.9 | 264.2 > 58.2 |
| Norfentanyl | 15.6 | 233.2 > 56.2 | Trazodone | 23.9 | 372.2 > 179.2 |
| Norketamine | 14.8 | 224.1 > 125.1 | Trifluoperazine | 28.8 | 408.2 > 113.2 |
| Normorphine | 3.8 | 272.1 > 165.2 | Trihexyphenidyl | 23.7 | 302.1 > 70.1 |
| Nornefopam | 19.7 | 240.9 > 166.1 | Varenicline | 12.3 | 212.2 > 168.1 |
| Noroxycodone | 13.0 | 302.1 > 284.1 | Venlafaxine | 19.1 | 278.2 > 58.2 |
| Norpropoxyphene | 23.0 | 308 > 44.2 | Verapamil | 23.9 | 455.2 > 150.1 |
| Norsertaline | 20.0 | 275.3 > 159 | Vigabatrin | 2.5 | 130.1 > 71.1 |
| Nortriptyline | 24.6 | 264.1 > 91.1 | Warfarin | 25.7 | 309.1 > 251.1 |
| Olanzapine | 13.4 | 313.1 > 84.1 | Zaleplon | 21.5 | 306.1 > 236.2 |
| Orphenadrine | 23.4 | 270.1 > 181.1 | Zolpidem | 18.8 | 308.2 > 235.2 |
| Oxazepam | 23.5 | 287.1 > 104.1 | Zolpidem phenyl COOH | 15.3 | 338 > 265.1 |
| Oxybutynin | 24.6 | 358.1 > 141.9 | Zopiclone | 16.5 | 389.1 > 217.1 |
| Oxycodone | 12.9 | 316.1 > 241.1 | Zopiclone N-oxide | 17.6 | 405.2 > 217.1 |
| Oxymorphone | 20.0 | 302 > 227 | | | |



Echinacea

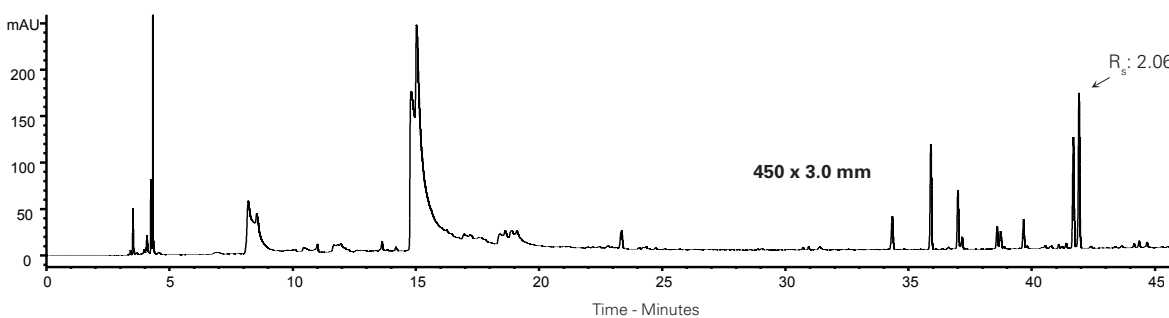
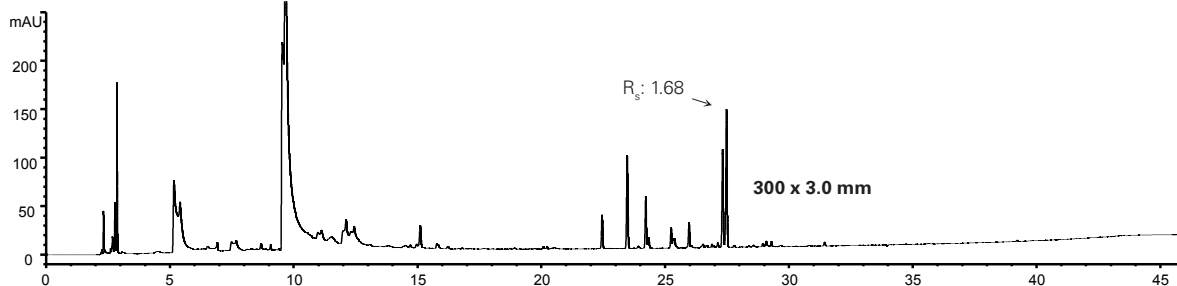
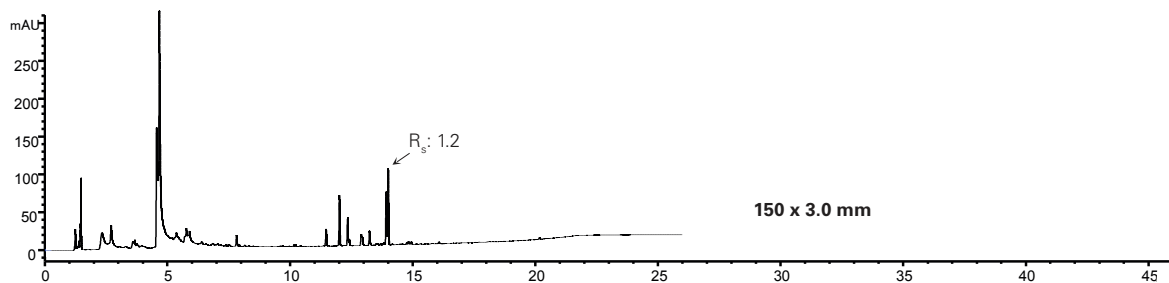
Application #AN4270

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 3.0 mm; 2 x 150 x 3.0 mm (coupled); 3 x 150 x 3.0 mm (coupled)
Part Number: CORE-25A-1503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

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



Entacapone

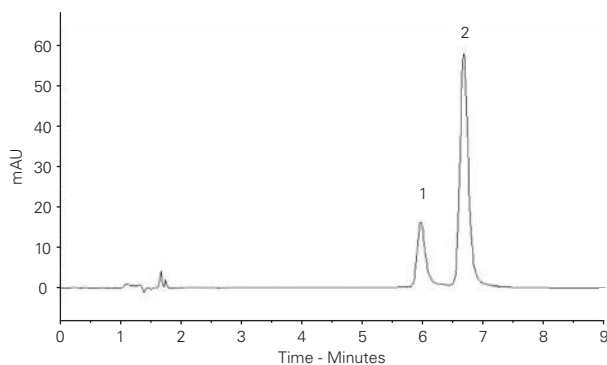
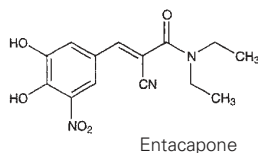
Application #AN3600

Conditions

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

Analytes

- Degradation Product
- Entacapone



Reproduced with permission of Brazilian Pharmacopoeia

Epanolol

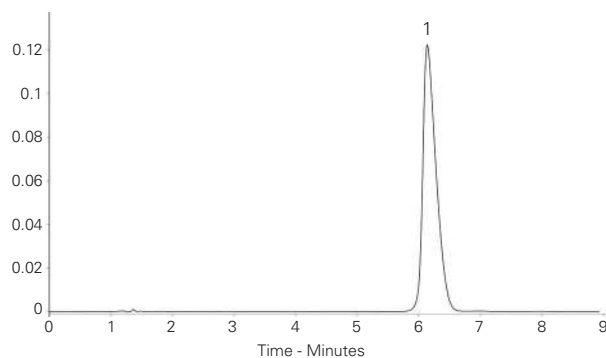
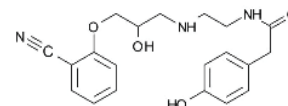
Application #AN3610

Conditions

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

Analyte

- Epanolol



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

Epinastine

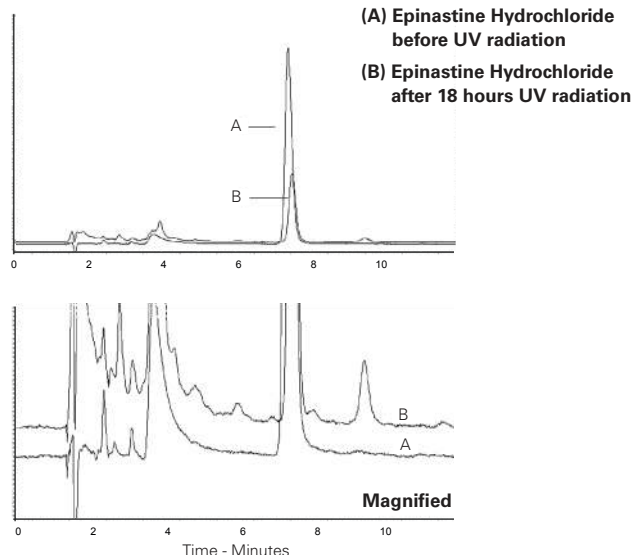
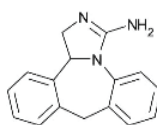
Application #AN3620

Conditions

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

Analyte

- Epinastine



Reproduced with permission of Brazilian Pharmacopoeia

Ethanol Extract from Seed Cover (*Acacia Farnesiana*)

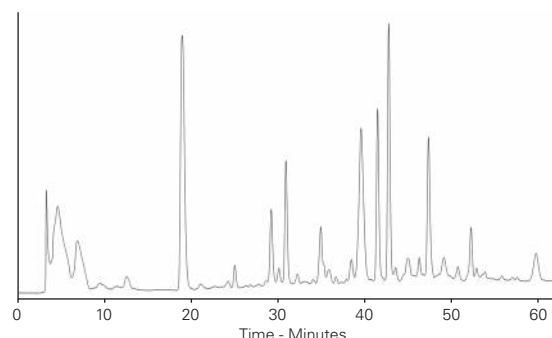
Application #AN2900

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: MeOH
 B: H₂O
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 85 |
| 2.5 | 85 |
| 60.0 | 50 |
| 62.5 | 50 |
| 70.0 | 85 |

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



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



Ethyl Glucuronide in Water by LC-MS/MS

Application #AN1100

Conditions

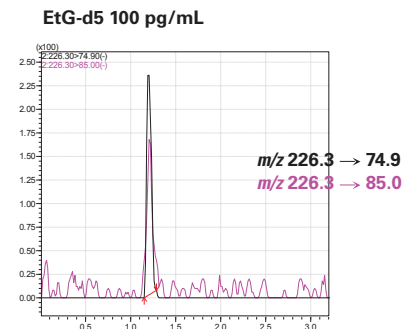
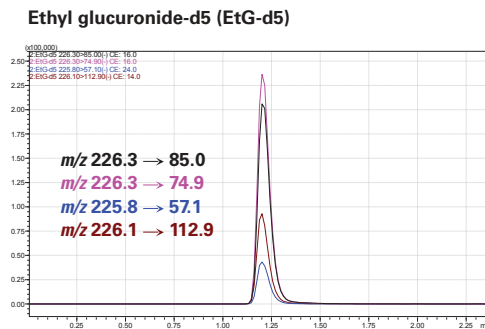
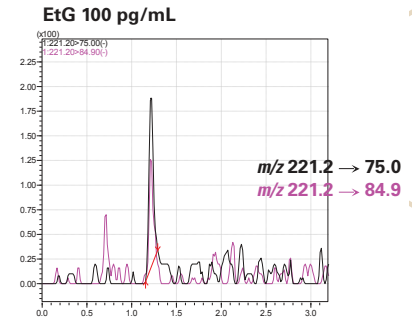
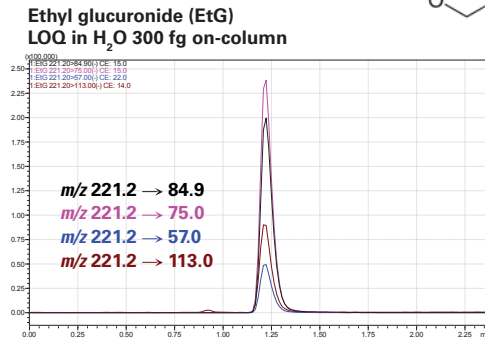
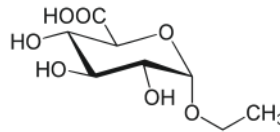
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 0.05% formic acid in H₂O
 B: MeOH
Gradient:

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

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

Analyte

1. Ethyl glucuronide



Reproduced with permission of Shimadzu Europa GmbH. Analysed on Shimadzu Nexera X2

Exploiting Selectivity by Adjusting pH

Application #AN2440

Conditions

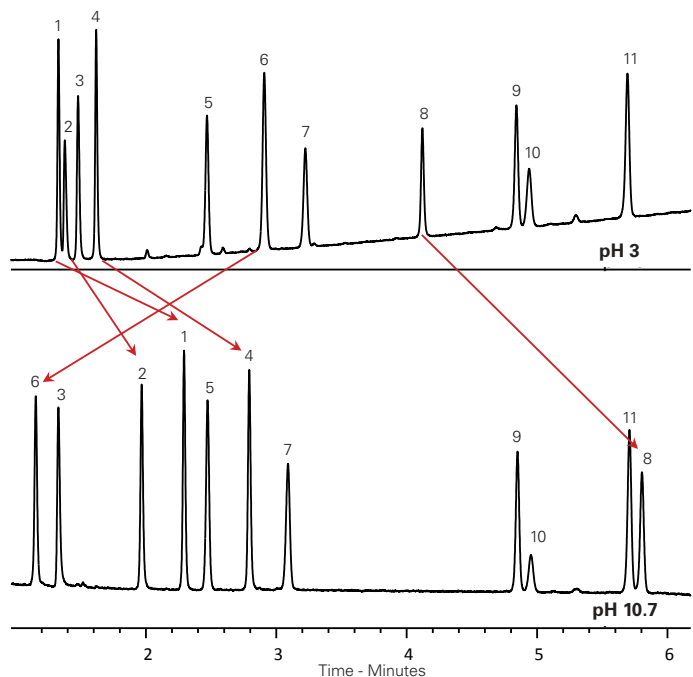
Column: ACE Excel 2 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: EXL-1011-0502U
Mobile Phase: A1: 10 mM ammonium formate pH 3.0 in H₂O
 A2: 0.1% ammonia pH 10.7 in H₂O
 B1: 10 mM ammonium formate pH 3.0 in MeCN/H₂O (90:10 v/v)
 B2: 0.1% ammonia pH 10.7 in MeCN/H₂O (90:10 v/v)
Gradient:

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

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

Analytes

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



Explosive Analytes (I)

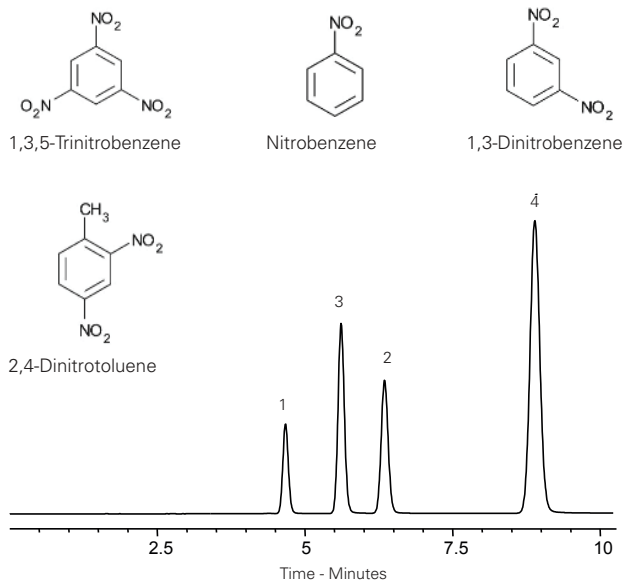
Application #AN1460

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeOH/H₂O (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 20 °C
Detection: UV, 254 nm

Analytes

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



Explosive Analytes (II)

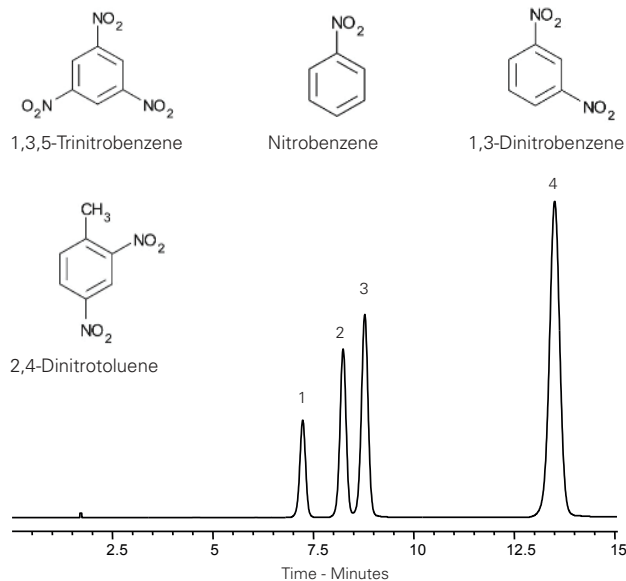
Application #AN1470

Conditions

Column: ACE 5 CN-ES
Dimensions: 150 x 4.6 mm
Part Number: EXL-1213-1546U
Mobile Phase: MeOH/H₂O (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 20 °C
Detection: UV, 254 nm

Analytes

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



Fingerprinting of *Cuscuta Chinensis* Flavonoids

Application #AN4250

Conditions

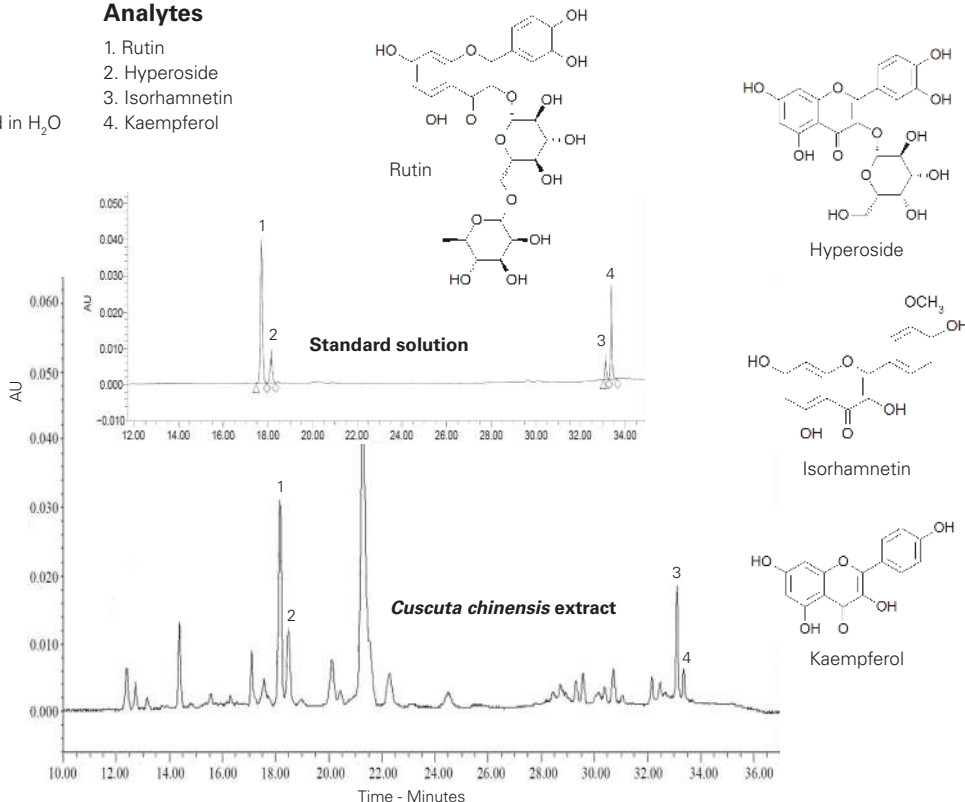
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.25% o-phosphoric acid in H₂O
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 5 |
| 2 | 5 |
| 7 | 10 |
| 10 | 15 |
| 23 | 20 |
| 28 | 30 |
| 32 | 50 |

Flow Rate: 1 mL/min
Injection: 10 µL
Detection: UV, 360 nm

Analytes

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



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

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



Flavone and Dibucaine

Application #AN2850

Conditions

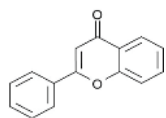
Column: ACE 3 C18
Dimensions: 30 x 4.6 mm
Part Number: ACE-111-0346
Mobile Phase: A: 6.5 mM ammonium acetate in H₂O
 B: MeCN
 C: MeOH
Gradient:

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

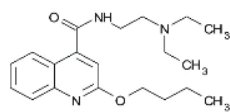
Flow Rate: 2 mL/min
Temperature: 60 °C
Detection: UV, 200-450 nm

Analytes

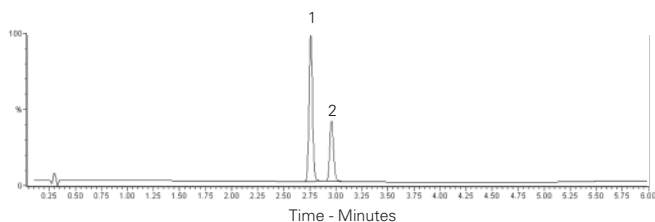
1. Flavone
2. Dibucaine



Flavone



Dibucaine



Reproduced with permission of Johnson & Johnson Pharmaceutical Research & Early Development, a division of Janssen-Cilag, S.A, Toledo, Spain

Flavonoids

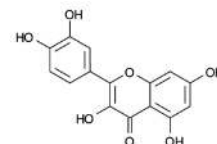
Application #AN2810

Conditions

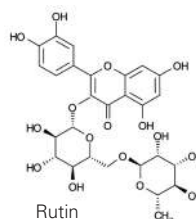
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/0.1% formic acid in H₂O (40:60 v/v)
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: Ambient
Detection: UV, 254 nm

Analytes

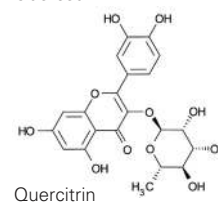
1. Rutin
2. Quercetin
3. Quercitrin
4. Kaempferol



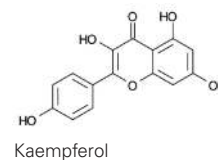
Quercetin



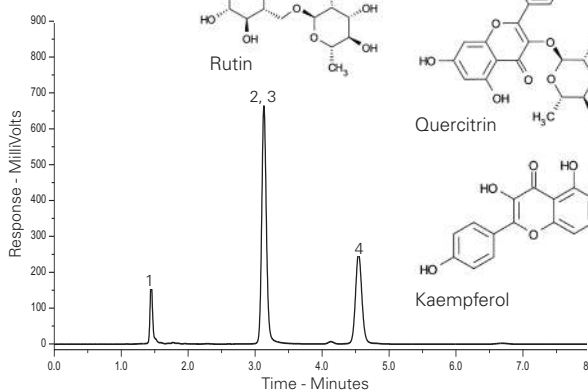
Rutin



Quercitrin



Kaempferol



Flurbiprofen and Related Substances

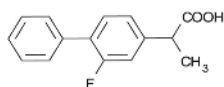
Application #AN3630

Conditions

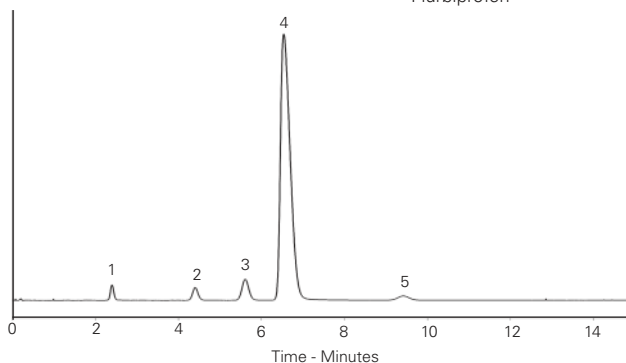
Column: ACE 3 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-111-0546
Mobile Phase: H₂O/MeCN/TFA (64:34:0.5 v/v/v)
Flow Rate: 2 mL/min
Injection: 20 µL
Temperature: 28 °C
Detection: UV, 254 nm

Analytes

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



Flurbiprofen



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

Formoterol from Human Plasma by LC-MS/MS

Application #AN3100

Conditions

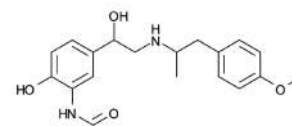
Column: ACE Excel 2 C18-AR
Dimensions: 50 x 2.1 mm
Part Number: EXL-109-0502U
Mobile Phase: A: 0.02% formic acid in H₂O
 B: 0.02% formic acid in H₂O/MeOH (2:98 v/v)
Gradient:

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

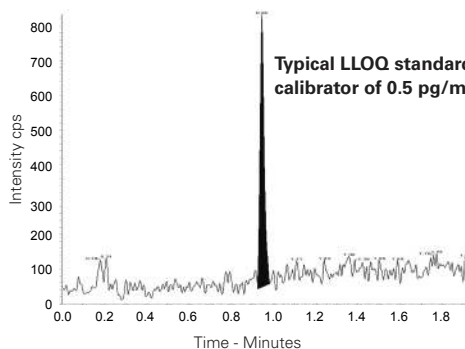
Flow Rate: 0.75 mL/min
Temperature: 60 °C
Detection: AB SCIEX QTRAP 5500 LC-MS/MS system
Sample: Extracted by mixed mode cation exchange SPE

Analyte

1. Formoterol
(*m/z* 345 → 149)



Formoterol



Typical LLOQ standard calibrator of 0.5 pg/mL

Reproduced with permission of Bioanalytical Systems, Inc

Galanthamine

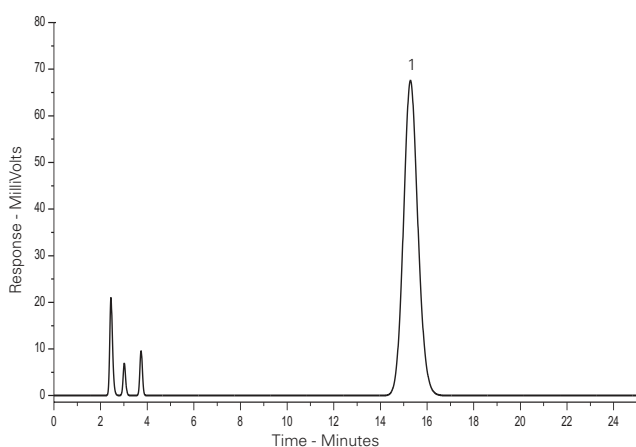
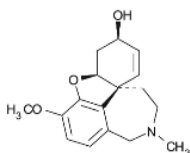
Application #AN3640

Conditions

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

Analyte

1. Galanthamine



Reproduced with permission of Neem Biotech, Cardiff, UK

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

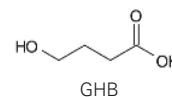
Application #AN1500

Conditions

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

Analytes

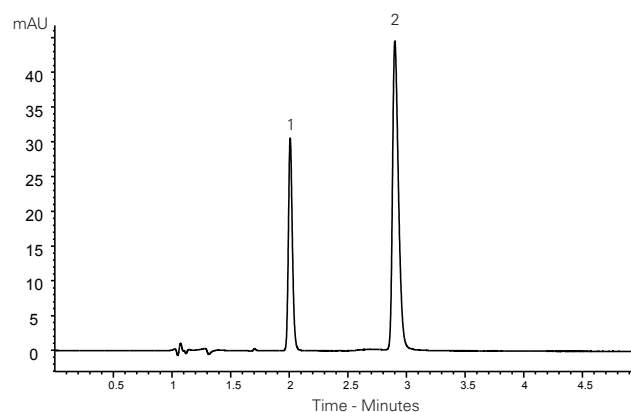
1. GHB
 2. GBL



GHB



GBL



Garlic Analysis (I)

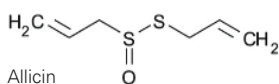
Application #AN2820

Conditions

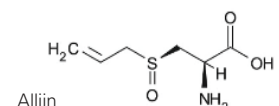
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: H₂O/MeOH (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 210 nm

Analytes

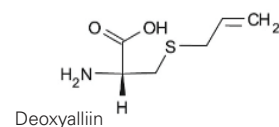
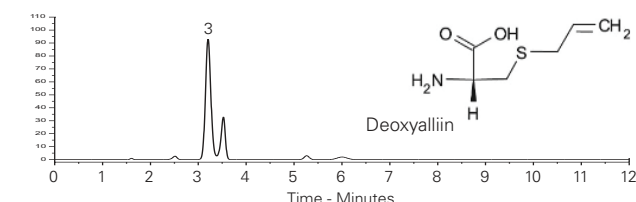
1. Allicin
 2. Alliin
 3. Deoxyalliin



Allicin



Alliin



Deoxyalliin

Reproduced with permission of Neem Biotech, Cardiff, UK

Garlic Analysis (II)

Application #AN2830

Conditions

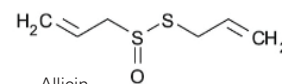
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: H₂O
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 40 |
| 20 | 100 |
| 25 | 100 |

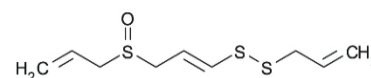
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 254 nm

Analytes

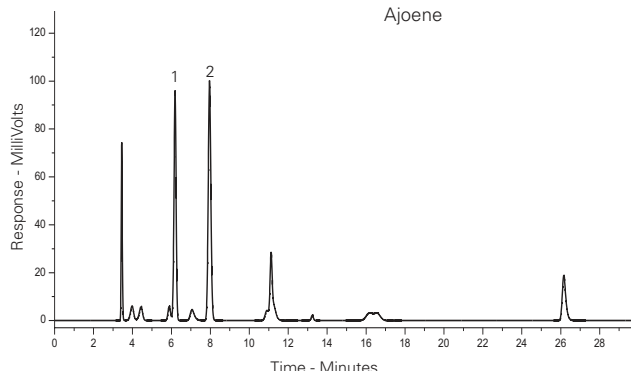
1. Allicin
 2. Ajoene



Allicin



Ajoene



Reproduced with permission of Neem Biotech, Cardiff, UK



Ginkgo Biloba – Ultra Resolution

Application #AN2270

Conditions

Column: ACE Excel 1.7 C18-PFP
Dimensions: 2 x 100 x 3.0 mm (coupled)
Part Number: 2 x EXL-1710-1003U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

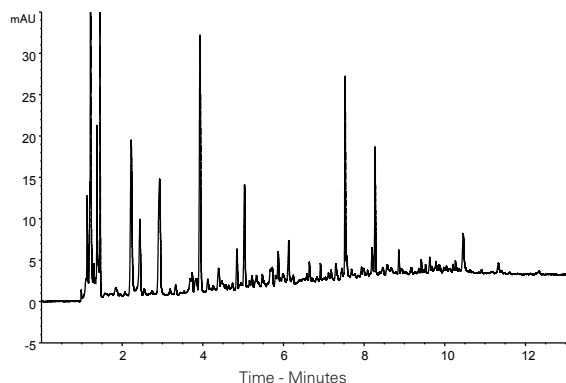
| Time (mins) | %B |
|-------------|-----|
| 0.00 | 5 |
| 0.72 | 5 |
| 15.72 | 50 |
| 18.72 | 100 |
| 20.72 | 100 |
| 22.72 | 5 |

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

Need a custom column for your application?

Please enquire

email: info@ace-hplc.com



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

Ginsenosides from Chinese Medicine by UHPLC-MS/MS

Application #AN3540

Conditions

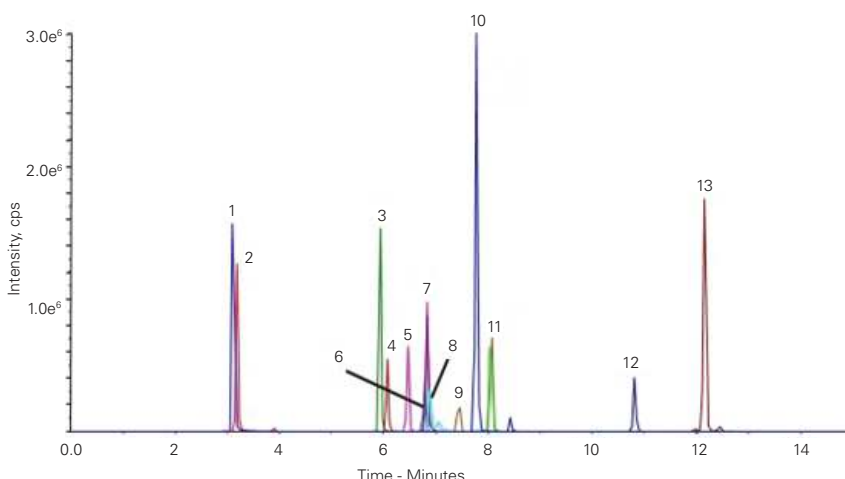
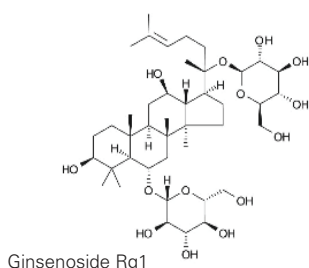
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 3.0 mm
Part Number: CORE-25A-1503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

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

Analytes

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



Reproduced with permission of Beijing University of Chinese Medicine, Beijing, China

Ginseng Extract

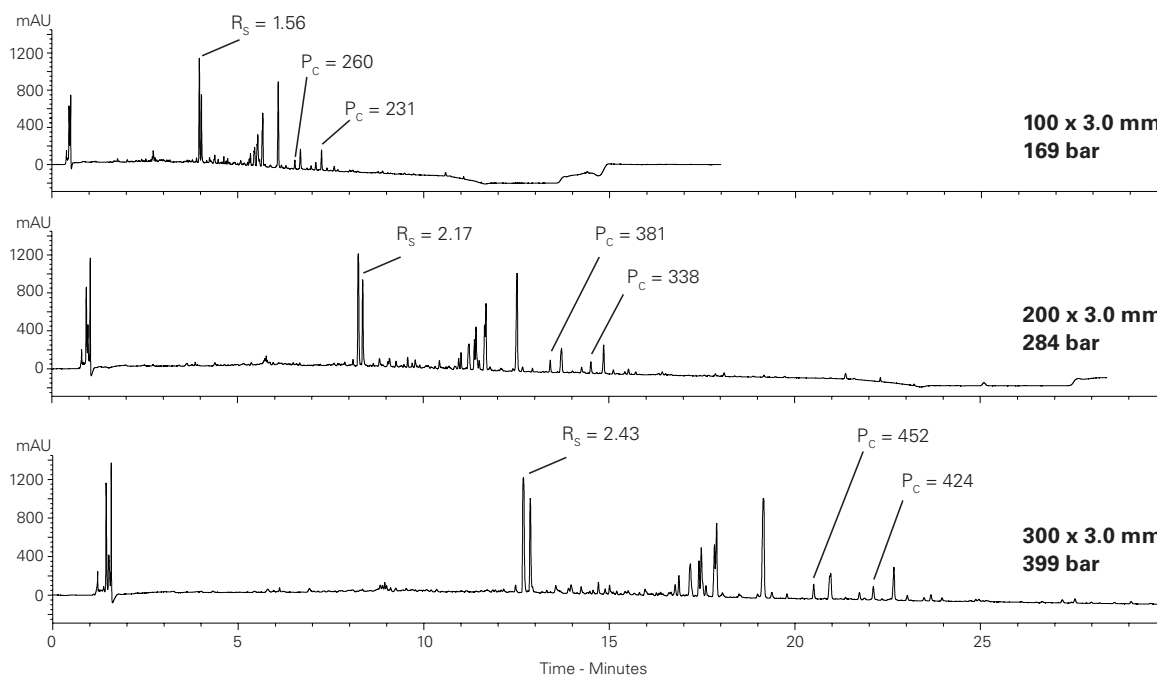
Application #AN4260

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 3.0 mm; 2 x 100 x 3.0 mm (coupled); 3 x 100 x 3.0 mm (coupled)
Part Number: CORE-25A-1003U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

Flow Rate: 0.8 mL/min
Injection: 2 µL (100 x 3.0 mm); 4 µL (200 x 3.0 mm); 6 µL (300 x 3.0 mm)
Temperature: 80 °C
Detection: UV, 203 nm
Sample: 5 x 75 mg tablets ground to fine powder and extracted with 10.0 mL MeCN/H₂O (1:1 v/v) for 15 minutes with ultrasonication. 100 µL supernatant diluted with 300 µL water and filtered using a Whatman Mini-Uniprep syringeless filter
System: Chromaster Ultra Rs





Gliotoxin from *Aspergillus Fumigatus* Liquid Culture

Application #AN3780

Conditions

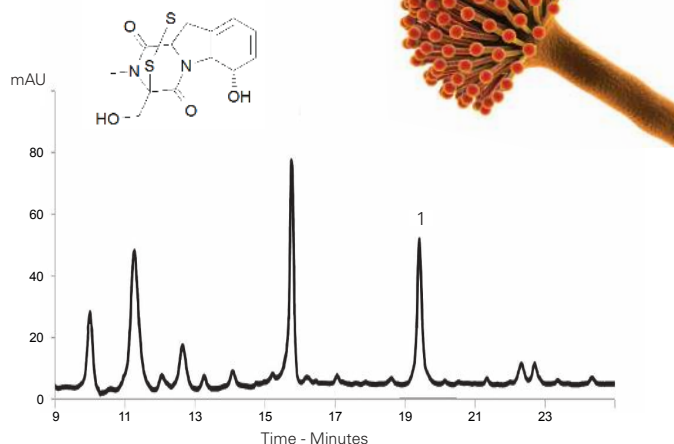
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.05% TFA in H₂O/MeCN (90:10 v/v)
 B: 0.05% TFA in H₂O/MeCN (40:60 v/v)
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 10 |
| 21 | 100 |

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

Analyte

1. Gliotoxin



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

Glyphosate and Related Compounds as FMOc Derivatives (Gradient)

Application #AN3850

Conditions

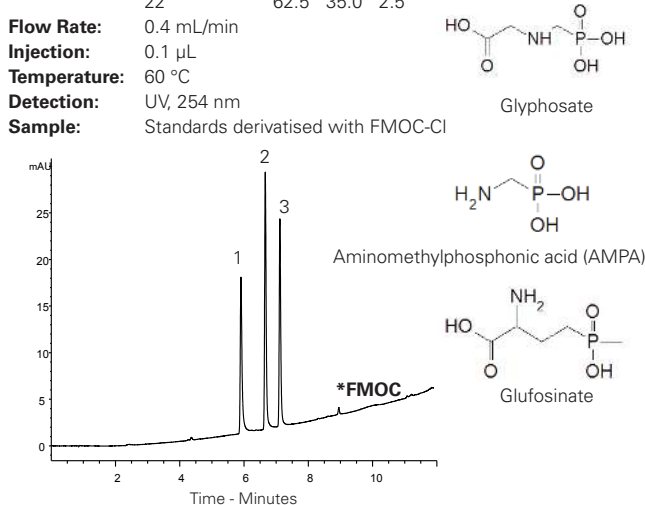
Column: ACE Excel 3 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: EXL-1111-1502U
Mobile Phase: A: H₂O
 B: MeOH
 C: 200 mM ammonium formate pH 3.0
Gradient:

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

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

Analytes

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



Glyphosate and Related Compounds as FMOc Derivatives (Isocratic)

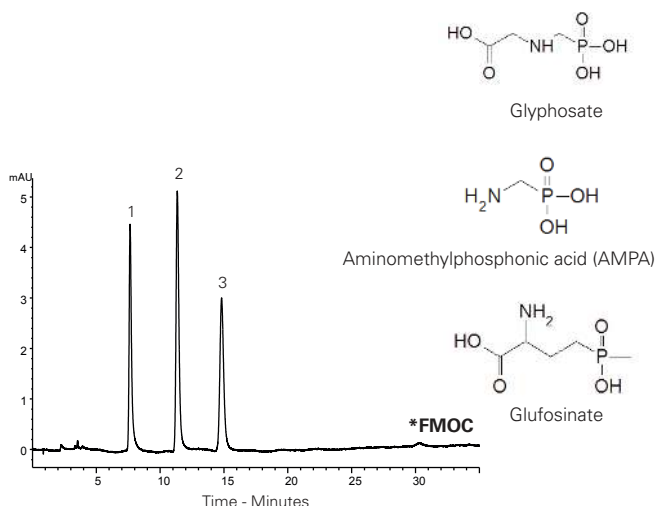
Application #AN3860

Conditions

Column: ACE Excel 3 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: EXL-1111-1502U
Mobile Phase: 5 mM ammonium formate pH 3.0 in H₂O/MeOH (55:45 v/v)
Flow Rate: 0.4 mL/min
Injection: 0.1 µL
Temperature: 25 °C
Detection: UV, 254 nm
Sample: Standards derivatised with FMOc-Cl

Analytes

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



Green Tea Extract

Application #AN4280

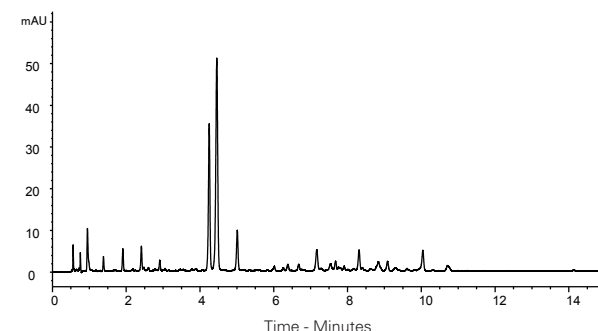
Conditions

Column: ACE Excel 1.7 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1711-1003U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

Flow Rate: 0.8 mL/min
Injection: 2 µL
Temperature: 80 °C
Detection: UV, 260 nm
Sample: Tablet ground to fine powder and extracted with MeCN/H₂O (1:1 v/v) with ultrasonication. Supernatant diluted with H₂O and filtered using Whatman Mini-Uniprep syringeless filter Chromaster Ultra Rs

System:



Green Tea Metabolite Profiling by LC-MS

Application #AN2580

Conditions

Column: ACE Excel 1.7 C18-Amide**Dimensions:** 100 x 2.1 mm**Part Number:** EXL-1712-1002U**Mobile Phase:** A: 0.01% formic acid in H₂O

B: 0.01% formic acid in MeCN

Gradient: **Time (mins)** **%B**

0.0 3

2.5 10

8.0 100

8.5 3

10.0 3

Flow Rate: 0.5 mL/min**Detection:** Exacte accurate mass MS system

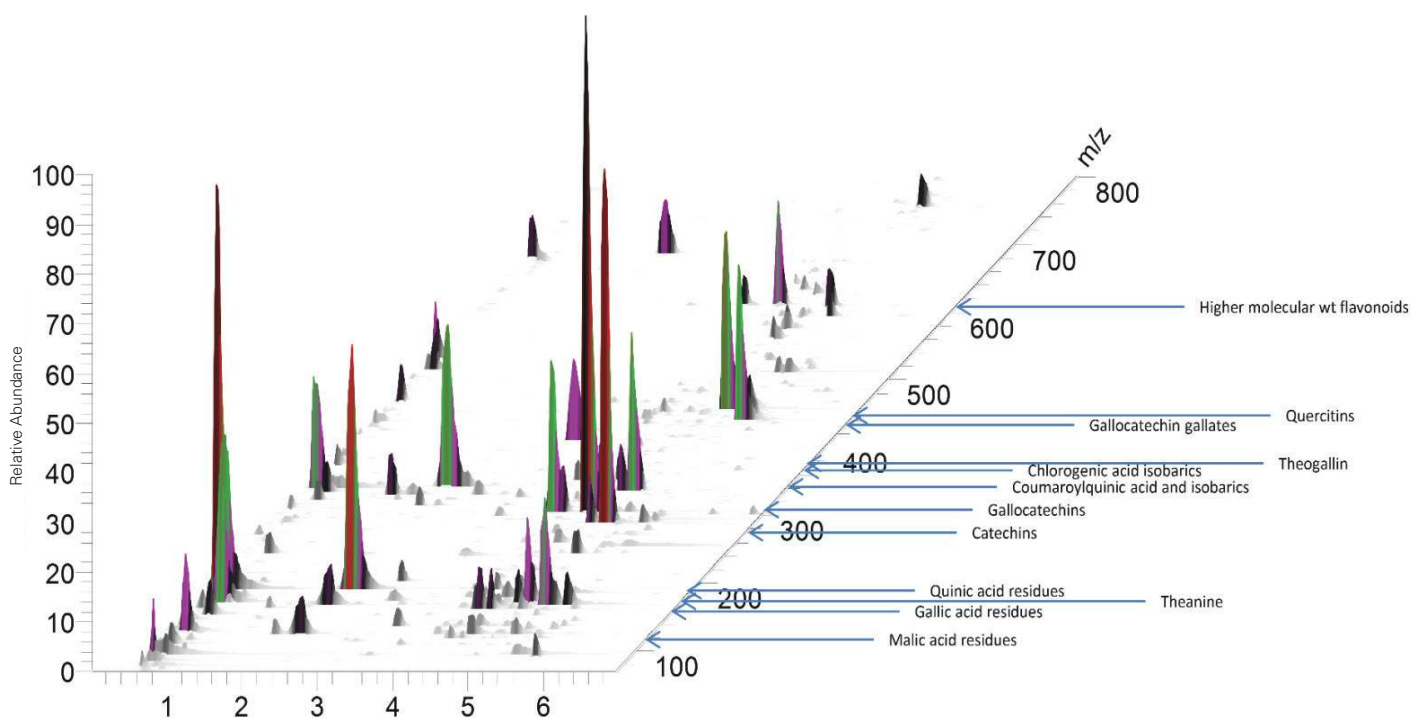
ESI in negative ion mode

Analytes between *m/z* 70-800 monitored**Sample:** Metabolites from green tea extracted into

cold water by vortexing for 20 mins.

Samples filtered prior to injection onto

column and modular Accela LC system



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



Hair Dye Restricted Components (I)

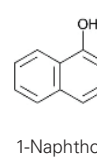
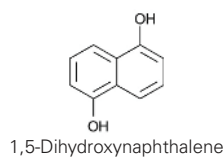
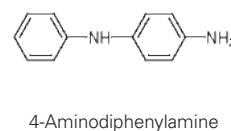
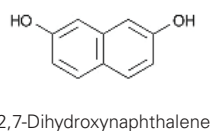
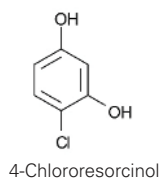
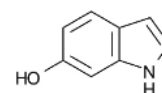
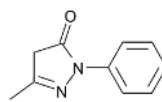
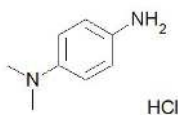
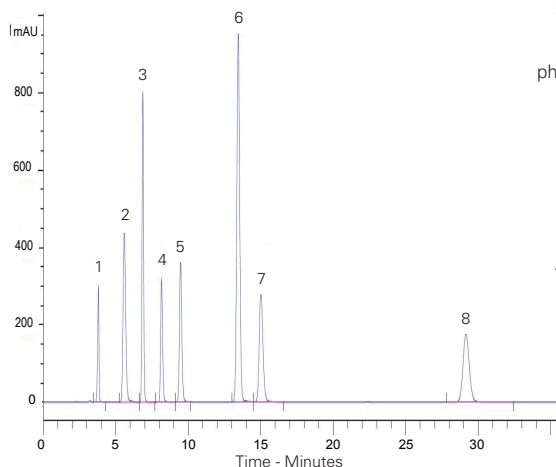
Application #AN2100

Conditions

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

Analytes

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



Hair Dye Restricted Components (II)

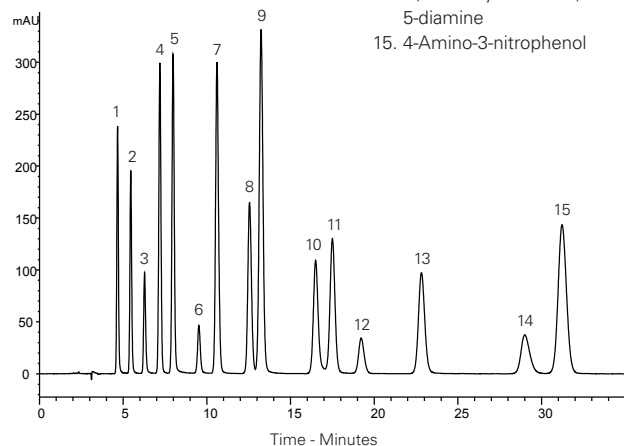
Application #AN2110

Conditions

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

Analytes

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



Halogenated Positional Isomer Separations

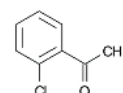
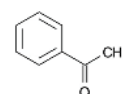
Application #AN1510

Conditions

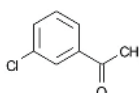
Column: ACE 5 C18
 ACE 5 C18-AR
 ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546,
 ACE-129-1546,
 ACE-1210-1546
Mobile Phase: H₂O/MeOH (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 254 nm

Analytes

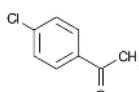
1. Acetophenone
2. o-Chloroacetophenone
3. m-Chloroacetophenone
4. p-Chloroacetophenone



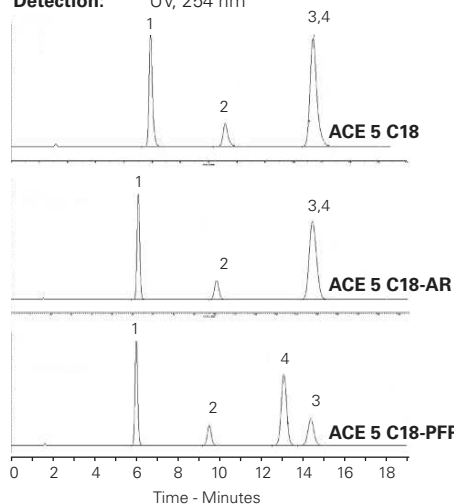
o-Chloroacetophenone



m-Chloroacetophenone



p-Chloroacetophenone



Hepcidin-25 and Truncated Isoforms by LC-HRMS

Application #AN3090

Conditions

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

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

Flow Rate: 0.25 mL/min**Injection:** 100 µL**Temperature:** 60 °C**Detection:** ThermoFisher Scientific Q-Exactive™ high resolution MS

Heated electrospray ionisation (positive mode)

Spray voltage: 4.5 kV

Vaporiser temperature: 200 °C

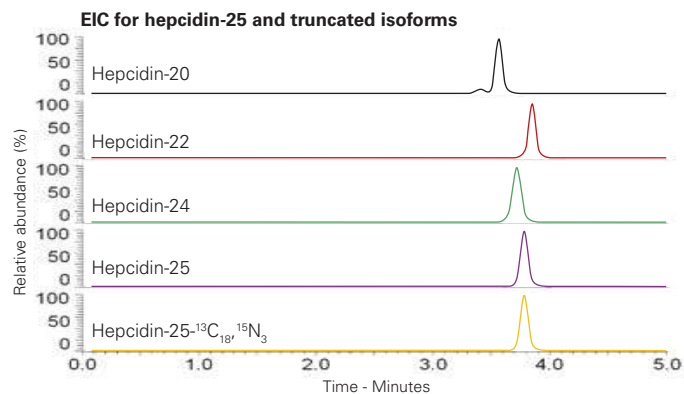
Capillary temperature: 320 °C

Detection: Full scan m/z 400 – 1000

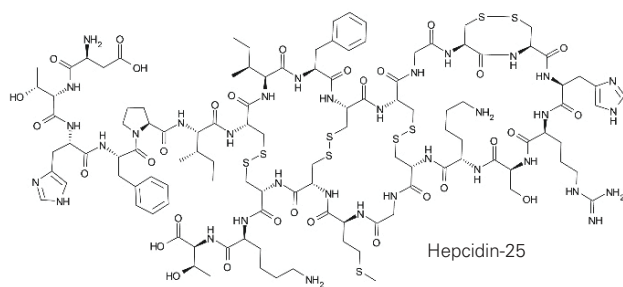
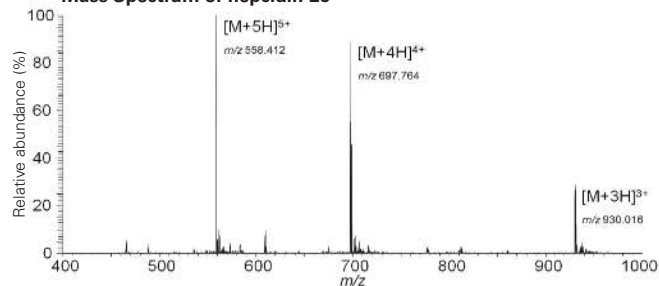
Extracted ion chromatogram from sum of 6 most abundant isotopes of +3, +4 and +5 charge states

Analyte

1. Hepcidin-25
 (MW 2789)



Mass Spectrum of hepcidin-25



Reproduced with permission of Viapath, Toxicology Unit, King's College Hospital London, UK

Herbicide – Benfluralin

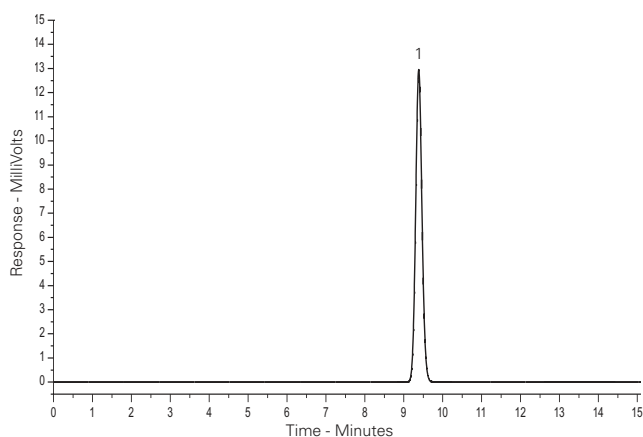
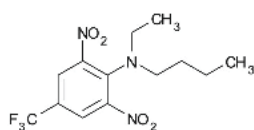
Application #AN2880

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: H₂O/MeOH (15:85 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Benfluralin



Herbicide – Trifluralin

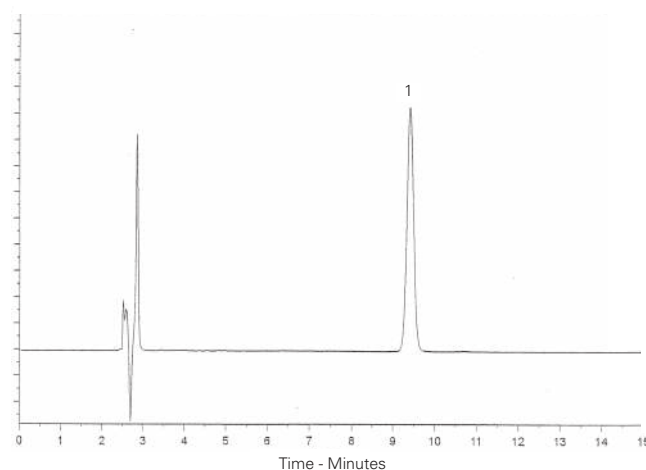
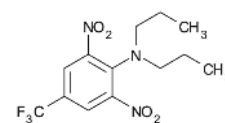
Application #AN2890

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: H₂O/MeOH (15:85 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Trifluralin





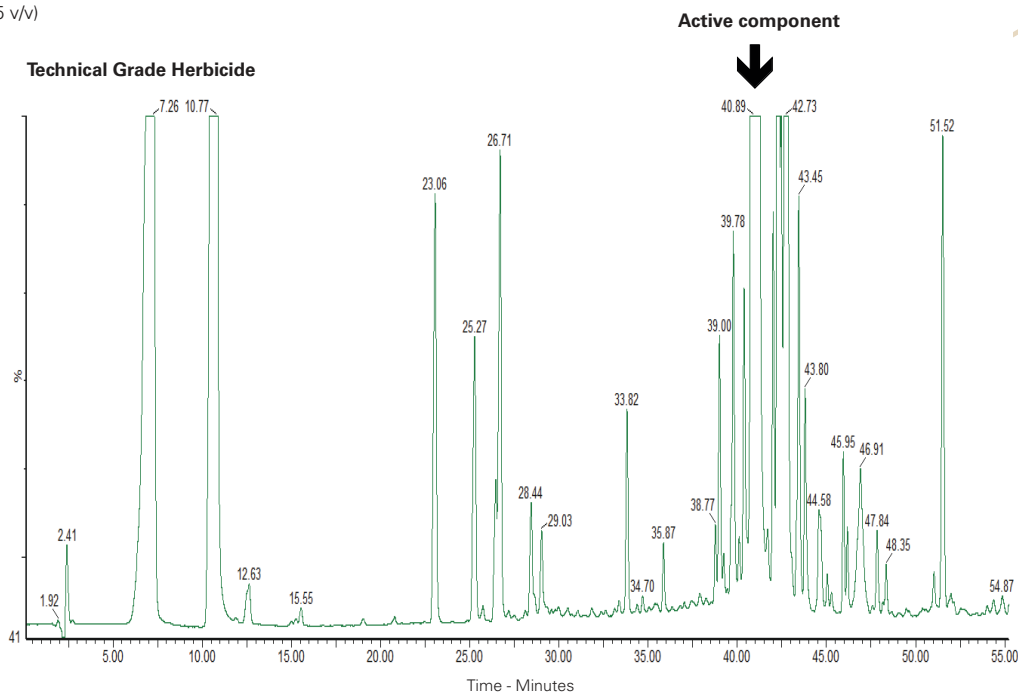
Herbicide Impurity Profile Application #AN2130

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: CORE-25A-1546U
Mobile Phase: A: MeCN/H₂O/TFA (5:95:0.05 v/v/v)
 B: MeCN/TFA (99.9:0.05 v/v)
Gradient:

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

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



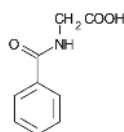
Hippuric Acid Application #AN2760

Conditions

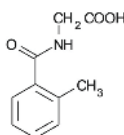
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM KH₂PO₄ pH 3.5 in H₂O/MeCN (15:85 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

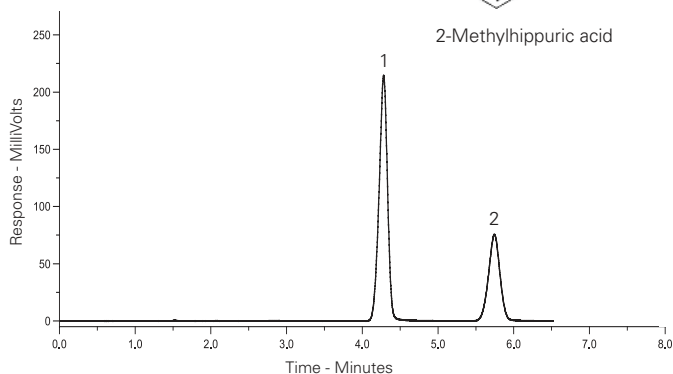
- Hippuric acid
- 2-Methylhippuric acid



Hippuric acid



2-Methylhippuric acid



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

email: info@ace-hplc.com

Human Urine Metabolite Profiling by LC-MS

Application #AN2600

Conditions

Column: ACE Excel 1.7 C18-Amide**Dimensions:** 100 x 2.1 mm**Part Number:** EXL-1712-1002U**Mobile Phase:** A: 0.01% formic acid in H₂O

B: 0.01% formic acid in MeCN

Gradient: **Time (mins)** **%B**

0.0 3

2.5 10

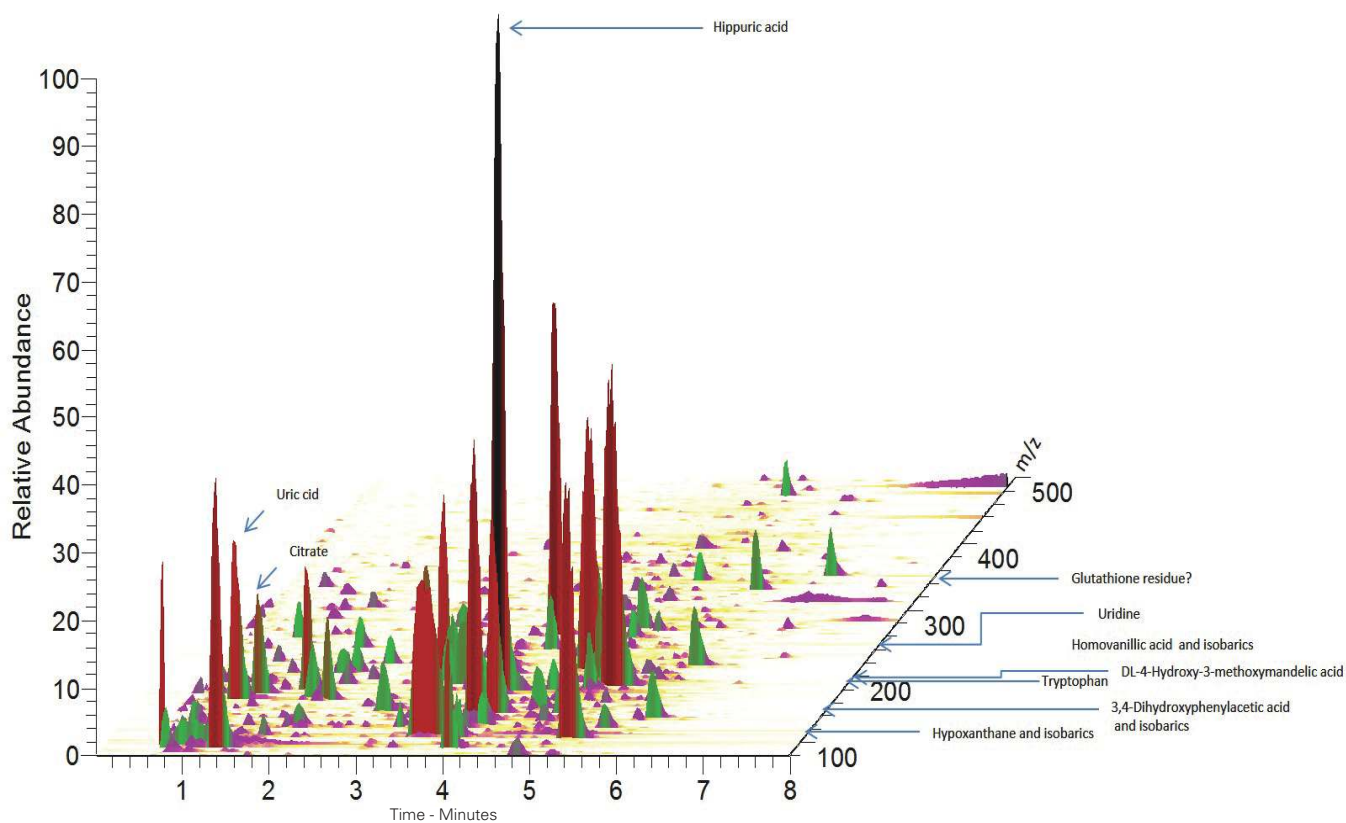
8.0 100

8.5 3

10.0 3

Flow Rate: 0.5 mL/min**Detection:** Exactive accurate mass MS system

ESI in negative ion mode

Analytes between *m/z* 70-800 monitored**Sample:** Urine of healthy adult volunteer, filtered prior to injection onto column and modular Accela LC system.

Human Urine Metabolite Profiling by LC-MS



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

Application #AN1120

Conditions

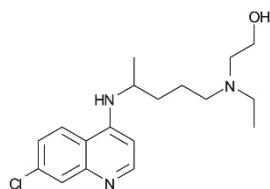
Column: ACE Excel 2 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: EXL-1011-0502U
Mobile Phase: A: 0.5% Ammonium hydroxide pH 10 in H₂O
 B: 0.5% Ammonium hydroxide in MeCN
Gradient:

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

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

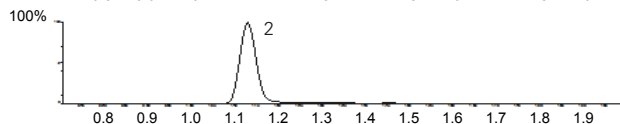
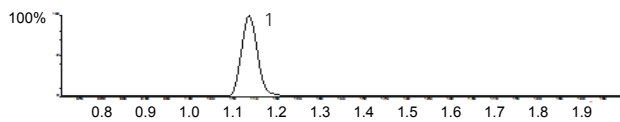
Analytes

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

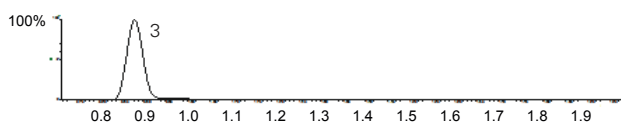
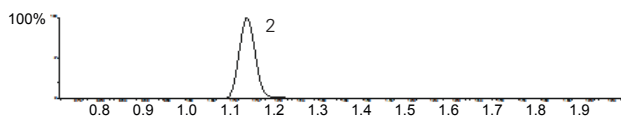
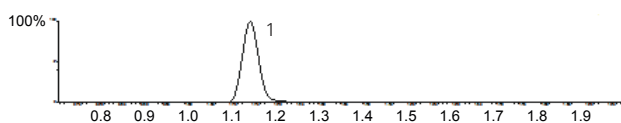


Hydroxychloroquine

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



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



Time - Minutes

Reproduced with permission of Leslie Brent Laboratory, Hammersmith Hospital, London, UK

Combined Hypertension Therapy Drugs

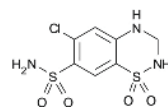
Application #AN4210

Conditions

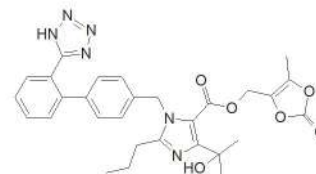
Column: ACE 5 CN
Dimensions: 200 x 4.6 mm
Part Number: ACE-124-2046
Mobile Phase: 10 mM phosphoric acid in H₂O, pH 2.5/MeCN/MeOH (80:7:13 v/v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 235 nm
Sample: 1 µg/mL each analyte

Analytes

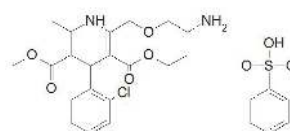
1. Hydrochlorothiazide
2. Olmesartan medoxomil
3. Amlodipine besylate
4. Valsartan



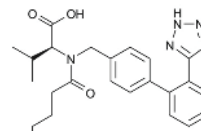
Hydrochlorothiazide



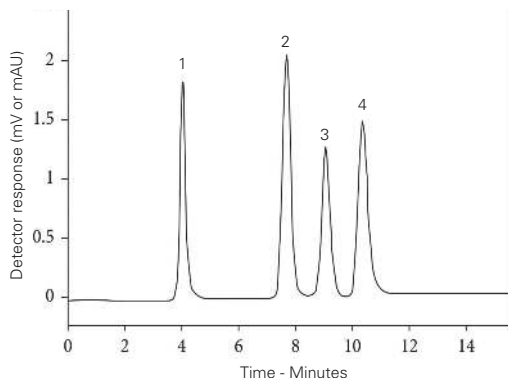
Olmesartan medoxomil



Amlodipine besylate



Valsartan



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

Ibuprofen and Related Impurities

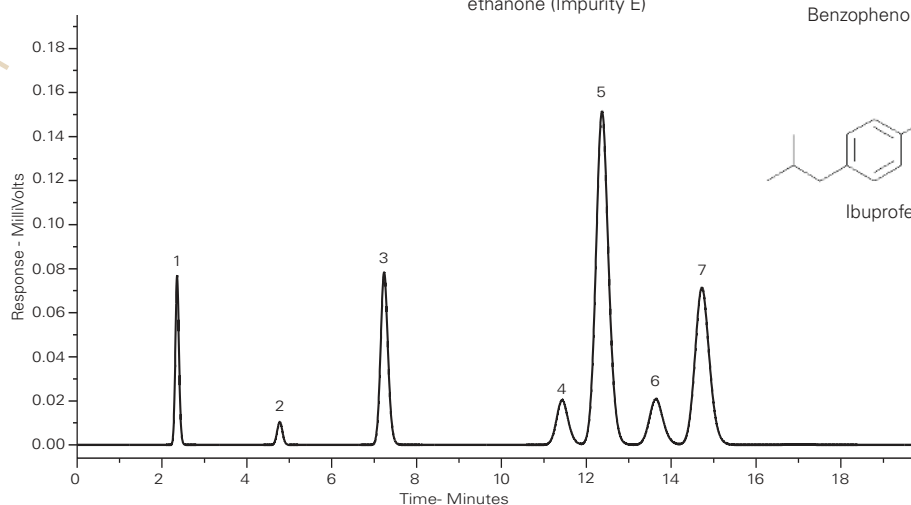
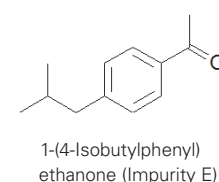
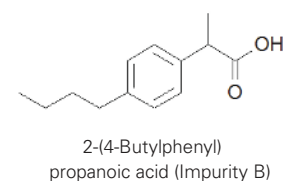
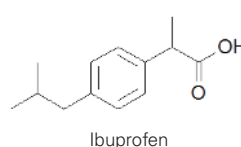
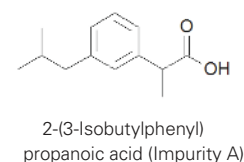
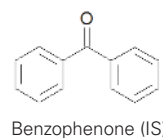
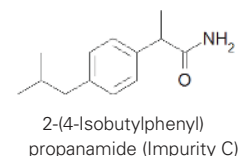
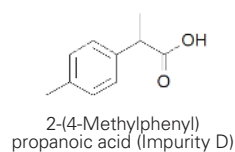
Application #AN4000

Conditions

Column: ACE 5 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-121-1503
Mobile Phase: 0.1% TFA in H₂O/MeCN (64:36 v/v)
Flow Rate: 1.5 mL/min
Temperature: 40 °C
Detection: UV, 214 nm

Analytes

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



Reproduced with permission of Boots Healthcare International, Nottingham, UK

Ibuprofen in Combination with Antihistamine and Decongestant

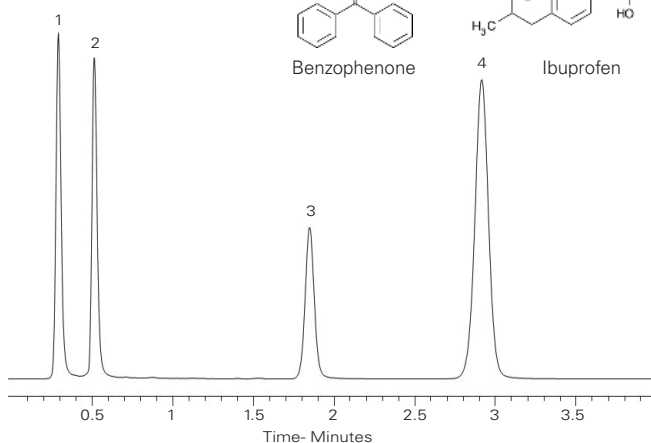
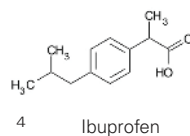
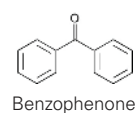
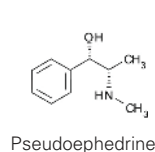
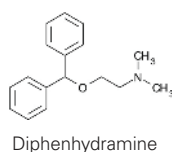
Application #AN2120

Conditions

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

Analytes

- Diphenhydramine
- Pseudoephedrine
- Benzophenone
- Ibuprofen



Alternative column dimensions available

Please enquire
 email: info@ace-hplc.com



Illegal Dyes in Spices

Application #AN2910

Conditions

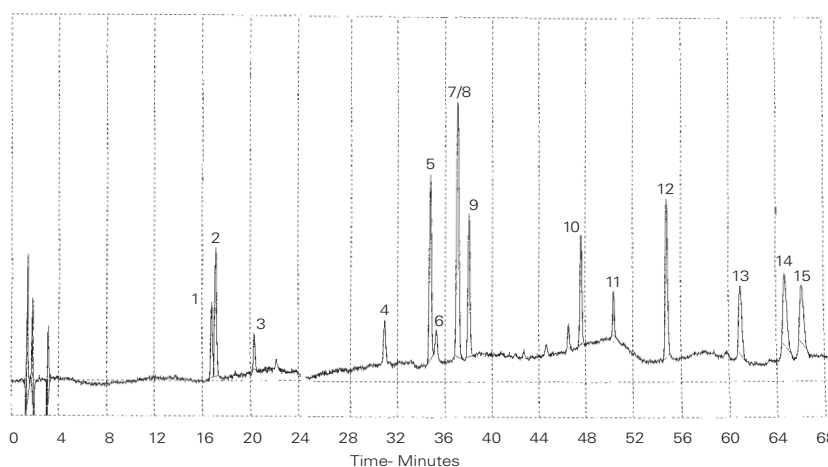
Column: ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-111-1046
Mobile Phase: A: H₂O
 B: MeOH
 C: 0.06 M Tetrabutylammonium bromide and 0.5 M KH₂PO₄ in H₂O pH 2.55
Gradient:

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

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

Analytes

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



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

Insulin Analogues in Clinical and Post-Mortem Analyses

Application #AN3350

Conditions

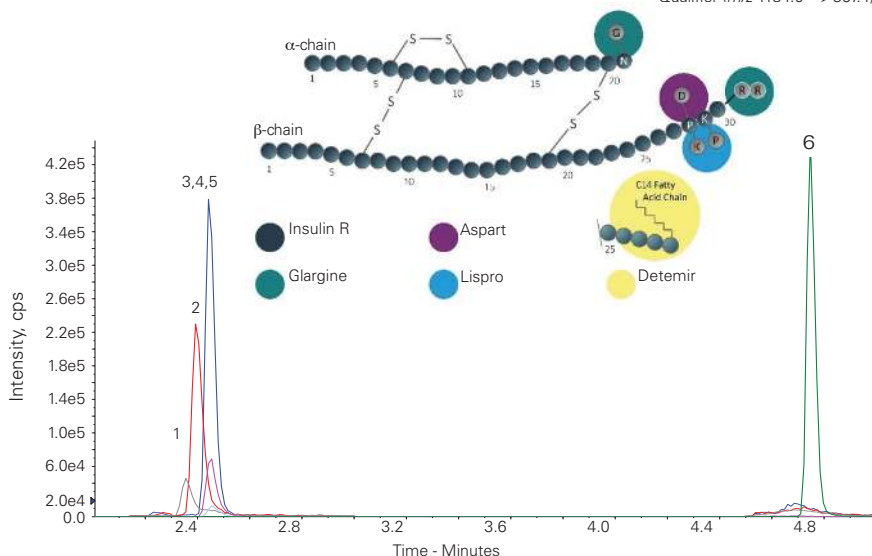
Column: ACE 5 C18-300
Dimensions: 50 x 2.1 mm
Part Number: ACE-221-0502
Mobile Phase: A: 0.1% acetic acid in H₂O
 B: 0.1% acetic acid in IPA/MeCN (25:75 v/v)
Gradient:

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

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

Analytes

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



Reproduced with permission of St Paul's Hospital, University of British Columbia, Vancouver, Canada

Insulins

Application #AN2770

Conditions

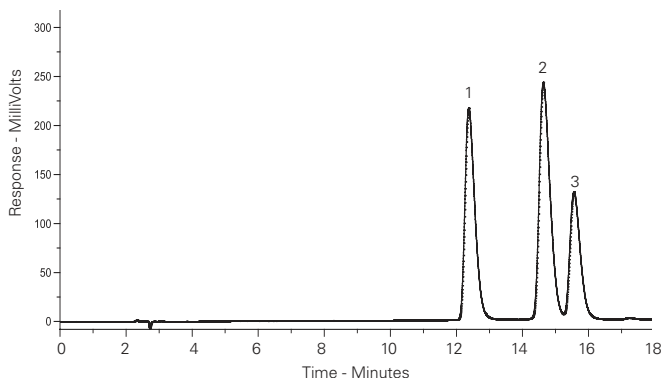
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% TFA in H₂O/MeCN (71:29 v/v)
 B: 0.1% TFA in H₂O/MeCN (68:32 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 10 |
| 16 | 90 |

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

Analytes

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



Isoflavones

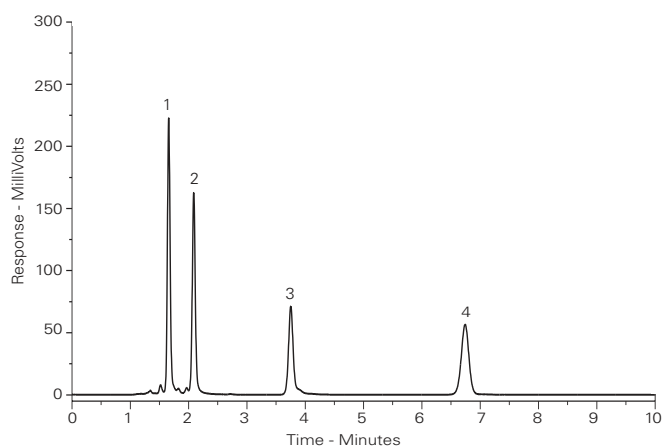
Application #AN2970

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/0.1% formic acid in H₂O (35:65 v/v)
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: Ambient
Detection: UV, 254 nm

Analytes

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



Isoflavones in Red Clover and Soy Extract

Application #AN1130

Conditions

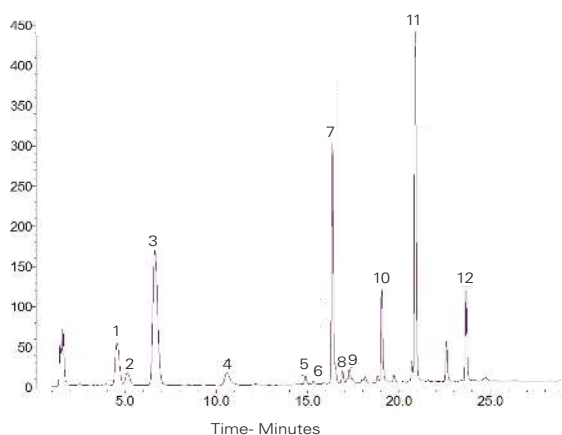
Column: ACE 3 C18-AR
Dimensions: 150 x 2.1 mm
Part Number: ACE-119-1502
Mobile Phase: A: Acetic acid in H₂O pH 2.8
 B: 0.6% Acetic acid in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 15 |
| 7 | 15 |
| 27 | 75 |

Flow Rate: 0.35 mL/min
Injection: 3 µL
Temperature: 25 °C
Detection: UV, 254 nm

Analytes

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



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

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



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

Application #AN3380

Conditions

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

Gradient:

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

Flow Rate: 0.7 mL/min

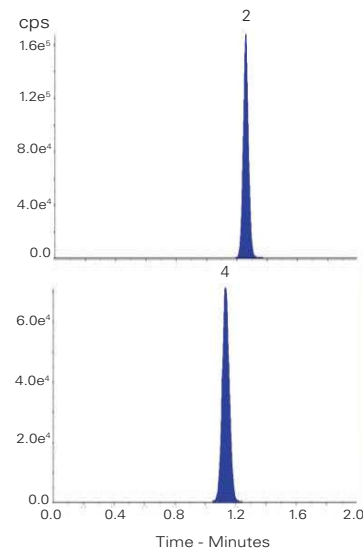
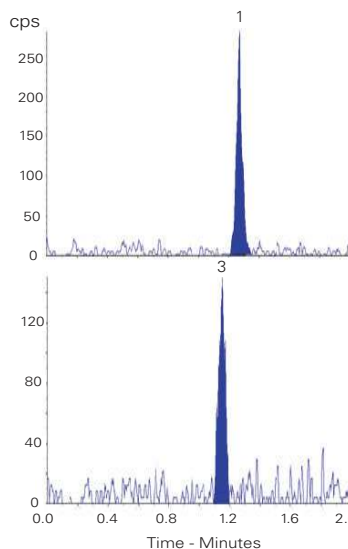
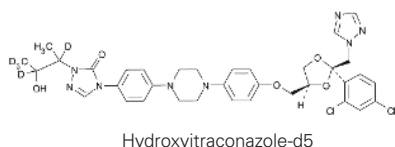
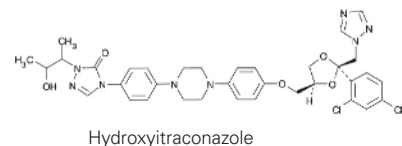
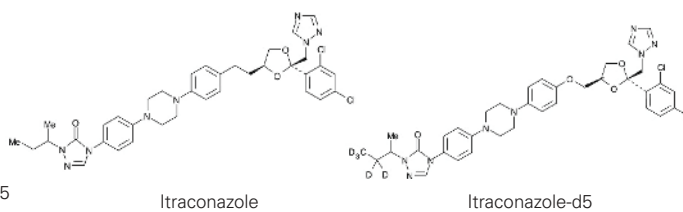
Temperature: 45 °C

Detection: AB Sciex 4000
 ESI positive ion mode

Sample: 1.0 ng/mL human whole blood (LLOQ)

Analytes

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



Reproduced with permission of Agilux Laboratories, USA



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

email: info@ace-hplc.com

Lansoprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl Application #AN1520

Conditions

Column: ACE Excel 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 0.1% ammonia in H₂O
 B: 0.1% ammonia in MeCN/H₂O (90:10 v/v)
Gradient:

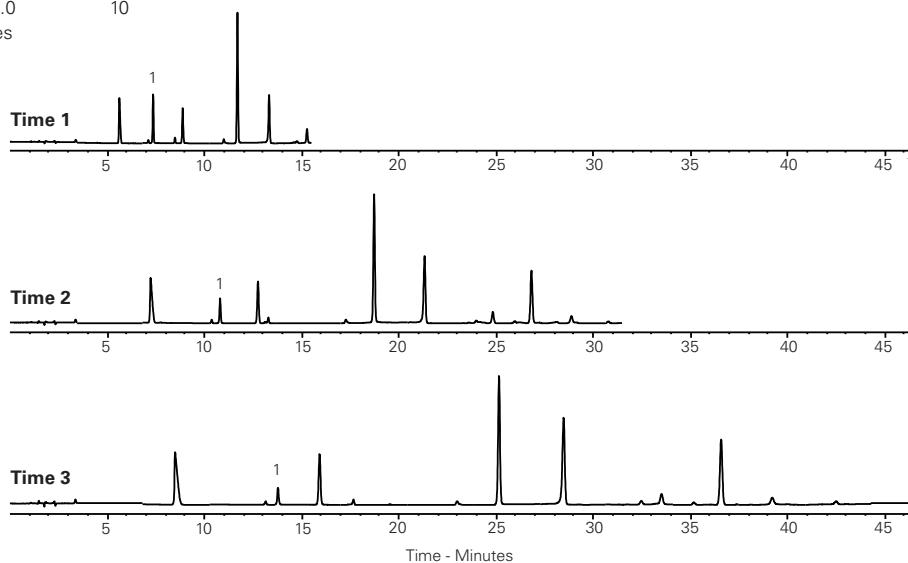
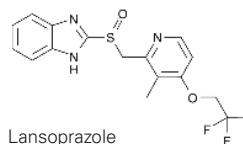
| Time 1 (mins) | Time 2 (mins) | Time 3 (mins) | %B |
|---------------|---------------|---------------|----|
| 0.0 | 0.0 | 0.0 | 10 |
| 15.0 | 30.0 | 45.0 | 90 |
| 15.5 | 30.5 | 45.5 | 90 |
| 18.0 | 33.0 | 48.0 | 10 |

Post time 10 minutes

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

Analyte

1. Lansoprazole



Lapatinib Anticancer Drug in Human Plasma by LC-MS/MS Application #AN3360

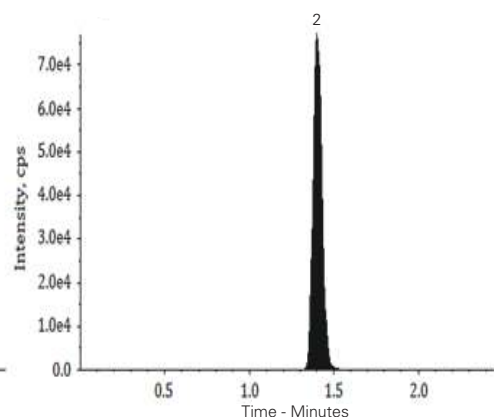
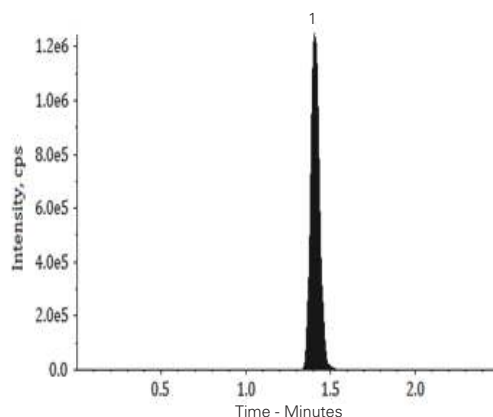
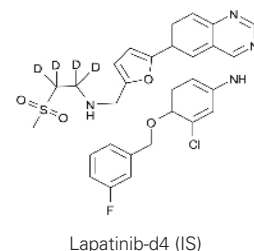
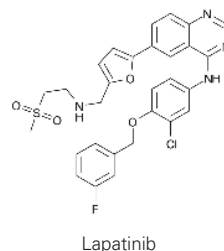
Conditions

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

Analytes

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

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



Reproduced with permission of Department of Chemistry, School of Science, Gujarat University, India



Lidocaine in Saliva by LC-MS/MS Application #AN2570

Conditions

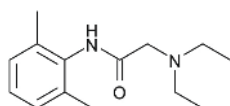
Column: ACE 3 C18
Dimensions: 100 x 3.0 mm
Part Number: ACE-111-1003
Mobile Phase: A: 0.1% formic acid in MeCN/H₂O (20:80 v/v)
 B: 0.1% formic acid in MeCN/H₂O (80:20 v/v)
Gradient:

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

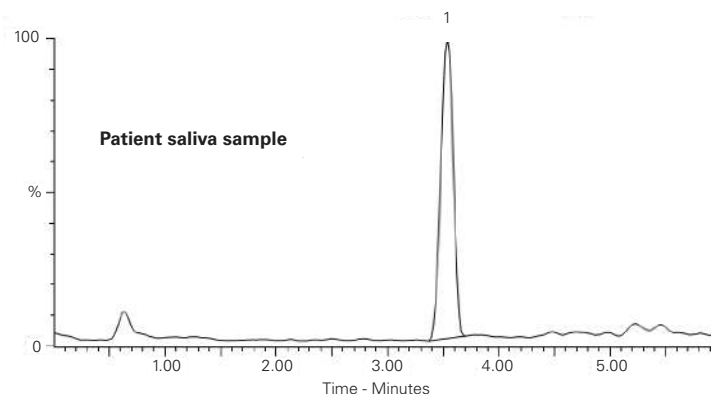
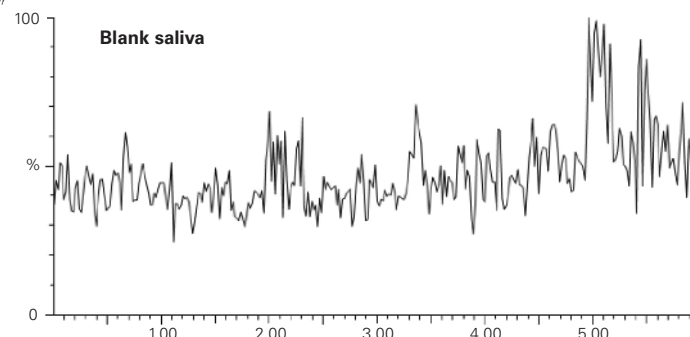
Flow Rate: 0.3 mL/min
Injection: 10 µL
Detection: Quattro-Micro triple quad MS
 Positive ion mode ESI

Analyte

1. Lidocaine
 (m/z 235 → 86)



1. Lidocaine



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

Reproduced with permission of Department of Analytical Chemistry, Stockholm University, Sweden

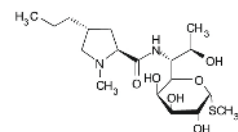
Lincosamide Antibiotics Application #AN2650

Conditions

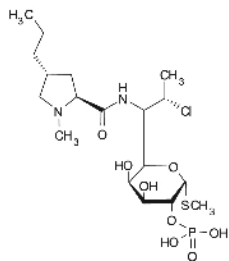
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 0.02 M sodium phosphate dibasic pH 3.0/MeCN (70:30 v/v)
Flow Rate: 1 mL/min
Injection: 25 µL
Temperature: 25 °C
Detection: UV, 205 nm

Analytes

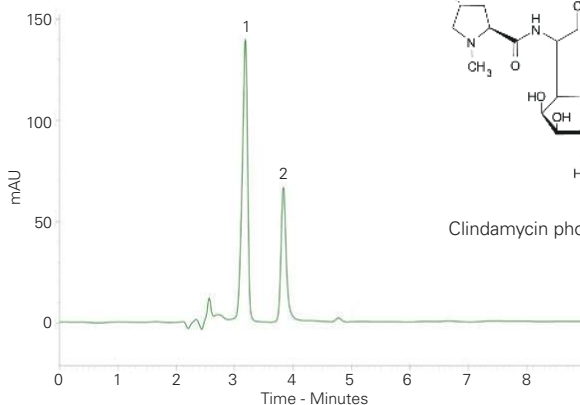
1. Lincomycin HCl
 2. Clindamycin phosphate



Lincomycin HCl



Clindamycin phosphate



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

Reproduced with permission of Department of Pharmacy, Faculty of Medicine and Surgery, University of Malta

Lipid Classes Separation from *Drosophila Melanogaster*

Application #AN1530

Conditions

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

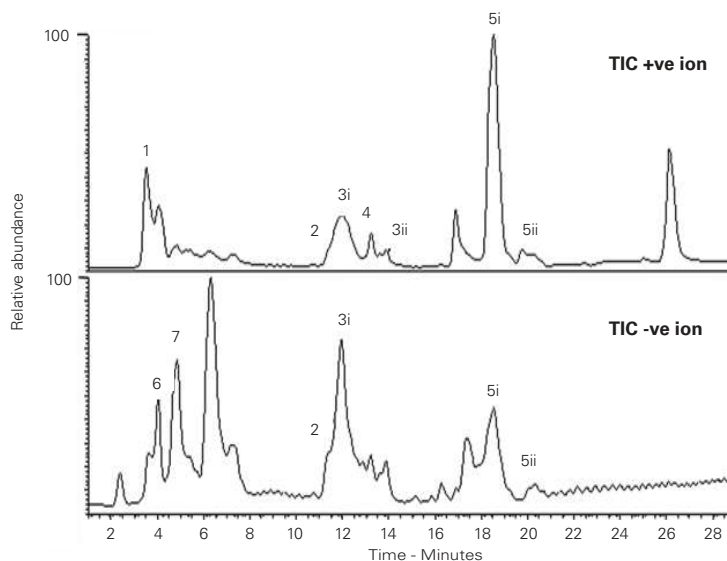
| Time (mins) | %B |
|-------------|----|
| 0.0 | 8 |
| 1.0 | 8 |
| 5.0 | 9 |
| 10.0 | 20 |
| 16.0 | 25 |
| 23.0 | 35 |
| 26.0 | 8 |

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

*Drosophila Melanogaster*

Analytes

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



Reproduced with permission of University of Strathclyde, Glasgow, UK

Liquorice Extracts Fingerprint

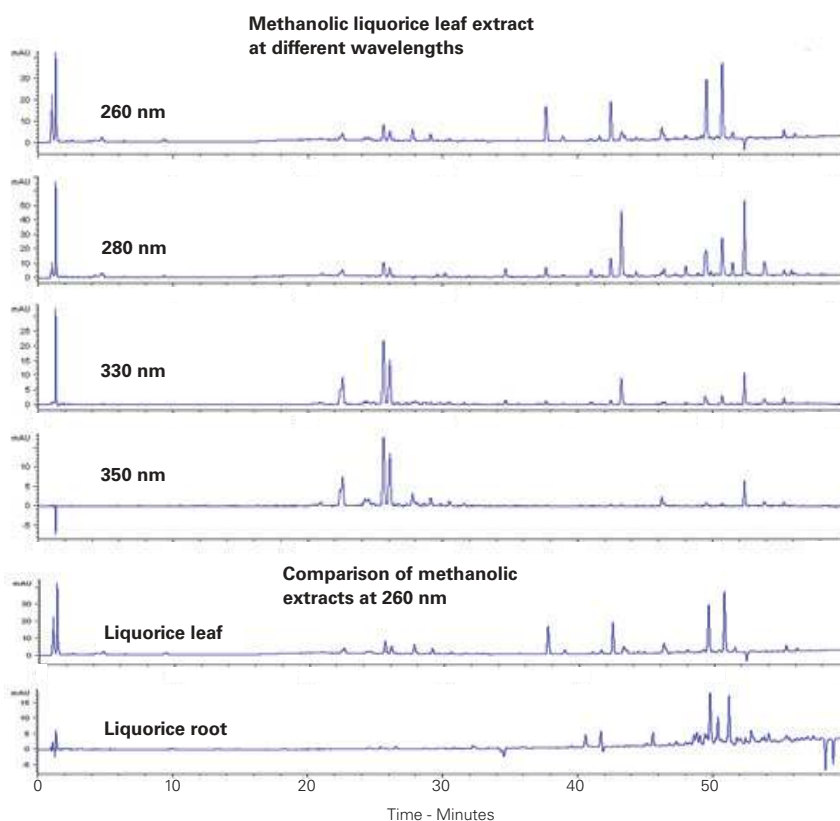
Application #AN2090

Conditions

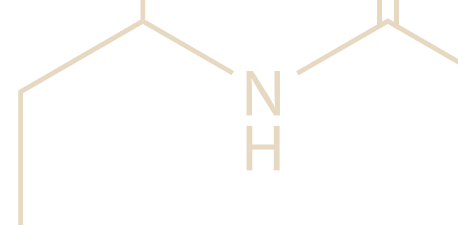
Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: Ammonium acetate in H₂O pH 4
 B: MeOH
Gradient:

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

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



Reproduced with permission of Unilever, Colworth Science Park, UK



Local Anaesthetics

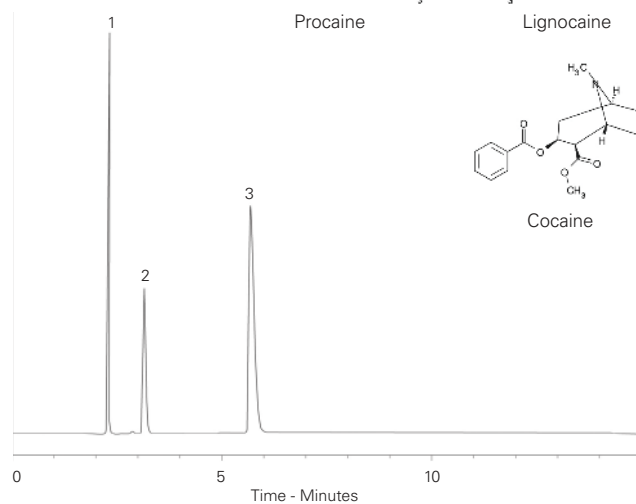
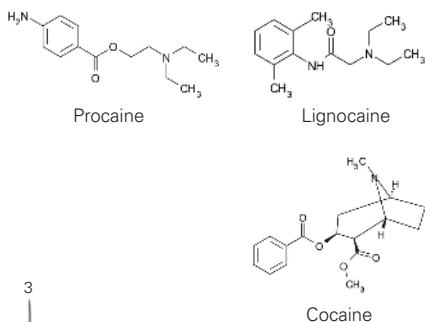
Application #AN3220

Conditions

Column: ACE 5 AQ
Dimensions: 250 x 4.6 mm
Part Number: ACE-126-2546
Mobile Phase: MeCN/H₂O/2.5 M H₂SO₄
 (21:79:0.1 v/v/v)
Flow Rate: 1.5 mL/min
Detection: UV

Analytes

1. Procaine
2. Lignocaine
3. Cocaine



Reproduced with permission of Forensic Science Laboratories, Lothian and Borders Police, UK

Need a custom column for your application?

Please enquire
 email: info@ace-hplc.com



15-Hydroxy Lubiprostone in Human Plasma

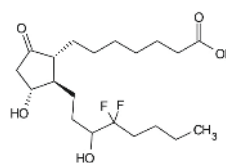
Application #AN1900

Conditions

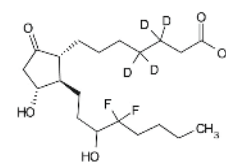
Column: ACE Excel 2 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-101-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: MeCN
Flow Rate: 0.65 mL/min
Injection: 15 µL
Temperature: 35 °C
Detection: MDS Sciex API 5000
 TurbolonSpray negative mode
 IonSpray voltage -4500 V
 Source Temperature 450 °C

Analytes

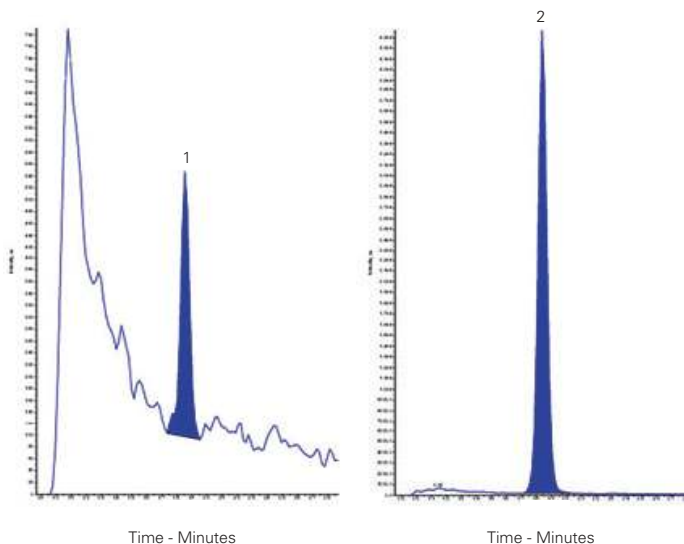
1. 15-Hydroxy lubiprostone
 (*m/z* 391.2 → 373.2)
2. 15-Hydroxy lubiprostone-d4 (IS)
 (*m/z* 395.2 → 377.2)



15-Hydroxy lubiprostone



15-Hydroxy lubiprostone-d4



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

Reproduced with permission of inVentiv Health Clinical, Quebec, Canada

Lubricant Additives: ADPA/OPNA Antioxidants

Application #AN1170

Conditions

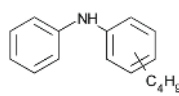
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: CORE-25A-1546U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN/IPA (1:2 v/v)
Gradient:

| Time (mins) | %B |
|-------------|------|
| 0.0 | 65.0 |
| 15.0 | 97.5 |
| 25.0 | 97.5 |
| 25.1 | 65.0 |

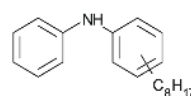
Flow Rate: 1 mL/min
Temperature: 60 °C
Detection: UV, 220 nm

Analytes

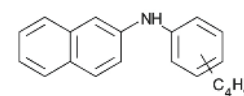
1. C4-ADPA
2. C8-ADPA
3. C4-OPNA
4. C12-ADPA
5. C16-ADPA



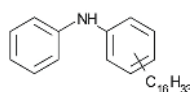
C4-ADPA



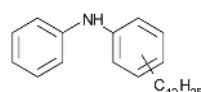
C8-ADPA



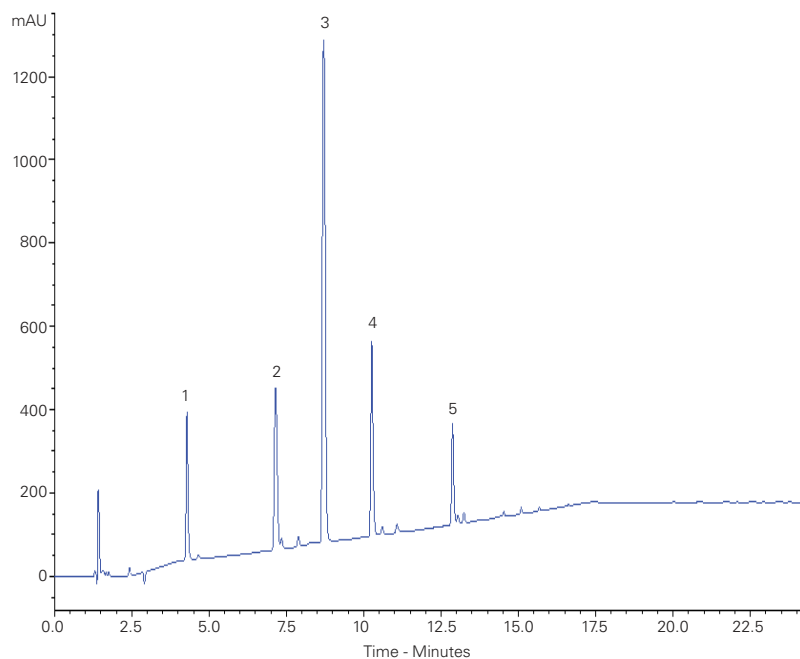
C4-OPNA



C16-ADPA



C12-ADPA



Reproduced with permission of Formulated Product Technology, BP Technology Centre, UK

Lurbinectedin in Plasma by LC-MS/MS

Application #AN3810

Conditions

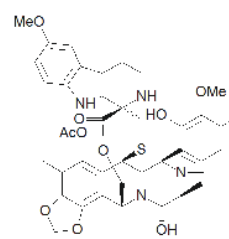
Column: ACE 3 C18-PFP
Dimensions: 30 x 2.1 mm
Part Number: ACE-1110-0302
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 10 |
| 2.5 | 90 |
| 3.5 | 90 |
| 3.6 | 10 |
| 5.0 | 10 |

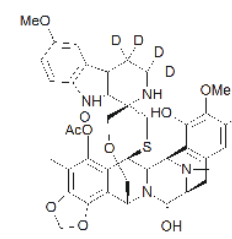
Flow Rate: 0.6 mL/min
Injection: 5 µL
Temperature: 50 °C
Detection: API 4000 triple quad
 TurbolonSpray, ESI positive ion mode
 Turbo Temperature: 650 °C
 Ion Spray Potential: 5000 V

Analytes

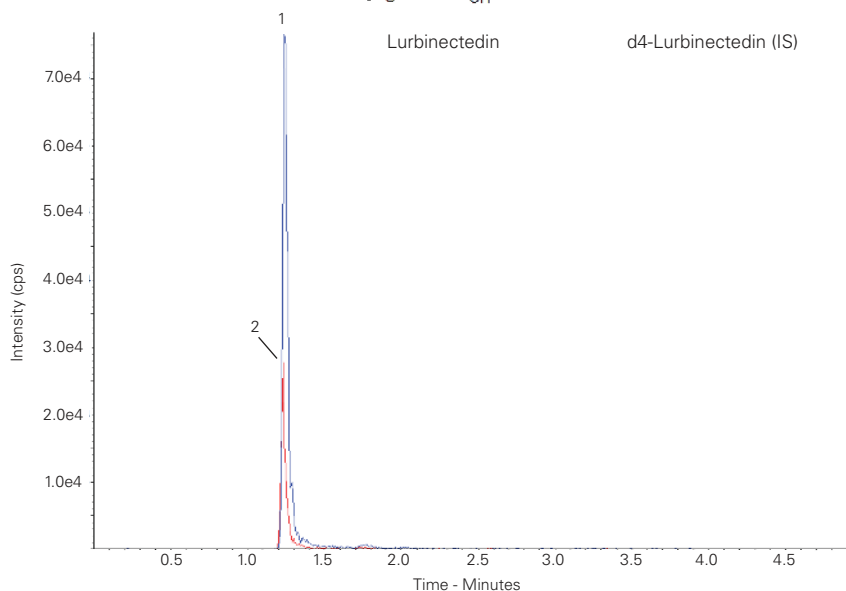
1. Lurbinectedin
(m/z 767.3 *→* 273.0)
 (LLOQ 0.1 ng/mL)
2. d4-Lurbinectedin (IS)
(m/z 771.4 *→* 277.0)



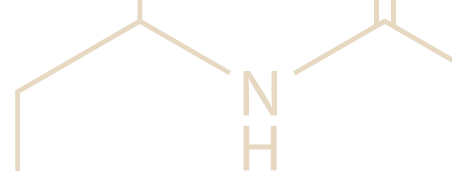
Lurbinectedin



d4-Lurbinectedin (IS)



Reproduced with permission of PharmaMar S.A., Madrid, Spain



Malachite Green

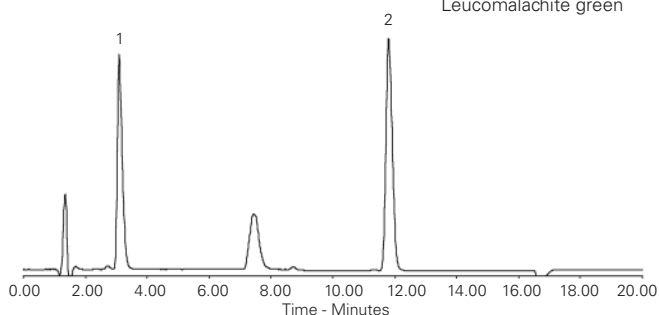
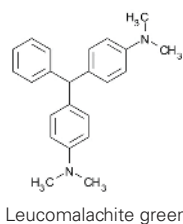
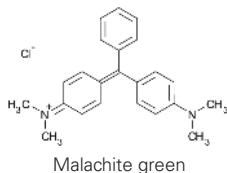
Application #AN2860

Conditions

Column: ACE 5 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-121-1503
Mobile Phase: 10 mM oxalic acid pH 2.9 in H₂O/MeCN (80:20 v/v)
Flow Rate: 0.4 mL/min
Temperature: Ambient
Detection: UV-Vis, 618 nm

Analytes

1. Malachite green
2. Leucomalachite green



Reproduced with permission of Fera Science Ltd, York, UK

Maleic and Fumaric Acids

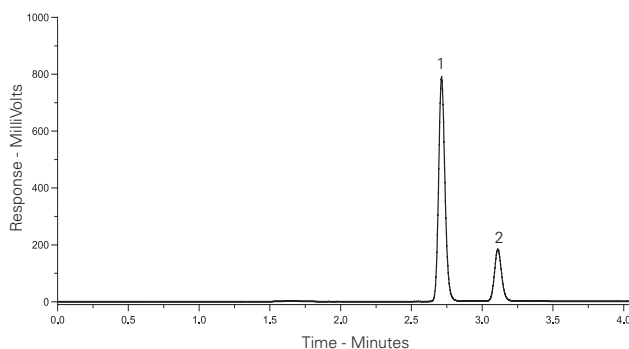
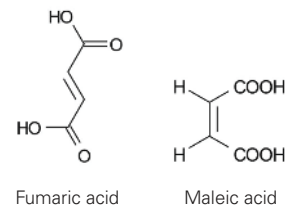
Application #AN3230

Conditions

Column: ACE 5 AQ
Dimensions: 250 x 4.6 mm
Part Number: ACE-126-2546
Mobile Phase: 50 mM KH₂PO₄ pH 7.0 in H₂O
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 210 nm

Analytes

1. Fumaric acid
2. Maleic acid



MDMA (Ecstasy) and PMA (Dr Death) Separation

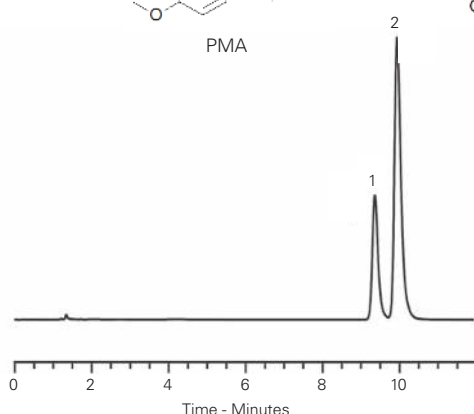
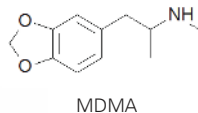
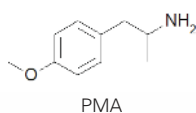
Application #AN4220

Conditions

Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: 0.05 M KH₂PO₄ pH 3.2 in H₂O/MeCN (90:10 v/v)
Flow Rate: 1.2 mL/min
Injection: 10 µL
Temperature: 22 °C
Detection: UV, 210 nm

Analytes

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



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

Melamine using Ion-Pairing Reagent

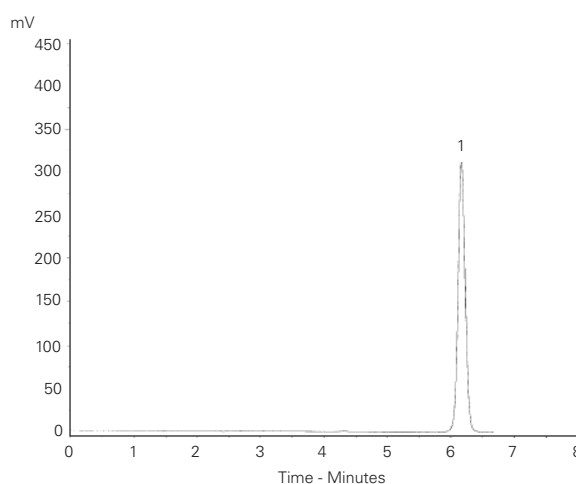
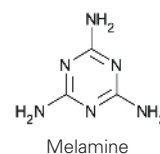
Application #AN2510

Conditions

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

Analyte

1. Melamine



Metabolomic Analysis of Extracted Jurkat T Cells by LC-HRMS

Application #AN3980

Conditions

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

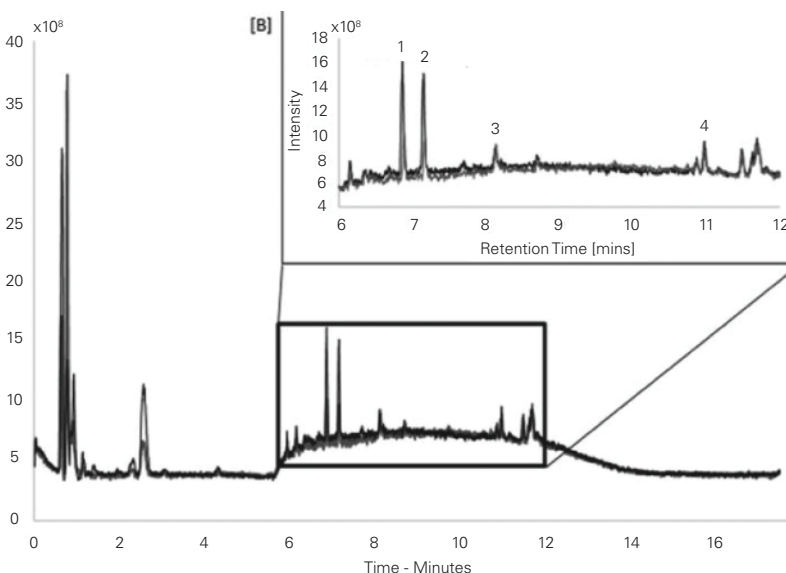
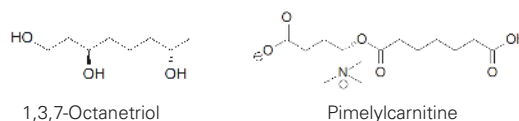
| Time (mins) | %B |
|-------------|----|
| 0 | 0 |
| 1 | 0 |
| 11 | 65 |
| 13 | 65 |
| 18 | 95 |
| 20 | 95 |

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

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

Analytes

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



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

Metabolomic Biomarkers in Ethylmalonic Encephalopathy

Application #AN4130

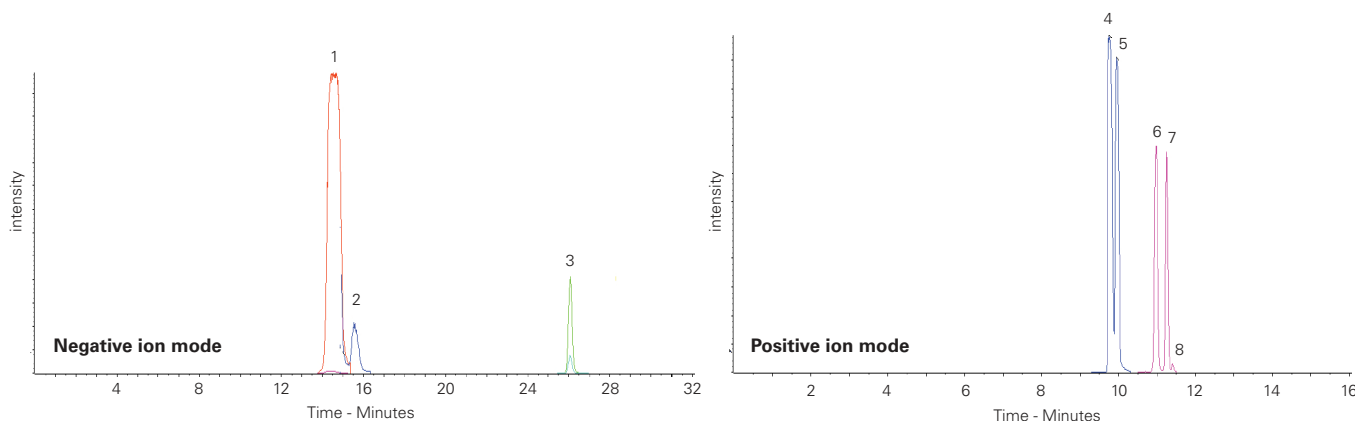
Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
 ESI in negative ion mode
Sample: Urine sample from patient with ethylmalonic encephalopathy is filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water

Analytes

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

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



Reproduced with permission of UCSD Biochemical Genetics, Department of Pediatrics, University of California San Diego, California, USA



Metabolomics and Biochemical Genetics - Acylglycines

Application #AN4080

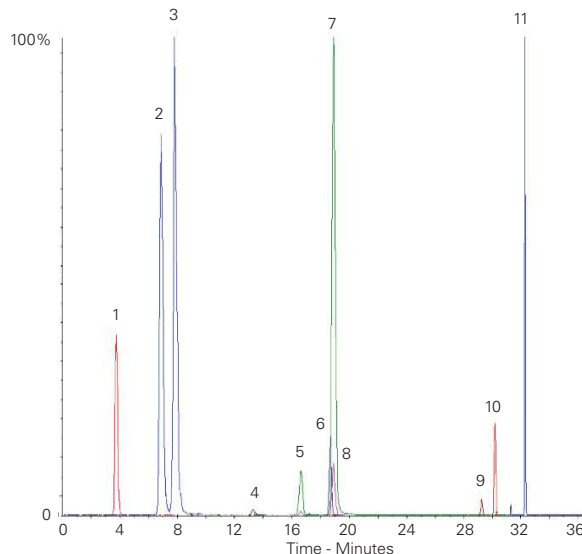
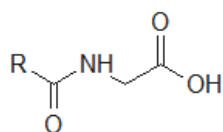
Conditions

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

Analytes

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

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



Reproduced with permission of UCSD Biochemical Genetics, Department of Pediatrics, University of California San Diego, California, USA

Metabolomics – C4 & C5 Hydroxy and Dicarboxylic Acids

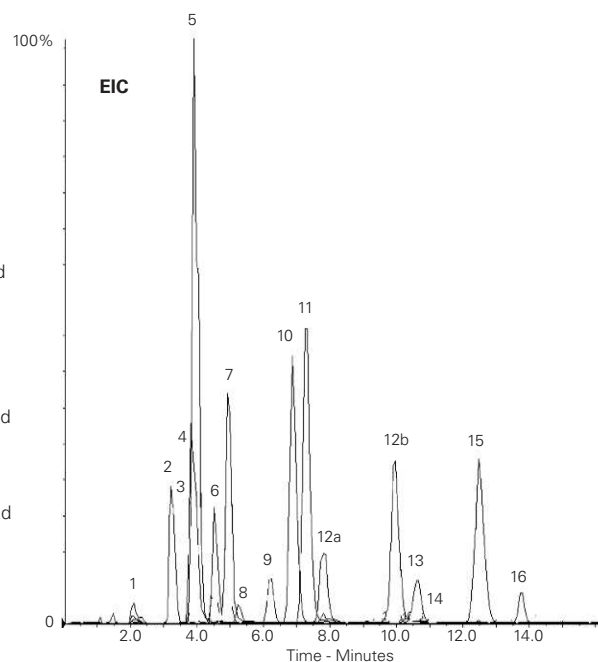
Application #AN4110

Conditions

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

Analytes

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



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

Reproduced with permission of UCSD Biochemical Genetics, Department of Pediatrics, University of California San Diego, California, USA

Metabolomics – C4 Hydroxy Acids

Application #AN4120

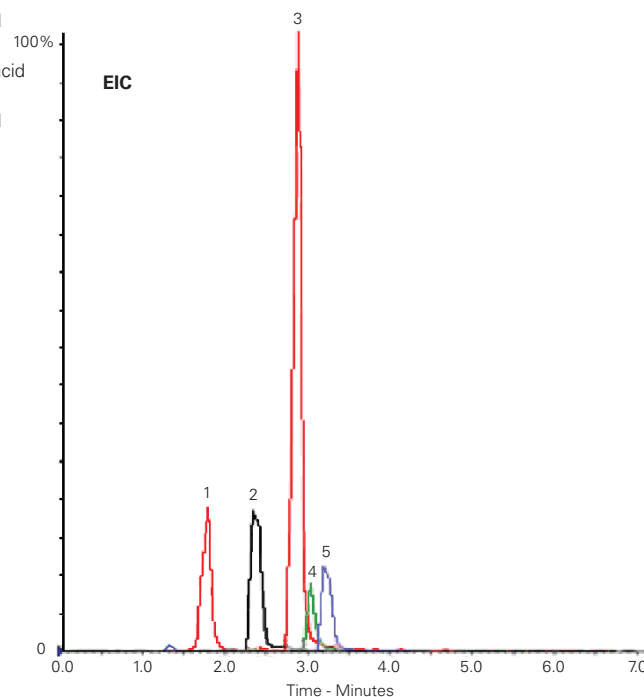
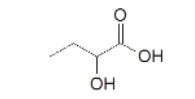
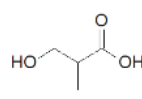
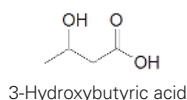
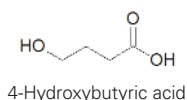
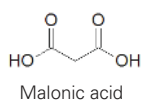
Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
 ESI in negative ion mode
Sample: Urine / plasma sample is filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water

Analytes

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

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



Reproduced with permission of UCSD Biochemical Genetics, Department of Pediatrics, University of California San Diego, California, USA

Metabolomics – C6 & C7 Hydroxy and Dicarboxylic Acids

Application #AN4100

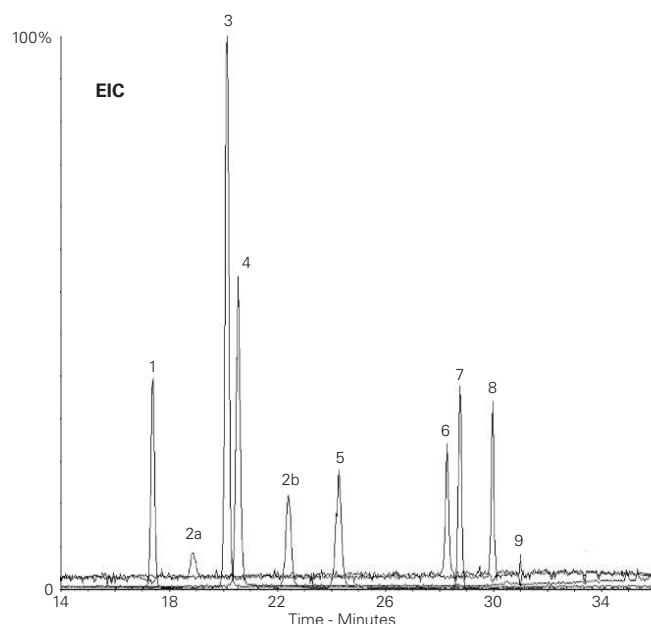
Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
 ESI in negative ion mode
Sample: Urine / plasma samples filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water.

Analytes

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

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



Reproduced with permission of UCSD Biochemical Genetics, Department of Pediatrics, University of California San Diego, California, USA

Methotrexate in K₃EDTA Human Plasma by LC-MS/MS

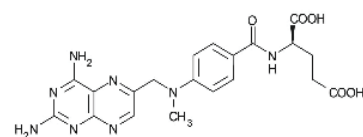
Application #AN3760

Conditions

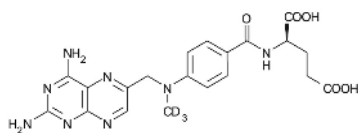
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: 10 mM ammonium formate
 pH 7.0/MeOH (60:40 v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: Quattro Premier XE triple quad MS
 Positive ion mode ESI
 Ion source temperature: 120 °C
 Desolvation temperature: 450 °C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

Analytes

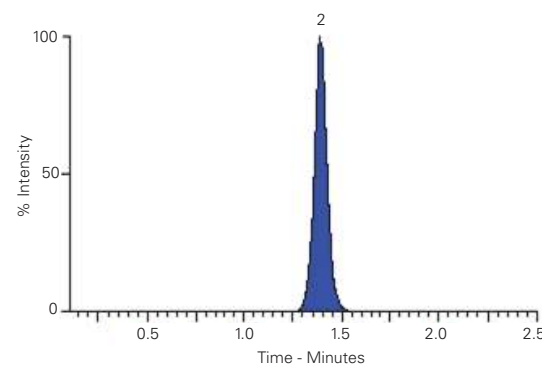
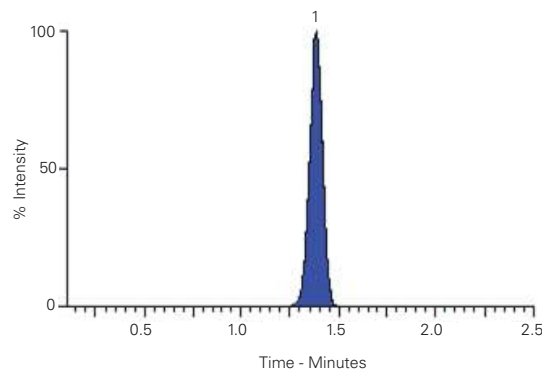
1. Methotrexate
 (m/z 455 → 308)
 (LLOQ 1.0 ng/mL)
 (Concentration 100 ng/mL)
2. Methotrexate-d3 (I.S.)
 (m/z 458 → 311)
 (Concentration 50 ng/mL)



Methotrexate



Methotrexate-d3 (I.S.)



Reproduced with permission of Chemistry Department, School of Sciences, Gujarat University, India

17 α -Methyltestosterone in Freshwater Tilapia Aquaculture

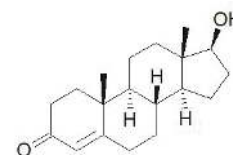
Application #AN4340

Conditions

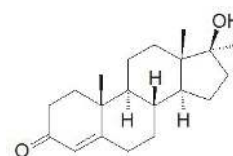
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/H₂O (45:55 v/v)
Flow Rate: 1 mL/min
Injection: 20 μ L
Temperature: 25 °C
Detection: UV, 245 nm

Analytes

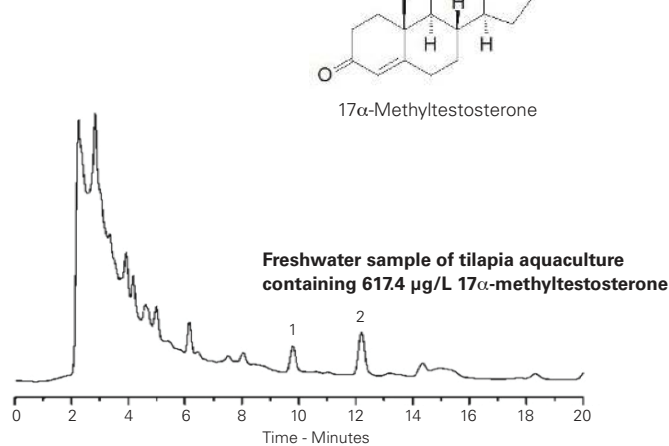
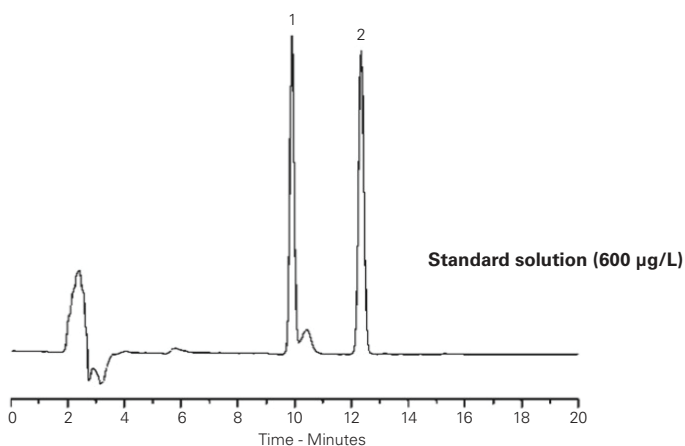
1. Testosterone (IS)
2. 17 α -Methyltestosterone



Testosterone (IS)

17 α -Methyltestosterone

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



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

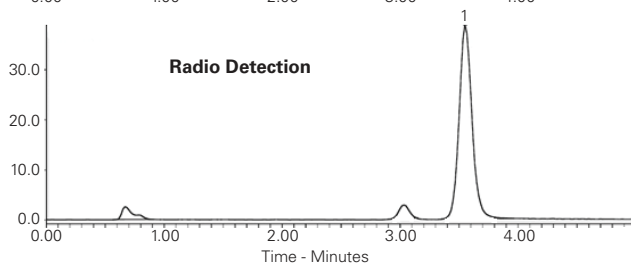
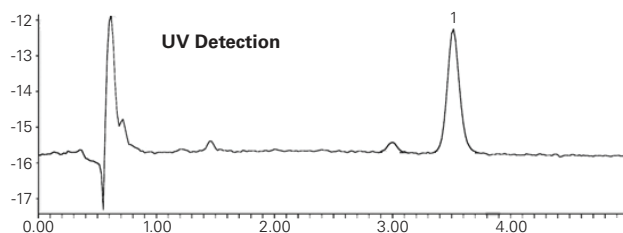
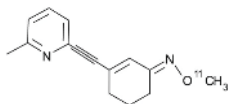
mGluR5 PET Tracer by Radio HPLC Analysis

Application #AN2700

Conditions

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

Analyte

1. ¹¹C-ABP688

Reproduced with permission of Centre of Radiopharmaceutical Science,
 University Hospital Zurich, Switzerland

For additional
 column dimensions

Please enquire
 email: info@ace-hplc.com

Microbial Extract by LC-MS

Application #AN1180

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: CORE-25A-1502U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

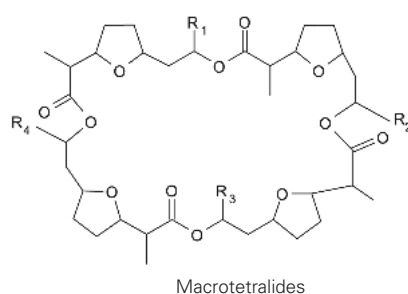
Flow Rate: 0.2 mL/min

Detection: Dionex 3000RS UHPLC system
 coupled with Bruker MaXis Q-TOF MS
 Electrospray MS positive mode
 Source end plate offset -500 V
 Nebuliser gas (N₂) 1.6 bar
 Drying gas (N₂) temp 180 °C
 Collision energy 5.0 eV
 Collision RF 600 Vpp

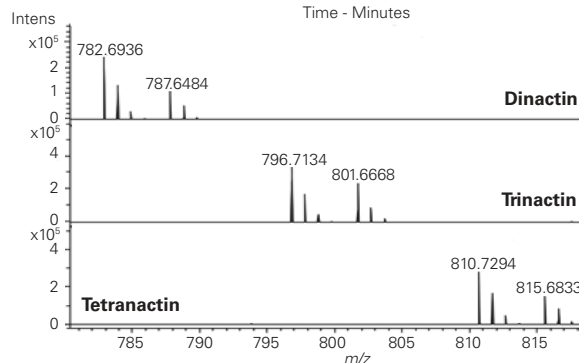
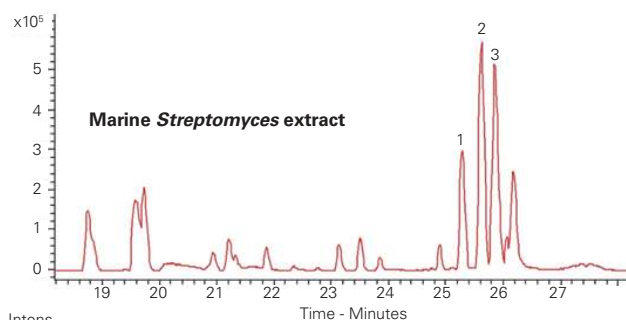
Analytes

Macrotetralides

1. Dinactin R₁ = R₃ = CH₂CH₃, R₂ = R₄ = CH₃
2. Trinactin R₁ = R₂ = R₃ = CH₂CH₃, R₄ = CH₃
3. Tetranactin R₁ = R₂ = R₃ = R₄ = CH₂CH₃



Macrotetralides



Reproduced with permission of Department of Chemistry, University of Warwick, UK



Microcystins from Blue/Green Algae in Drinking Water

Application #AN1190

Conditions

Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 0.1 % formic acid in H₂O
 B: MeCN
Gradient:

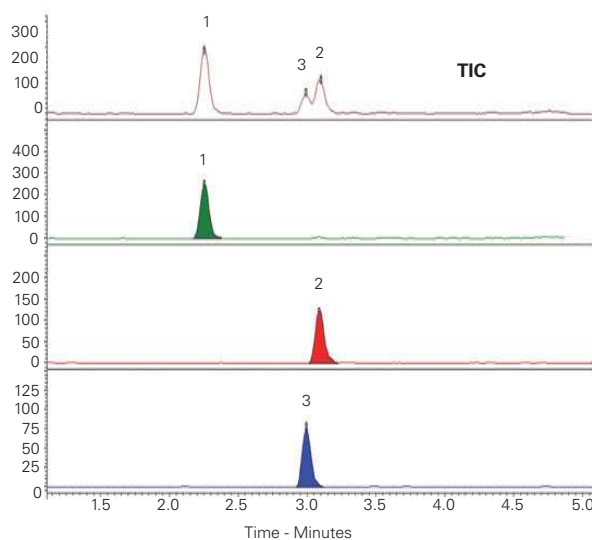
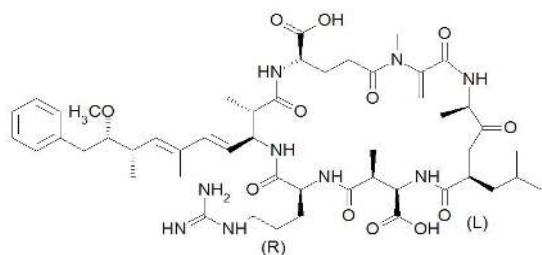
| Time (mins) | %B |
|-------------|----|
| 0.0 | 30 |
| 1.0 | 30 |
| 7.0 | 95 |
| 7.1 | 30 |
| 10.0 | 30 |

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

Analyses

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

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



Reproduced with permission of Bruker UK Ltd

Milk Proteins

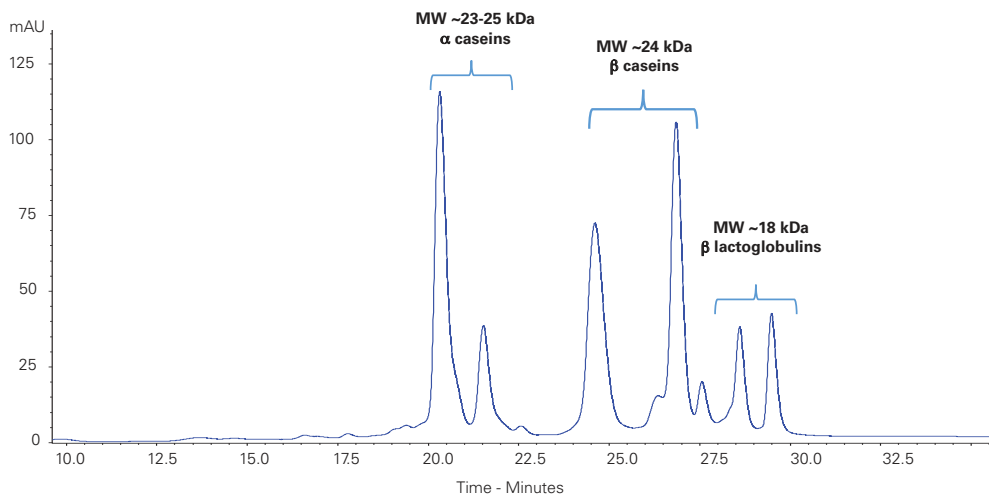
Application #AN1540

Conditions

Column: ACE 5 C18-300
Dimensions: 150 x 2.1 mm
Part Number: ACE-221-1502
Mobile Phase: A: 0.01 % TFA in H₂O
 B: 0.01 % TFA in MeCN
Gradient:

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

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



Reproduced with permission of The Chemical Analysis Facility, University of Reading, UK

Mycotoxins by LC-MS/MS

Application #AN2330

Conditions

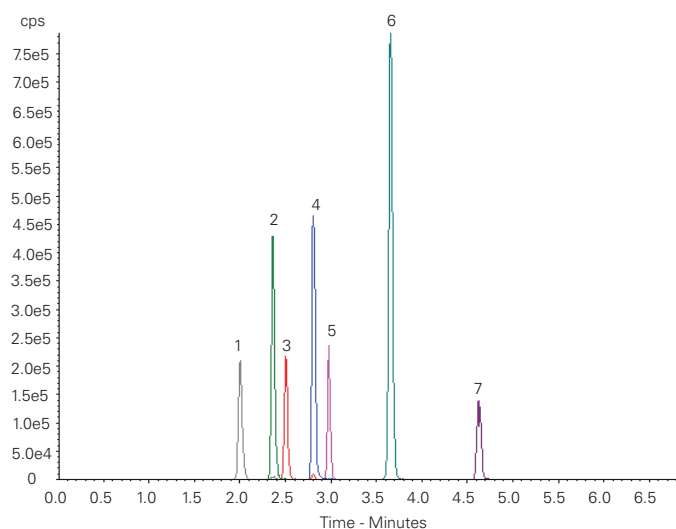
Column: ACE Excel 2 C18-AR
Dimensions: 50 x 2.1 mm
Part Number: EXL-109-0502U
Mobile Phase: A: 1 mM ammonium acetate, 0.5% acetic acid in H₂O
 B: 1 mM ammonium acetate, 0.5% acetic acid in 95% MeOH
Gradient:

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

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

Analytes

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



Reproduced with permission of Biotage GB Ltd, UK

Mycotoxins/Aflatoxins from Peppers

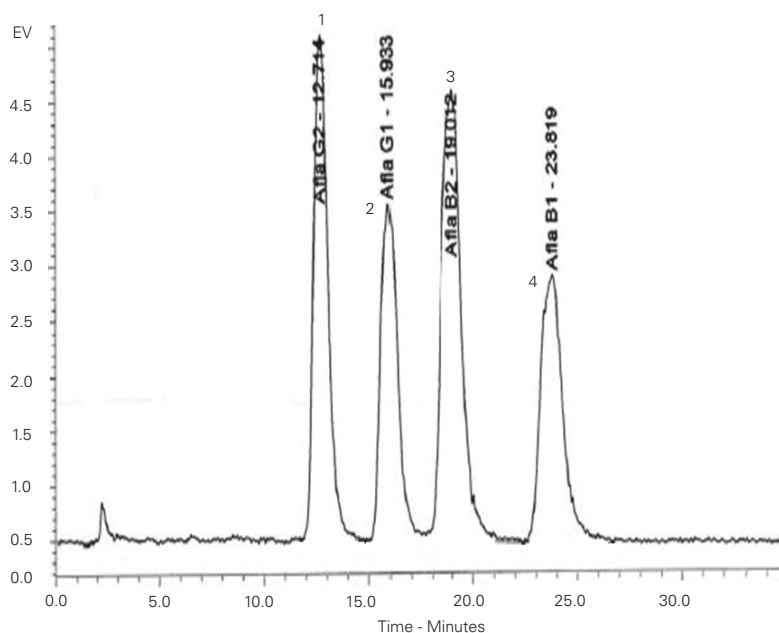
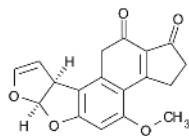
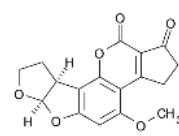
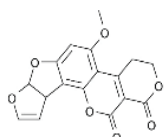
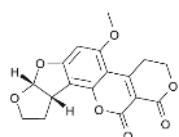
Application #AN1200

Conditions

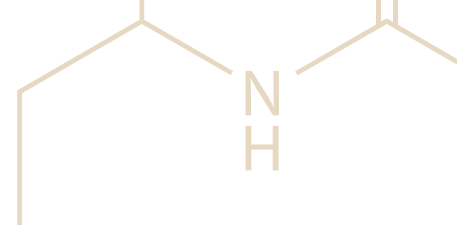
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: H₂O/MeOH (60:40 v/v)
Flow Rate: 1 mL/min
Injection: 100 µL
Temperature: 45 °C
Detection: Fluorescence, λ_{Ex} 362 nm,
 λ_{Em} 425 nm

Analytes

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



Reproduced with permission of Public Health Laboratory of Soria, Spain



Naphthalenes (Substituted)

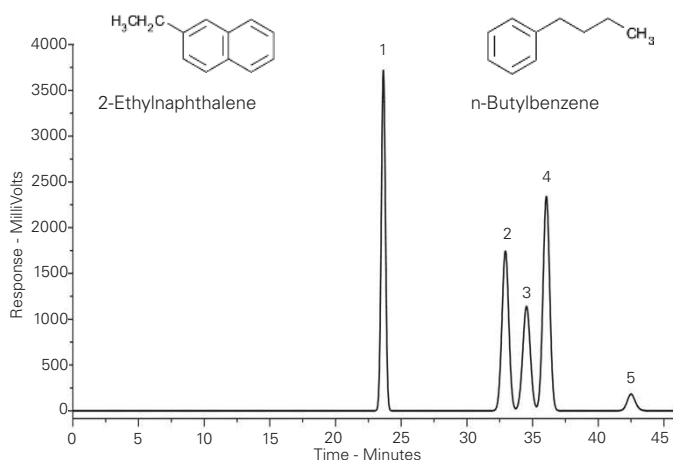
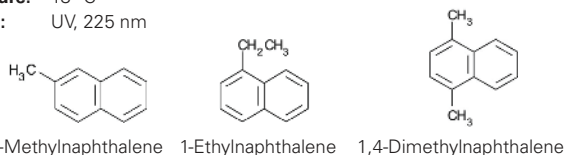
Application #AN3690

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/H₂O (51:49 v/v)
Flow Rate: 1.5 mL/min
Temperature: 18 °C
Detection: UV, 225 nm

Analytes

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



Reproduced with permission of Department of Environmental Chemistry, University of Glasgow, UK

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

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

Neonicotinoids in Honey by LC-MS/MS

Application #AN4050

Conditions

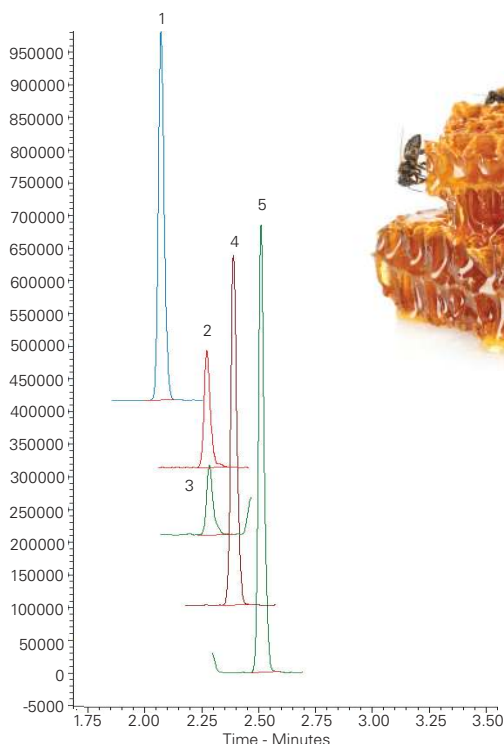
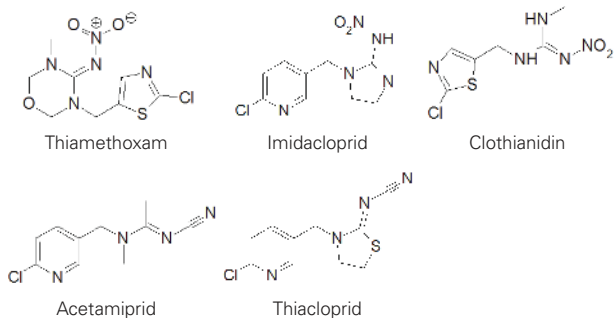
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 0.05% ammonia in H₂O
 B: 0.05% ammonia in MeOH
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 5 |
| 3 | 100 |

Flow Rate: 0.6 mL/min
Injection: 1 µL (POISe mode)
Temperature: 30 °C
Detection: Shimadzu LCMS-8060
 Positive ion mode HESI
Sample: Honey spiked at 0.1 ppb (QuEChERS extract)

Analytes

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



Reproduced with permission of Shimadzu, France

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

Application #AN3870

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: A: 0.2% formic acid in H₂O
 B: MeCN

Gradient:

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

Flow Rate: 0.6 mL/min

Injection: 5 µL

Temperature: 25 °C

Detection: Agilent 6410 triple quad
 ESI in positive ion mode (negative ion mode for MHPG)

Capillary Voltage: 1950 kV

Sample: Rat brain samples homogenised in aqueous formic acid, centrifuged and proteins removed by precipitation with acetonitrile

Analytes

- Adrenaline
- Noradrenaline
- Glutamic acid
- GABA
- Dopamine
- MHPG (3-Methoxy-4-hydroxyphenylglycol)
- Isoprenaline (IS)
- 5-Hydroxyindoleacetic acid
- Serotonin

Quantifier

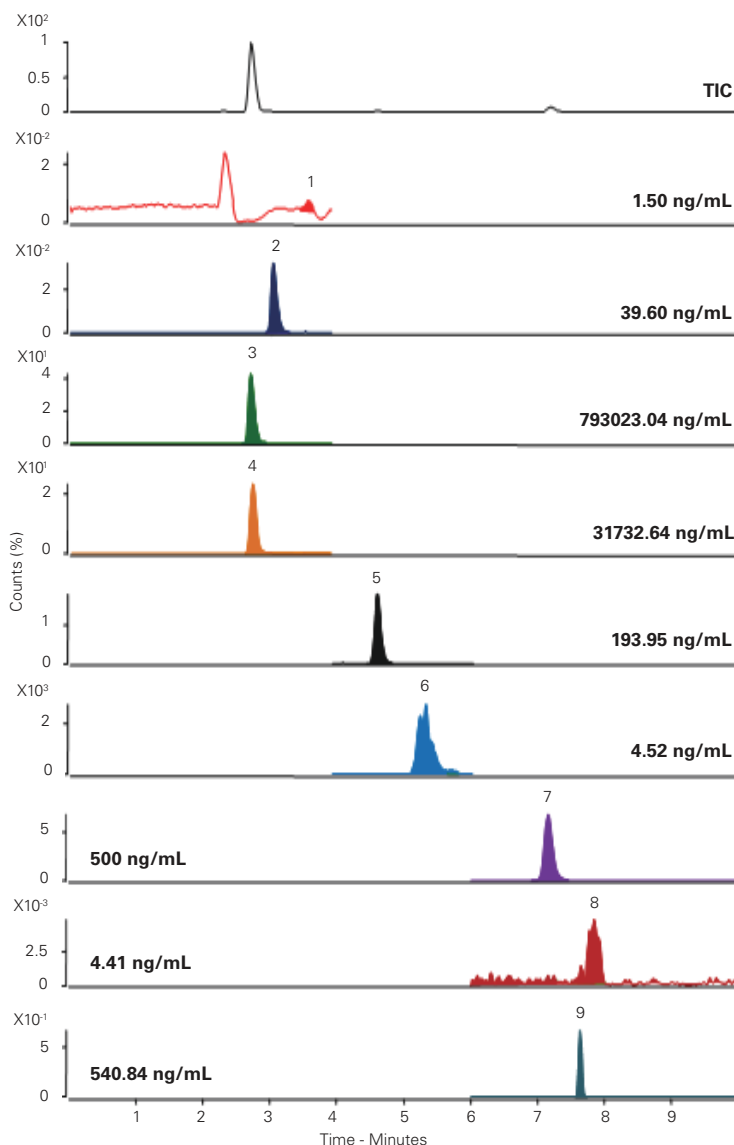
m/z 184.2 → 166.2
m/z 170.2 → 107.1
m/z 148.1 → 84.1
m/z 104 → 45
m/z 154.1 → 137.1
m/z 263 → 165.1
m/z 212.2 → 194.1
m/z 192 → 145.9
m/z 177.2 → 160.2

Qualifier

m/z 184.2 → 57.1
m/z 170.2 → 152.1
m/z 148.1 → 130.1
m/z 104 → 87
m/z 154.1 → 91.1
m/z 263 → 165.1
m/z 192 → 90.9
m/z 177.2 → 132.1

LLOQ (ng/mL)

0.25
 0.5
 250
 250
 0.25
 1
 1
 10

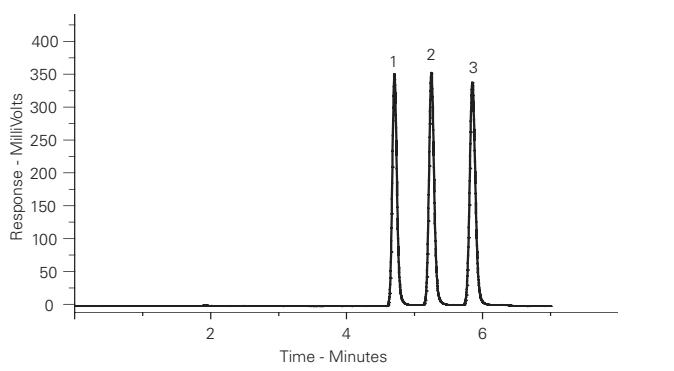


Reproduced with permission of Hospital Universitario de la Princesa, Servicio Farmacologia Clinica, Madrid, Spain



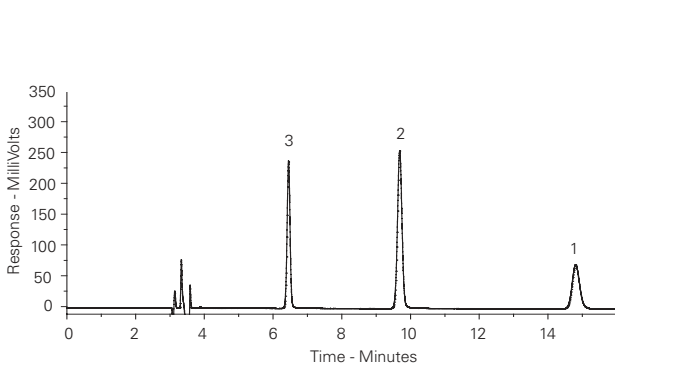
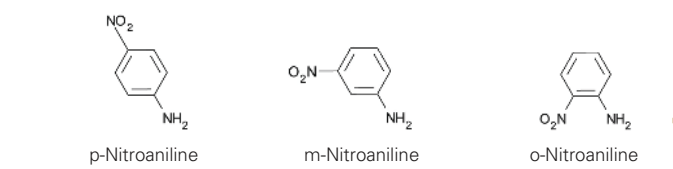
Nitroanilines (I) Application #AN3240

Conditions
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM KH₂PO₄ pH 3.15/ MeCN (50:50 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm



Nitroanilines (II) Application #AN3250

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

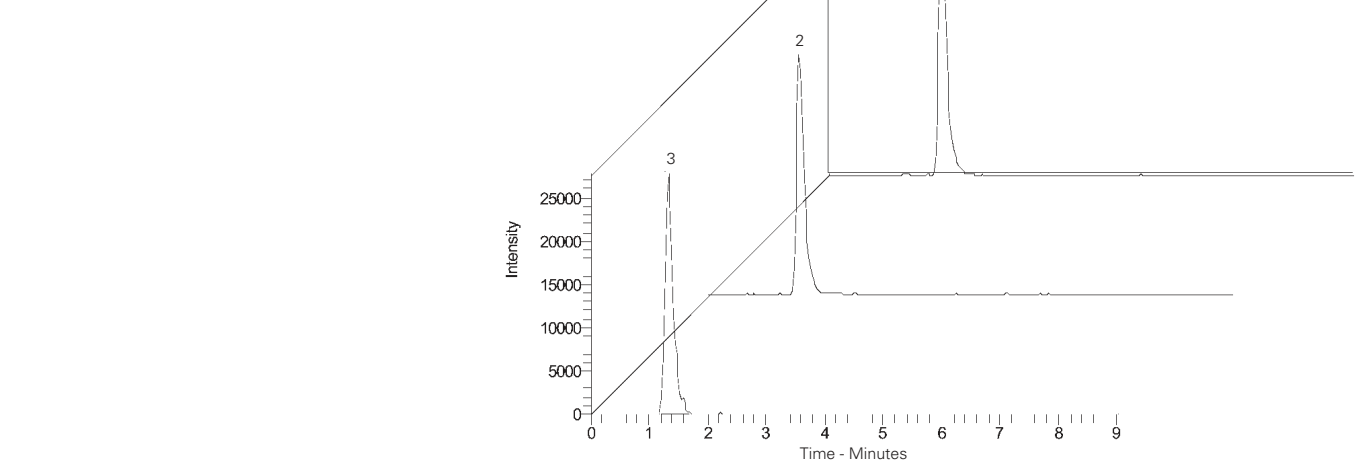


Nitrofuran Metabolites by LC-MS/MS Application #AN3050

Conditions
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: MeOH/0.5 mM ammonium acetate in H₂O (50:50 v/v)
Flow Rate: 0.2 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: ESI MS/MS (+ve mode)
Sample: Metabolites derivatised with 2-nitrobenzaldehyde to form nitrophenyl derivatives, prior to LC-MS analysis

Analytes

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



Reproduced with permission of Agricultural Ministry, Brazil

Nitrosamines European Toy Standard Method by LC-MS/MS

Application #AN1110

Conditions

Column: ACE Excel 2 C18-PFP
Dimensions: 150 x 3.0 mm
Part Number: EXL-1010-1503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

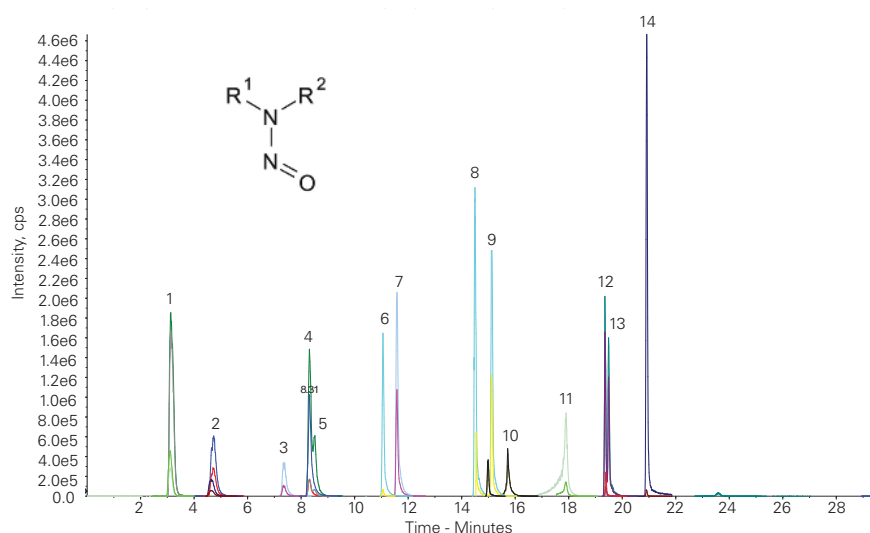
| Time (mins) | %B |
|-------------|----|
| 0.0 | 5 |
| 1.0 | 5 |
| 10.0 | 65 |
| 14.0 | 65 |
| 15.0 | 90 |
| 20.0 | 90 |
| 21.0 | 5 |
| 30.0 | 5 |

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

Analytes

| | | |
|---|--|--|
| 1. NDELA (<i>m/z</i> 135.2 → 74.2, 135.2 → 104.2) | 6. NDEA (<i>m/z</i> 103.1 → 75.2, 103.1 → 472) | 11. NEPhA (<i>m/z</i> 151.1 → 77.1, 151.1 → 95.3) |
| 2. NDMA (<i>m/z</i> 74.9 → 43.2, 74.9 → 58.2) | 7. NPIP (<i>m/z</i> 115.1 → 69.1, 115.1 → 41.2) | 12. NDIBA (<i>m/z</i> 159.3 → 57.2, 159.3 → 103.2) |
| 3. Nmorph (<i>m/z</i> 117.1 → 86.3, 117.1 → 73.3) | 8. NDnPA (<i>m/z</i> 131.2 → 89.2, 131.2 → 43.3) | 13. NDnBA (<i>m/z</i> 159.3 → 103.2, 159.3 → 57.2) |
| 4. Npyrr (<i>m/z</i> 101.2 → 55.3, 101.2 → 59.2) | 9. NdiPA (<i>m/z</i> 131.2 → 89.2, 131.2 → 43.3) | 14. NDBzA (<i>m/z</i> 227.2 → 91.1, 227.2 → 181.2) |
| 5. NMEA (<i>m/z</i> 89.2 → 61.1, 89.2 → 43.3) | 10. NMPHA (<i>m/z</i> 137.2 → 107.2, 137.2 → 66.1) | |

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



Reproduced with permission of LGC Limited, UK

Non-Steroidal Anti-Inflammatory Drugs (I)

Application #AN1210

Conditions

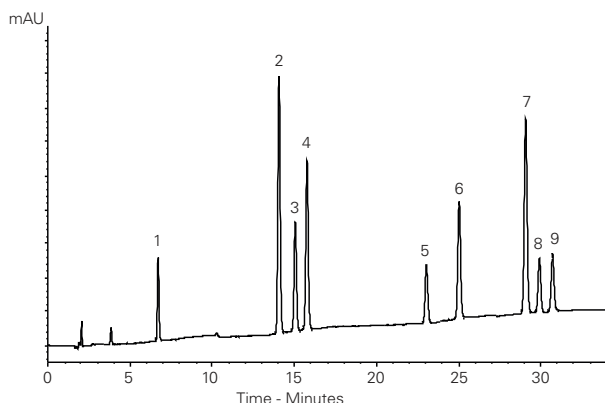
Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 52 |
| 28 | 74 |
| 33 | 74 |
| 38 | 52 |
| 48 | 52 |

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

Analytes

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



Non-Steroidal Anti-Inflammatory Drugs (II)

Application #AN1220

Conditions

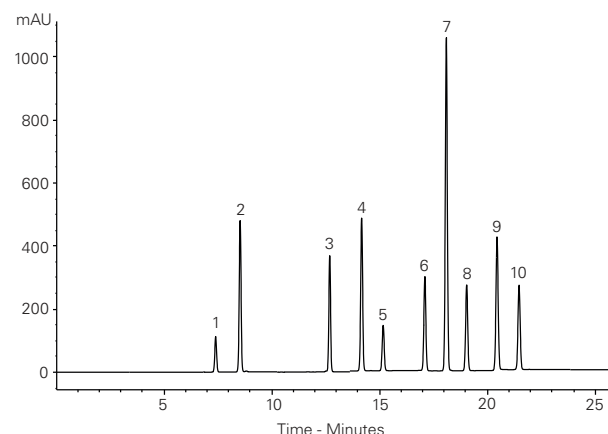
Column: ACE Excel 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

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

Analytes

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





Non-Steroidal Anti-Inflammatory Drugs (III)

Application #AN3570

Conditions

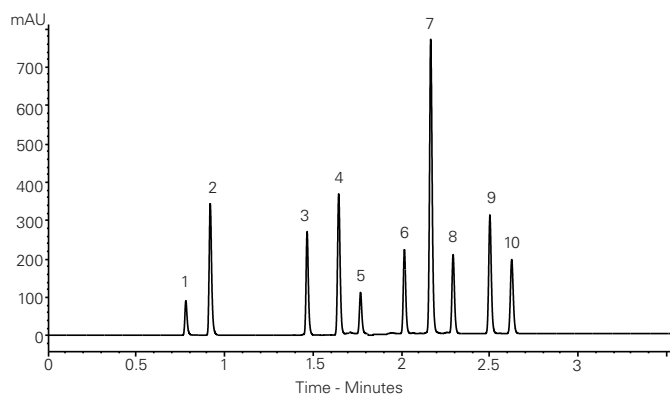
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.02 | 20 |
| 2.71 | 70 |
| 3.39 | 70 |
| 3.52 | 20 |

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

Analytes

- Aspirin
- Phenacetin
- Sulindac
- Tolmetin
- Naproxen
- Nimesulide
- Flurbiprofen
- Diclofenac
- Phenylbutazone
- Meclofenamic acid



Non-Steroidal Anti-Inflammatory Drugs – Fast Analysis

Application #AN2080

Conditions

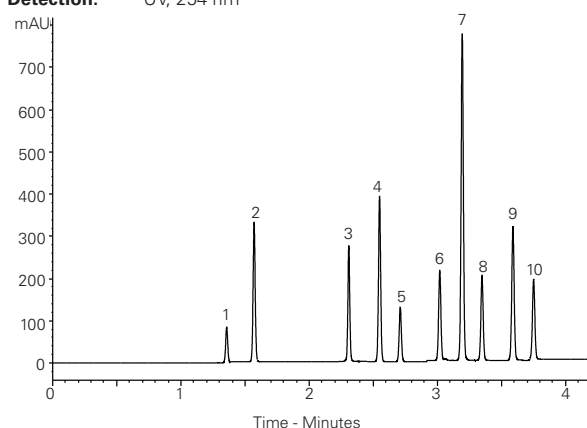
Column: ACE Excel 2 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: EXL-1011-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.00 | 20 |
| 0.25 | 20 |
| 3.50 | 70 |
| 4.00 | 20 |
| 4.25 | 20 |

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

Analytes

- Aspirin
- Phenacetin
- Sulindac
- Tolmetin
- Naproxen
- Nimesulide
- Flurbiprofen
- Diclofenac
- Phenylbutazone
- Meclofenamic acid



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

Application #AN2630

Conditions

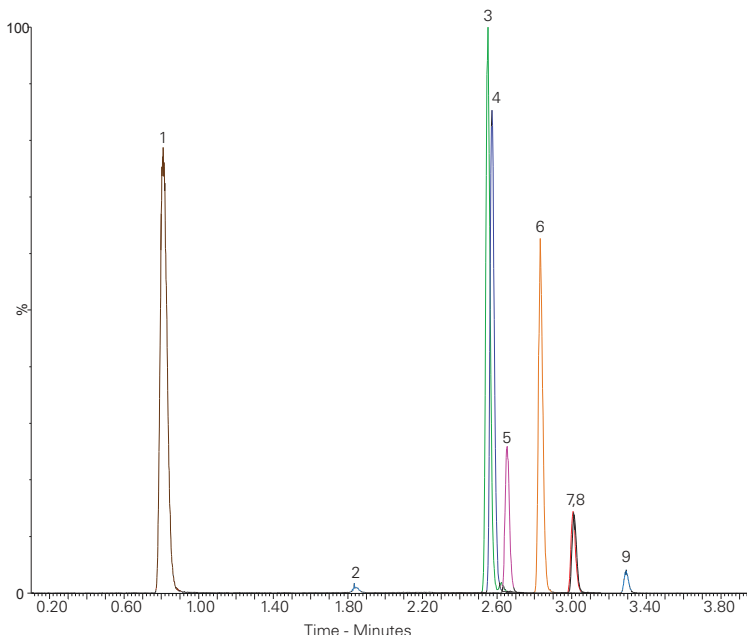
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O
 B: 2 mM ammonium acetate, 0.1% formic acid in MeOH
Gradient:

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

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

Analytes

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



Nucleic Acids / Disease Biomarker Profiling (I)

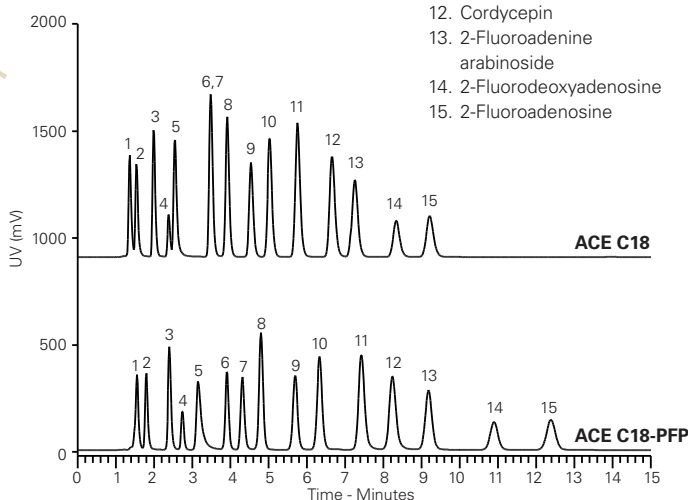
Application #AN1080

Conditions

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

Analytes

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



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

Nucleosides and Vitamins

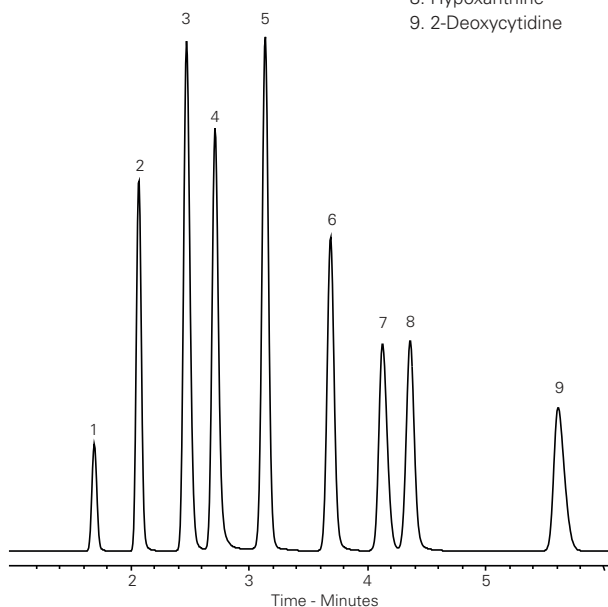
Application #AN1330

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: 20 mM H₃PO₄ in H₂O
Flow Rate: 1 mL/min
Temperature: 22 °C
Detection: UV, 254 nm

Analytes

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



Nucleic Acids / Disease Biomarker Profiling (II)

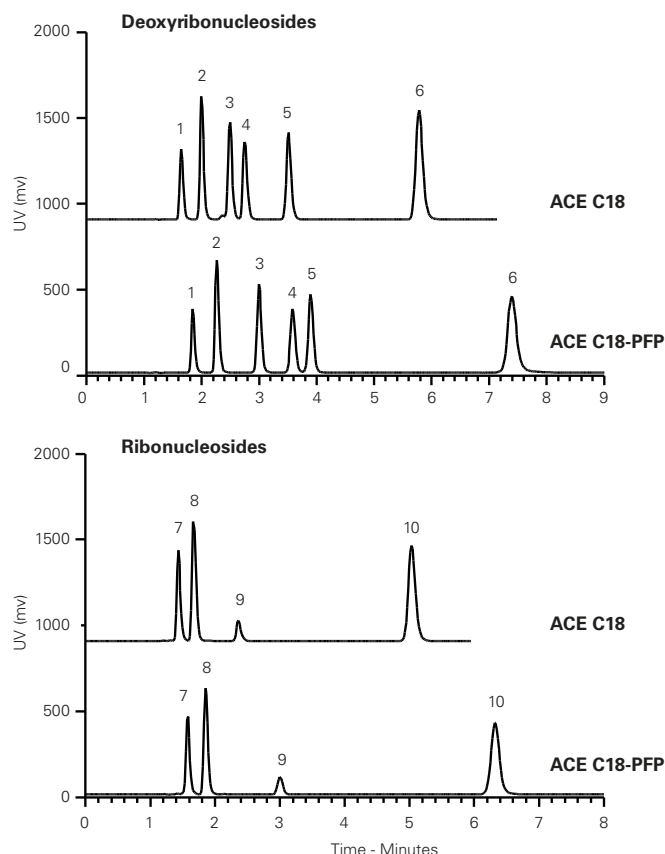
Application #AN1090

Conditions

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

Analytes

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

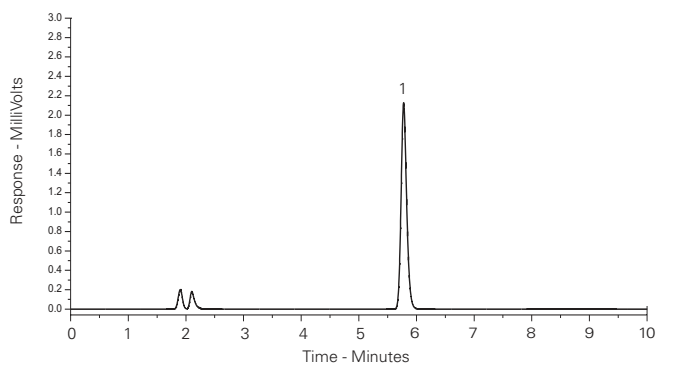
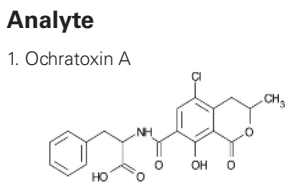


Reproduced with permission of Department of Medical Biochemistry and Biophysics, Umeå University, Sweden



Ochratoxin A Application #AN2870

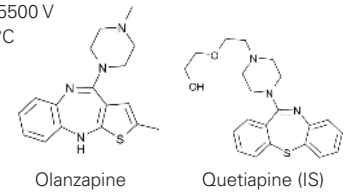
Conditions
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/H₂O/Acetic acid (51:47:2 v/v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: Fluorescence – λ_{ex} 333 nm, λ_{em} 443 nm



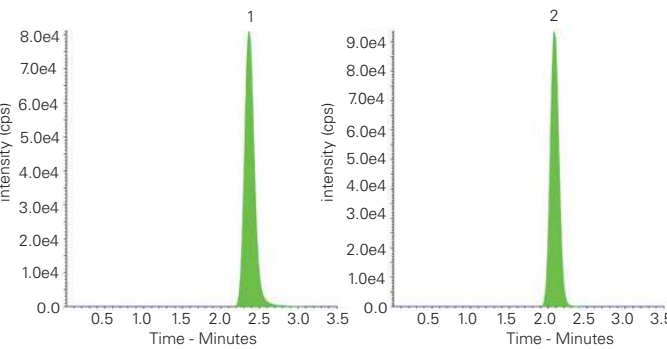
Reproduced with permission of R-Biopharm Rhone Ltd, Glasgow, UK

Olanzapine in Human Plasma by LC-MS/MS Application #AN2520

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



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



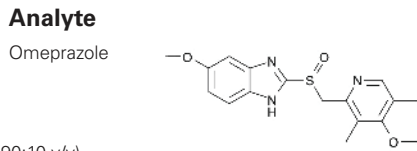
Reproduced with permission of Department of Chemistry, School of Sciences, Gujarat University, India

Omeprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl Application #AN1560

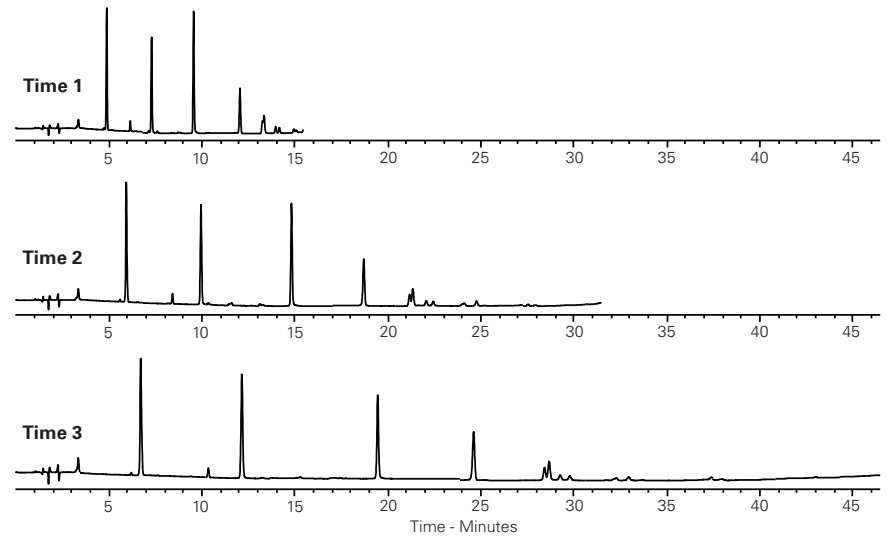
Conditions
Column: ACE Excel 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 0.1% ammonia in H₂O
 B: 0.1% ammonia in MeCN/H₂O (90:10 v/v)
Gradient:

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

Post time 10 minutes



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



Opiates from Drugs of Abuse Screen (#AN2190)

Application #AN2340

Conditions

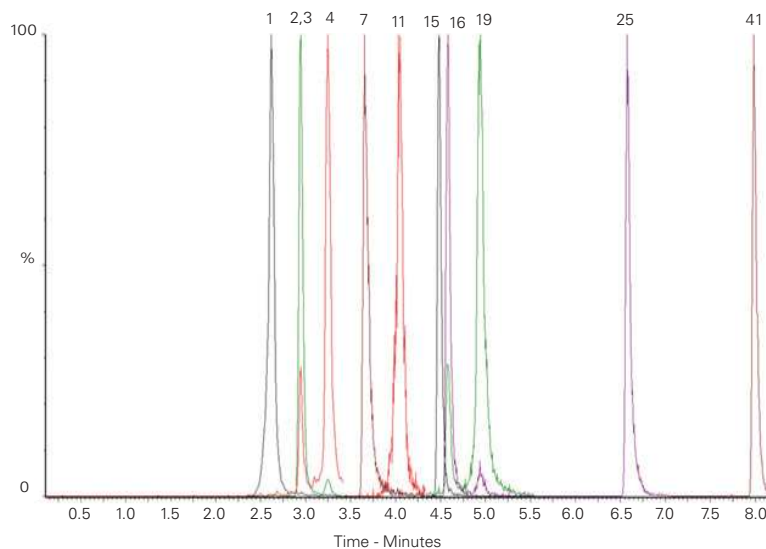
Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 5 mM ammonium acetate in H₂O
 B: 5 mM ammonium acetate in MeOH
Gradient:

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

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

Analytes

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



Reproduced with permission of Biotage GB Ltd

Opiates in Urine by LC-MS/MS

Application #AN1230

Conditions

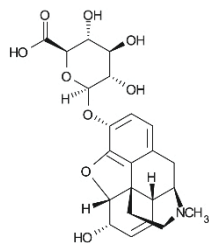
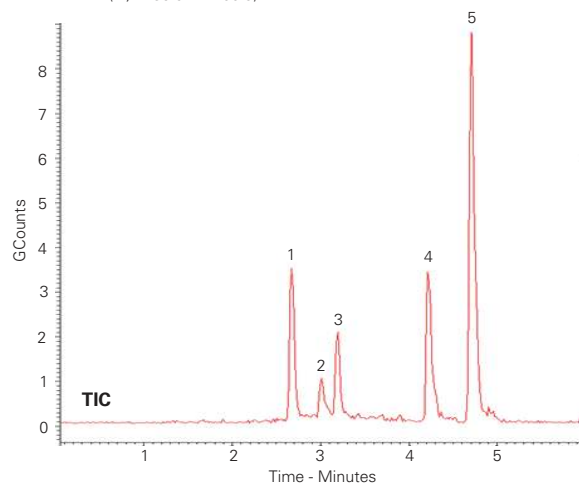
Column: ACE Excel 3 SuperC18
Dimensions: 75 x 2.1 mm
Part Number: EXL-1111-7502U
Mobile Phase: A: 5 mM ammonium hydroxide pH 10.8 in H₂O
 B: 5 mM ammonium hydroxide pH 10.8 in MeOH/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 30 |
| 5 | 95 |

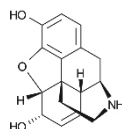
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: Varian 320 Triple Quadrupole MS
 Electrospray voltage: +5 kV
 Inlet capillary voltage: 30 V
 CID with argon at 1.5 mTorr
 Collision cell potential ranges from 5 to 17 V
 Drying gas (nitrogen) temperature: 325 °C
 Nebulizing gas (nitrogen)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

Analytes

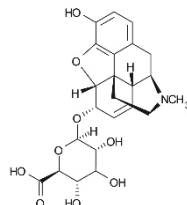
- | | | |
|---|---|--|
| 1. Morphine 3-β-D-glucuronide LOD (est) 100 ppb (<i>m/z</i> 462.0 → 285.9) | 3. Morphine 6-β-D-glucuronide LOD (est) 100 ppb (<i>m/z</i> 462.0 → 285.9) | 5. 6-Acetylmorphine LOD (est) 10 ppb (<i>m/z</i> 328.0 → 164.9) |
| 2. Normorphine LOD (est) 100 ppb (<i>m/z</i> 272.0 → 165.0) | 4. Morphine LOD (est) 20 ppb (<i>m/z</i> 286.0 → 200.9) | |



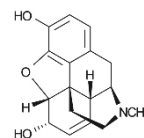
Morphine 3-β-D-glucuronide



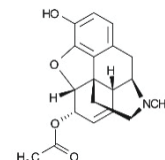
Normorphine



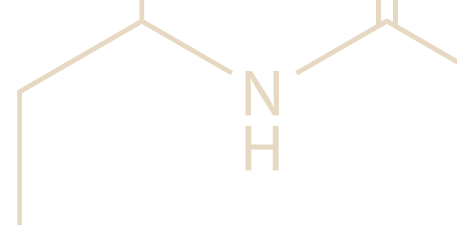
Morphine 6-β-D-glucuronide



Morphine



6-Acetylmorphine



Organic Acids

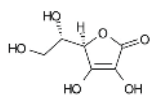
Application #AN2780

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM KH₂PO₄ pH 5.7 in H₂O/MeOH (70:30 v/v)
Flow Rate: 1 mL/min
Temperature: 22 °C
Detection: UV, 220 nm

Analytes

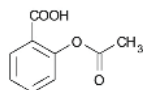
1. L-Ascorbic acid
2. Maleic acid
3. Acetylsalicylic acid
4. Benzoic acid
5. Salicylic acid



L-Ascorbic acid



Maleic acid



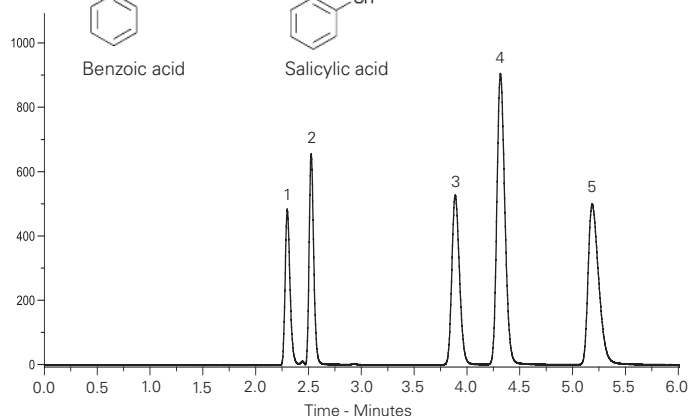
Acetylsalicylic acid



Benzoic acid



Salicylic acid



For further applications

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

Organic Acids – Fast Separation

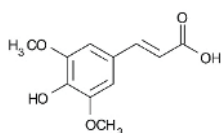
Application #AN2200

Conditions

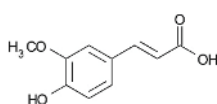
Column: ACE Excel 3 C18-Amide
 ACE Excel 1.7 C18-Amide
Dimensions: 250 x 2.1 mm, 50 x 3.0 mm
Part Number: 250 x 2.1 mm (EXL-1112-2502U),
 50 x 3 mm (EXL-1712-0503U)
Mobile Phase: 20 mM H₃PO₄ in MeOH/H₂O (40:60 v/v)
Flow Rate: 0.21 mL/min (250 x 2.1 mm)
 0.8 mL/min (50 x 3.0 mm)
Injection: 5 µL (250 x 2.1 mm)
 2 µL (50 x 3.0 mm)
Temperature: 20 °C
Detection: UV, 210 nm

Analytes

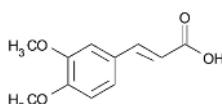
1. Sinapic acid
2. Ferulic acid
3. 3,4-Dimethoxycinnamic acid
4. Cinnamic acid
5. 4-Methoxycinnamic acid



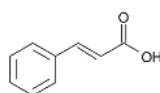
Sinapic acid



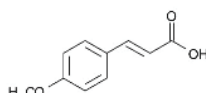
Ferulic acid



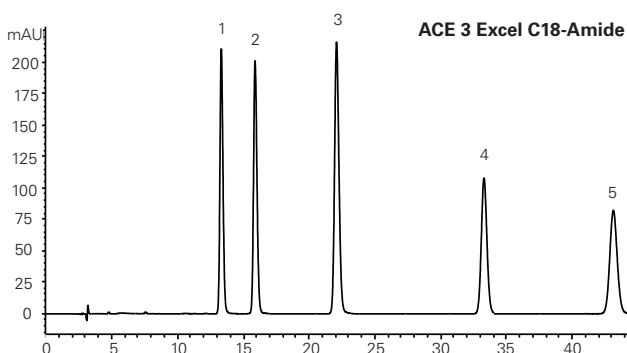
3,4-Dimethoxycinnamic acid



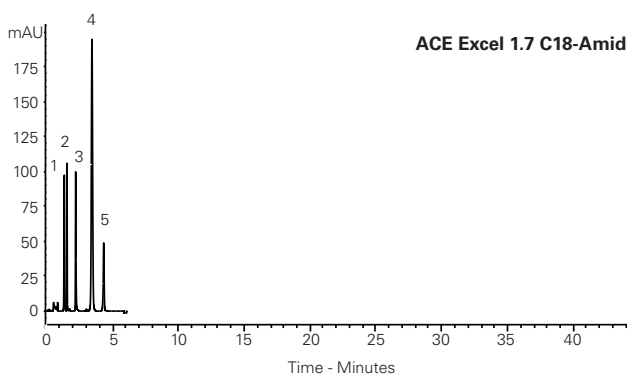
Cinnamic acid



4-Methoxycinnamic acid



ACE 3 Excel C18-Amide



ACE Excel 1.7 C18-Amide

Organophosphorus Flame Retardants in Water by LC-MS/MS

Application #AN1240

Conditions

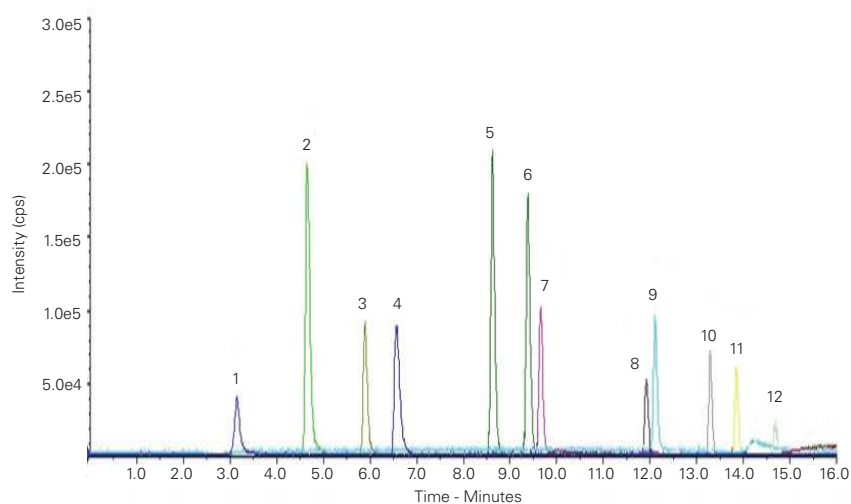
Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.05 mM ammonium formate + 0.005% formic acid in H₂O
 B: MeOH/MeCN (95:5 v/v)
Gradient:

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

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

Analytes

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



Reproduced with permission of Ontario Ministry of the Environment and Climate Change, Canada

Organophosphorus (Isomeric) Flame Retardants in Water

Application #AN1140

Conditions

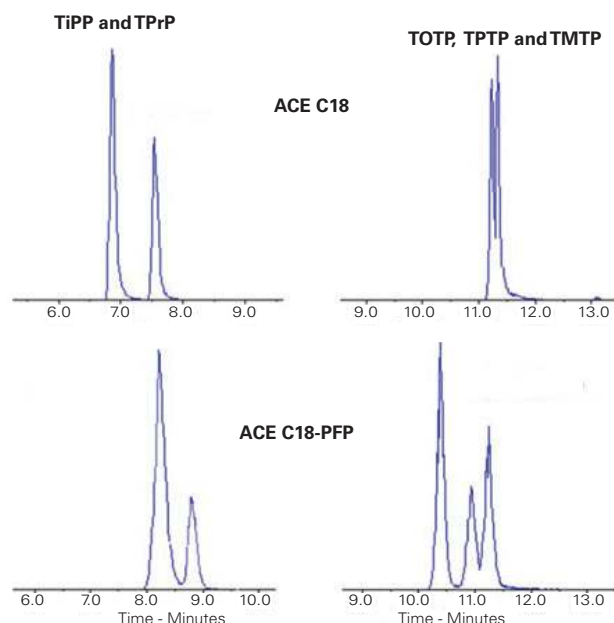
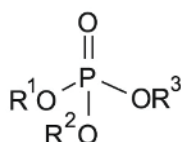
Column: ACE 3 C18
 ACE 3 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002, ACE-1110-1002
Mobile Phase: A: 0.05 mM ammonium formate + 0.005% formic acid in H₂O
 B: MeOH/MeCN (95:5 v/v)
Gradient:

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

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

Analytes

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



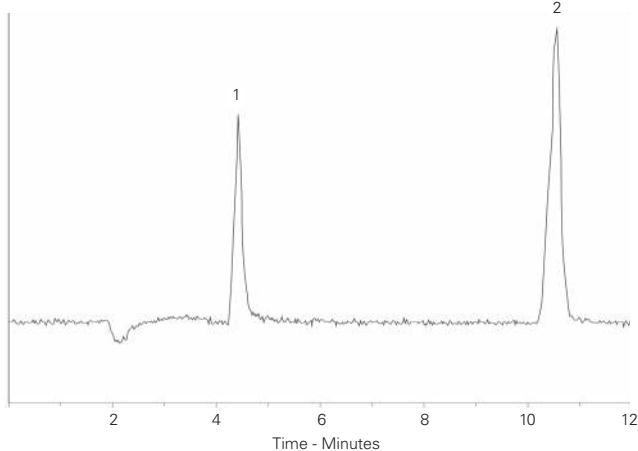
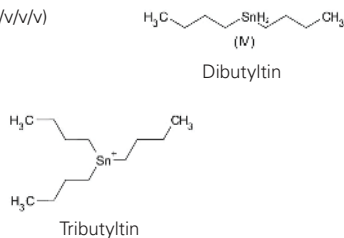
Reproduced with permission of Ontario Ministry of the Environment and Climate Change, Canada



Organotin Compounds Application #AN3650

Conditions
Column: ACE 3 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-111-1502
Mobile Phase: H₂O/MeCN/acetic acid/TEA (23:65:12:0.05 v/v/v/v)
Flow Rate: 0.2 mL/min
Detection: ICP-MS

Analytes
 1. Dibutyltin
 2. Tributyltin

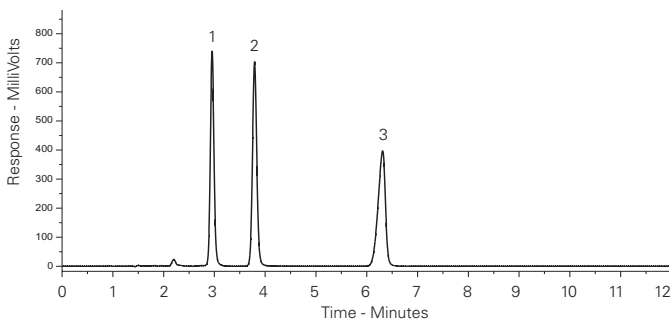
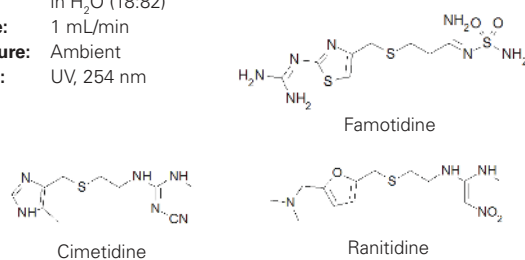


Reproduced with permission of LGC Ltd, Middlesex, UK

OTC Gastric Drugs Application #AN3940

Conditions
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/10 mM ammonium bicarbonate pH 8.0 in H₂O (18:82)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes
 1. Famotidine
 2. Cimetidine
 3. Ranitidine



Oxysterols by LC-MS/MS Application #AN2380

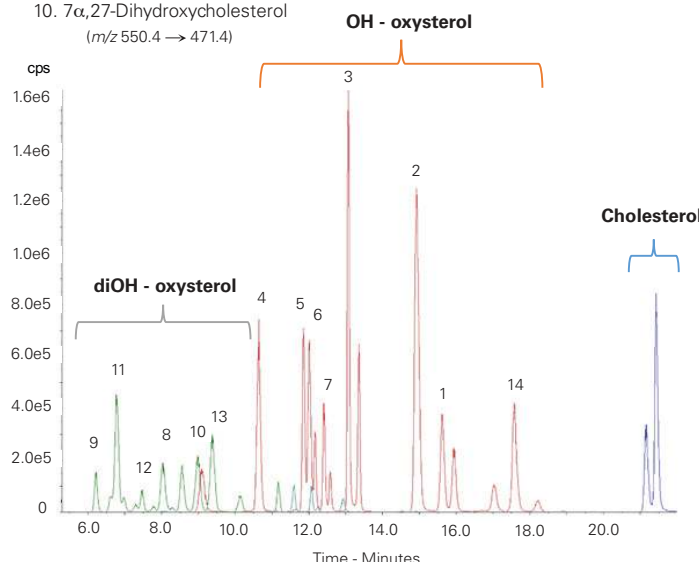
Conditions
Column: ACE 3 C18-AR
Dimensions: 150 x 2.1 mm
Part Number: ACE-119-1502
Mobile Phase: A: 0.1% formic acid in H₂O/MeOH (70:30 v/v)
 B: 0.1% formic acid in MeOH
Gradient:

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

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

Analytes

- 7 α -Hydroxycholesterol (*m/z* 534.4 → 455.4)
- 7 β -Hydroxycholesterol (*m/z* 534.4 → 455.4)
- 22(S)-Hydroxycholesterol (*m/z* 534.4 → 455.4)
- 22(R)-Hydroxycholesterol (*m/z* 534.4 → 455.3)
- 24(S)-Hydroxycholesterol (*m/z* 534.5 → 455.4)
- 25-Hydroxycholesterol (*m/z* 534.4 → 455.4)
- 27-Hydroxycholesterol (*m/z* 534.4 → 455.4)
- 7 α ,25-Dihydroxycholesterol (*m/z* 550.4 → 471.4)
- 7 β ,25-Dihydroxycholesterol (*m/z* 550.4 → 471.4)
- 7 α ,27-Dihydroxycholesterol (*m/z* 550.4 → 471.4)
- 7 β ,27-Dihydroxycholesterol (*m/z* 550.4 → 471.4)
- 3 β ,25-Dihydroxy-5-cholesten-7-one (*m/z* 550.4 → 471.4)
- 3 β ,27-Dihydroxy-5-cholesten-7-one (*m/z* 550.4 → 471.4)
- 5 α ,6 α -Epoxycholestanol (*m/z* 534.4 → 455.4)



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

Oxymetazoline in Nasal Spray Formulation

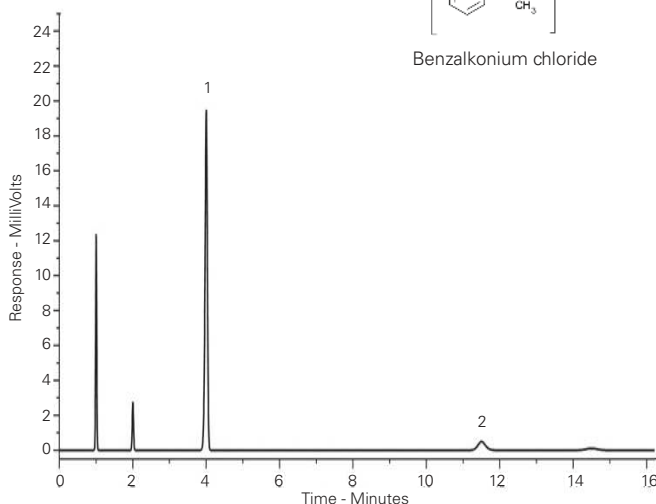
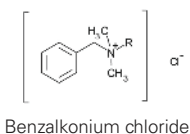
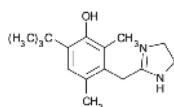
Application #AN3660

Conditions

Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: aq. Na₂HPO₄ pH 7.0/MeCN (50:50 v/v)
Flow Rate: 1.5 mL/min
Temperature: 30 °C
Detection: UV, 214 nm

Analytes

1. Oxymetazoline
2. Benzalkonium chloride



Reproduced with permission of Thornton & Ross Ltd, Huddersfield, UK

Paclitaxel

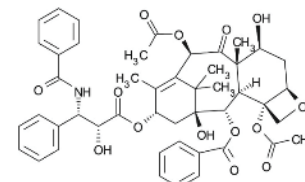
Application #AN3670

Conditions

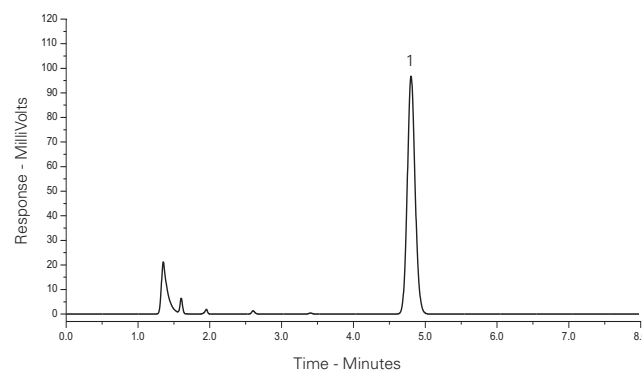
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: H₂O/MeCN (45:55 v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: UV, 227 nm

Analyte

1. Paclitaxel



Paclitaxel



Reproduced with permission of Biointeractions Ltd, Reading, UK

Paeonia Lactiflora Extract HPLC Fingerprint

Application #AN3820

Conditions

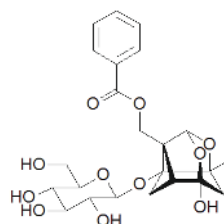
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% phosphoric acid in H₂O
 B: MeCN
Gradient:

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

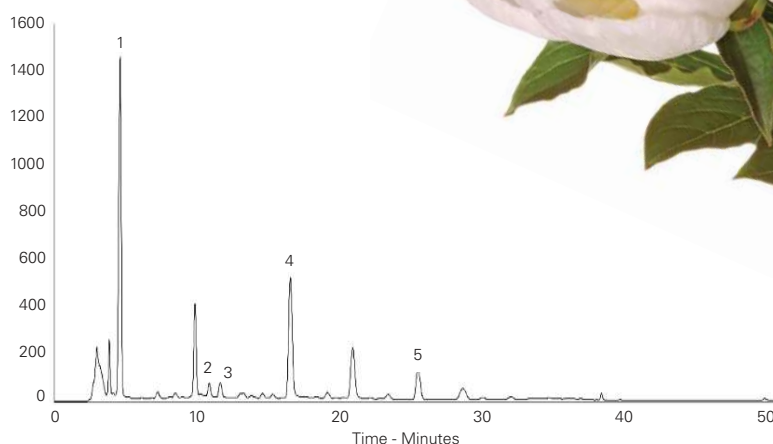
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 25 °C
Detection: UV, 254 nm
Sample: *P. lactiflora* root extracted with boiling water and polysaccharides removed by precipitation

Analytes

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



Paeoniflorin



Choi H-J, Chung T-W, Park M-J, Lee KS, Yoon Y, Kim HS, Lee JH, Kwon S-M, Lee S-O, Kim K-J, Baek J-H, Ha K-T. (2016) *Paeonia lactiflora* Enhances the Adhesion of Trophoblast to the Endometrium via Induction of Leukemia Inhibitory Factor Expression. PLoS ONE 11(2): e0148232. doi:10.1371/journal.pone.0148232



Paraben Preservatives

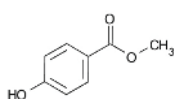
Application #AN1250

Conditions

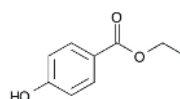
Column: ACE 3 Phenyl
Dimensions: 150 x 2.1 mm
Part Number: ACE-115-1502
Mobile Phase: 25 mM ammonium acetate pH 6.8 in H₂O/MeOH (50:50 v/v)
Flow Rate: 0.2 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: UV, 240 nm

Analytes

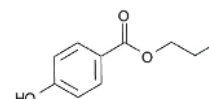
1. Methyl paraben
2. Ethyl paraben
3. n-Propyl paraben
4. i-Butyl paraben
5. n-Butyl paraben
6. Benzyl paraben



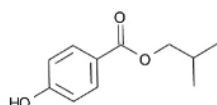
Methyl paraben



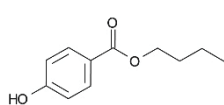
Ethyl paraben



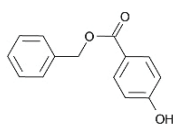
n-Propyl paraben



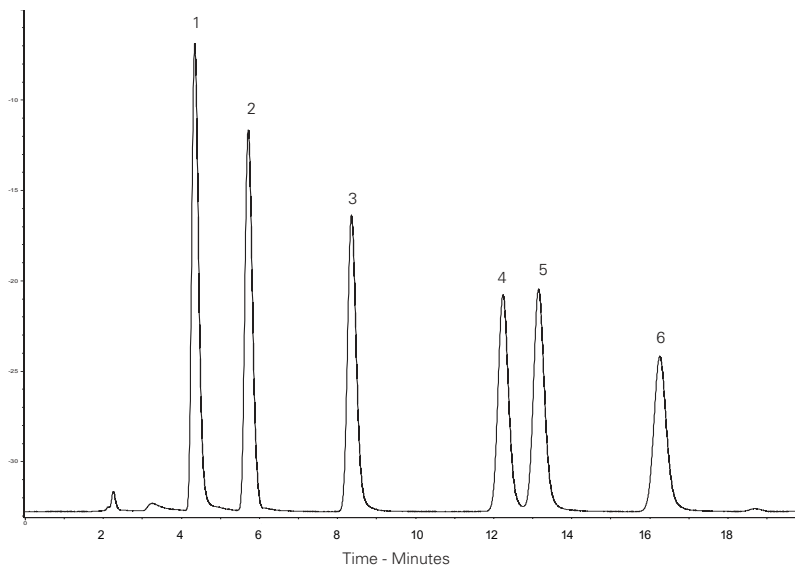
i-Butyl paraben



n-Butyl paraben



Benzyl paraben



Reproduced with permission of The Chemical Analysis Facility, University of Reading

Paracetamol and Related Compounds

Application #AN1260

Conditions

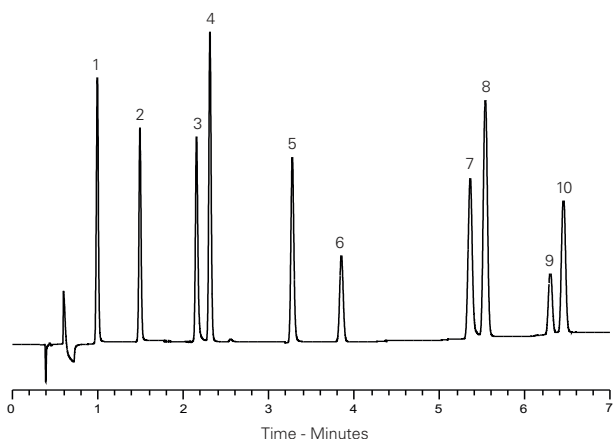
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 3.0 mm
Part Number: EXL-1010-1003U
Mobile Phase: A: 20 mM ammonium acetate pH 6.0 in H₂O
 B: 20 mM ammonium acetate pH 6.0 in MeOH/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 6 |
| 5.5 | 63 |

Flow Rate: 1.2 mL/min
Injection: 2 µL
Temperature: 27 °C
Detection: UV, 220 nm

Analytes

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



Paracetamol and Related Substances – Fast Analysis (I)

Application #AN2210

Conditions

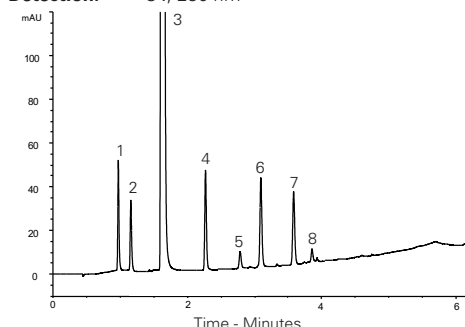
Column: ACE Excel 1.7 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-171-0503U
Mobile Phase: A: 10 mM ammonium acetate pH 6.0 in H₂O
 B: 10 mM ammonium acetate pH 6.0 in MeOH/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.00 | 5 |
| 0.08 | 5 |
| 5.08 | 95 |
| 6.76 | 95 |
| 7.09 | 5 |
| 10.00 | 5 |

Flow Rate: 0.51 mL/min
Injection: 0.7 µL
Temperature: 40 °C
Detection: UV, 230 nm

Analytes

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



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

Paracetamol and Related Substances – Enhanced Resolution

Application #AN2220

Conditions

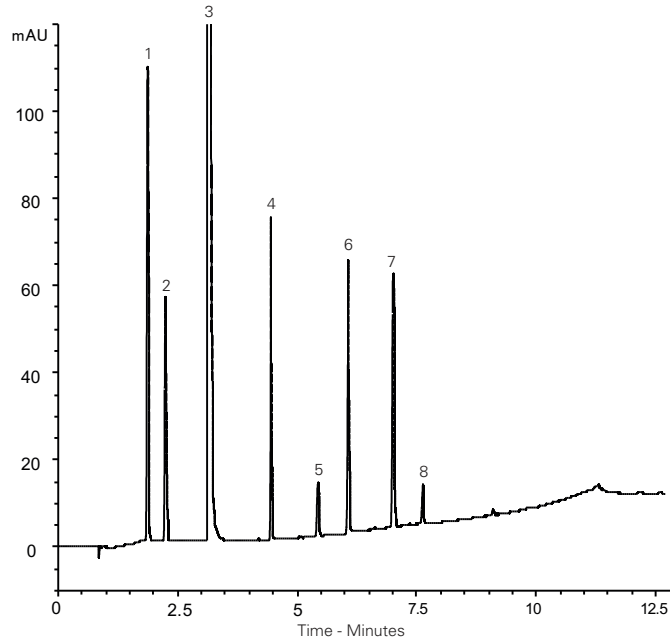
Column: ACE Excel 1.7 C18
Dimensions: 100 x 3.0 mm
Part Number: EXL-171-1003U
Mobile Phase: A: 10 mM ammonium acetate
 pH 6.0 in H₂O
 B: 10 mM ammonium acetate
 pH 6.0 in MeOH/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.00 | 5 |
| 0.21 | 5 |
| 10.23 | 95 |
| 13.56 | 95 |
| 14.16 | 5 |
| 20.24 | 5 |

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

Analytes

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



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

Paracetamol and Related Substances – Phase Selectivity

Application #AN3580

Conditions

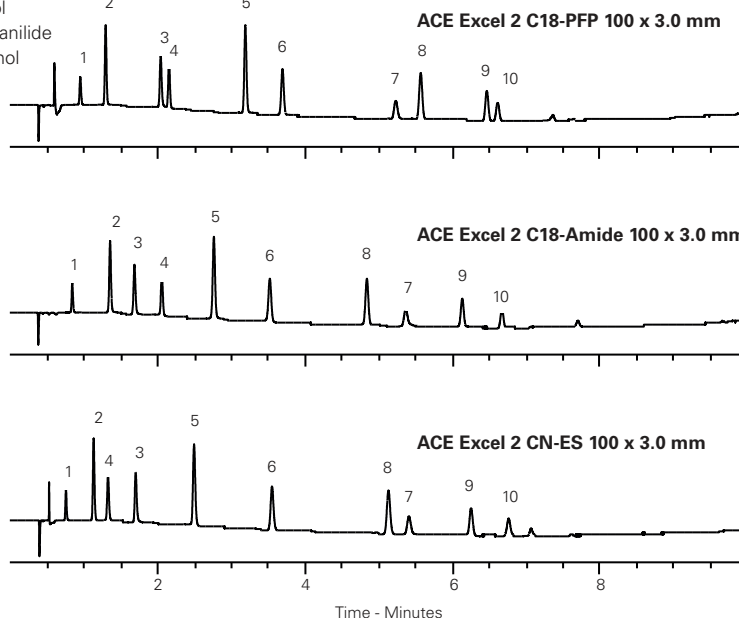
Column: ACE Excel 2 C18-PFP,
 ACE Excel 2 C18-Amide,
 ACE Excel 2 CN-ES
Dimensions: 100 x 3.0 mm
Part Number: EXL-1010-1003U,
 EXL-1012-1003U,
 EXL-1013-1003U
Mobile Phase: A: 20 mM ammonium acetate
 pH 6.0 in H₂O
 B: 20 mM ammonium acetate
 pH 6.0 in MeOH/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 5 |
| 10.0 | 95 |
| 12.5 | 95 |
| 13.0 | 5 |

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

Analytes

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





Paralytic Shellfish Poisoning (PSP) Toxins

Application #AN3180

Conditions

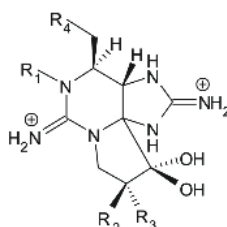
Column: ACE UltraCore 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: CORE-5A-1546U
Mobile Phase: A: 0.1 M ammonium formate in H₂O
 B: 0.1 M ammonium formate in H₂O/MeOH (95:5 v/v)
Gradient:

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

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

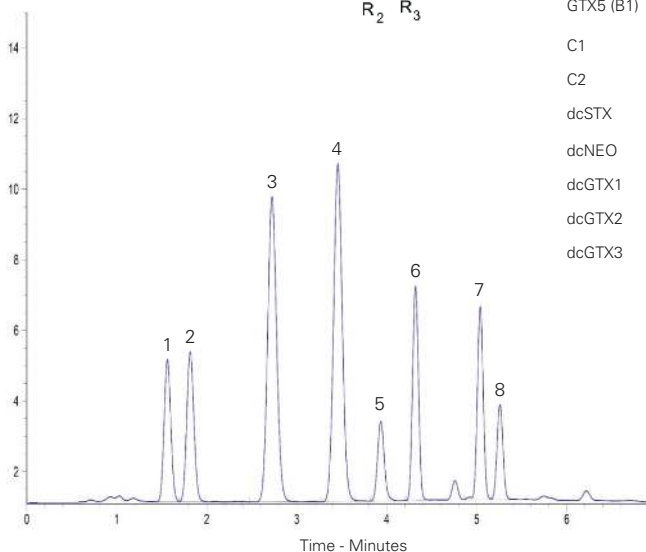
Analytes

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



PST Variant

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



Reproduced with permission of CEFAS, Weymouth, UK

Parotoid Macrogland Secretions from South American Toads

Application #AN3970

Conditions

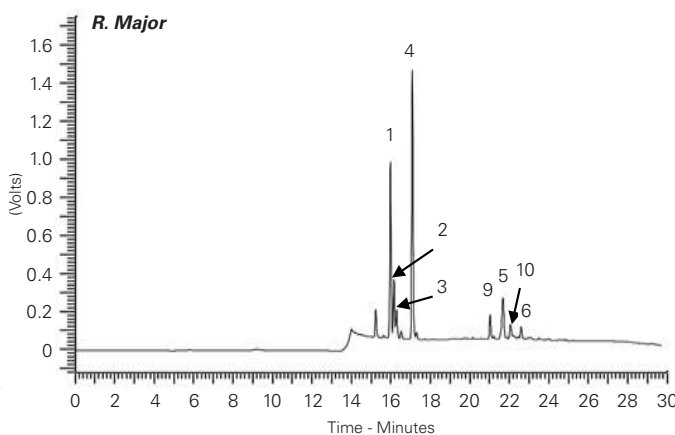
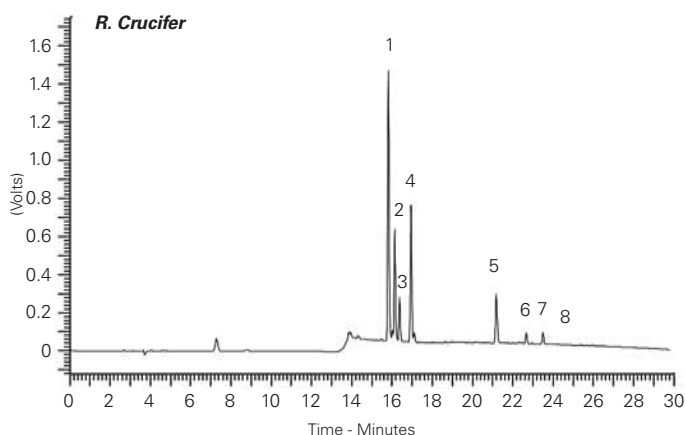
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in MeCN/H₂O (90:10 v/v)
Gradient:

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

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

Analytes

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



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

Paroxetine and Desfluoro Analogue

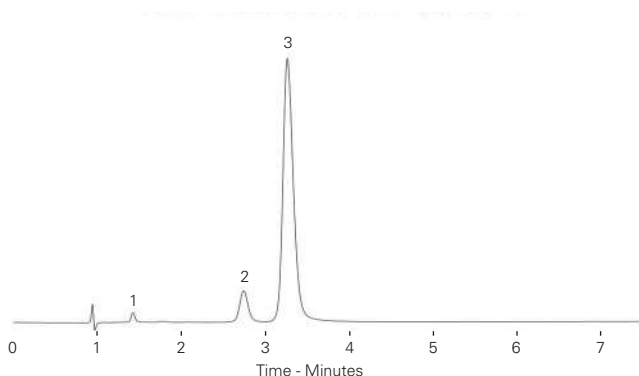
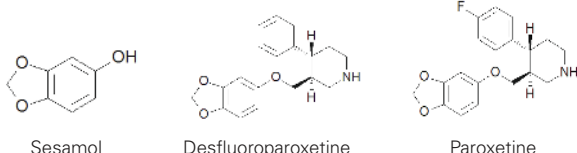
Application #AN3890

Conditions

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

Analytes

1. Sesamol
2. Desfluoroparoxetine
3. Paroxetine



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

Peptide Test Mix

Application #AN3930

Conditions

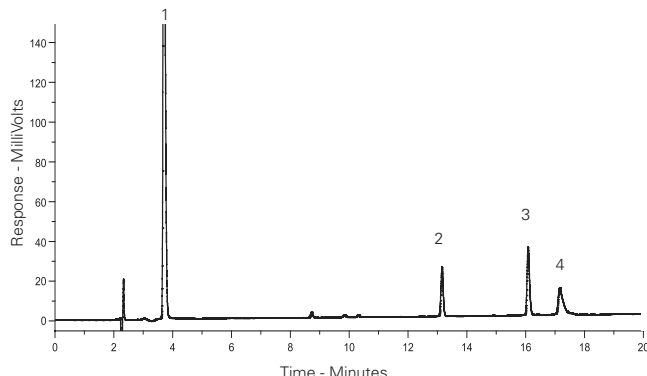
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 10 |
| 25 | 40 |

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

Analytes

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



Peptides – Varying pH

Application #AN3990

Conditions

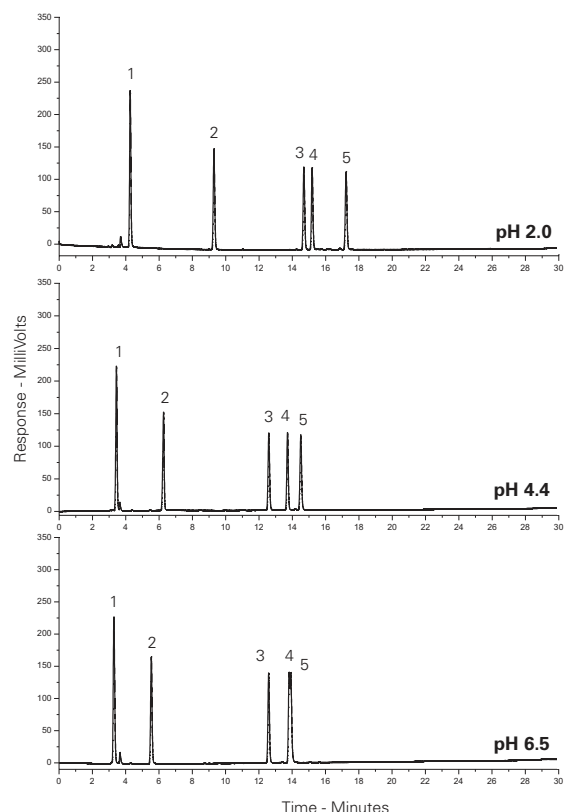
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 20 mM KH₂PO₄ in
 H₂O (pH as indicated)
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 10 |
| 25 | 40 |

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

Analytes

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





Peptides – Selectivity Changes with Bonded Phase and Mobile Phase

Application #AN3430

Conditions

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

Dimensions: 250 x 4.6 mm

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

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

Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 10 |
| 25.0 | 40 |

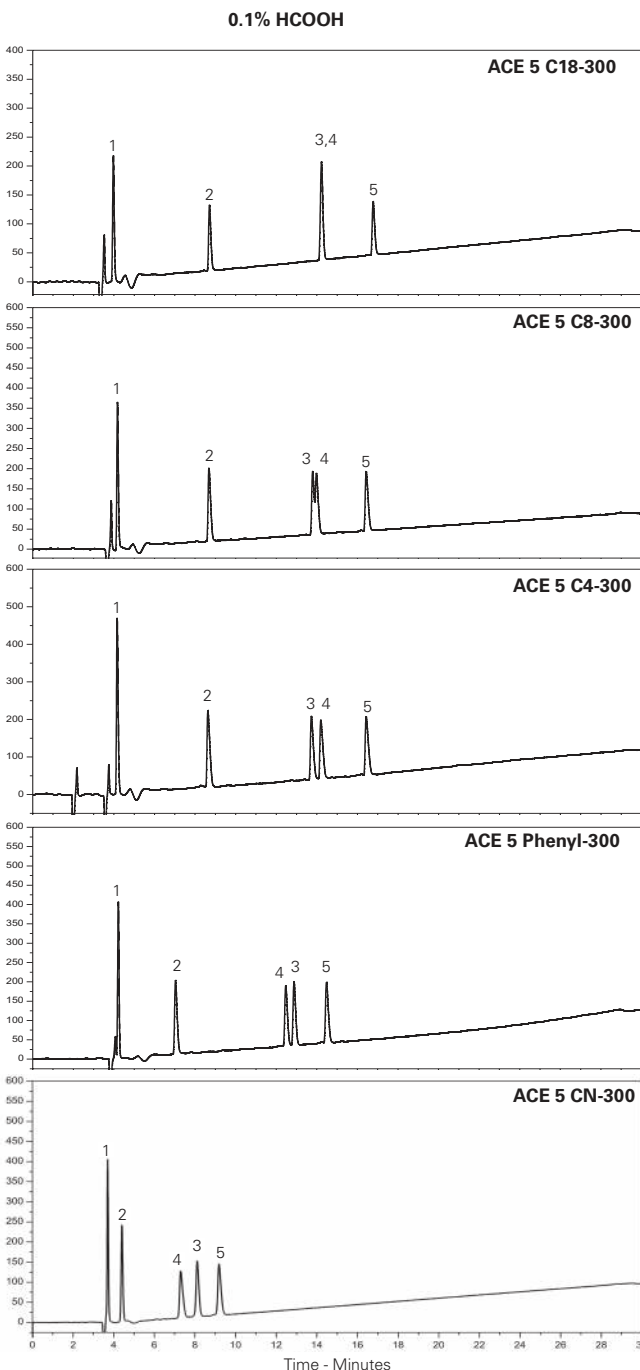
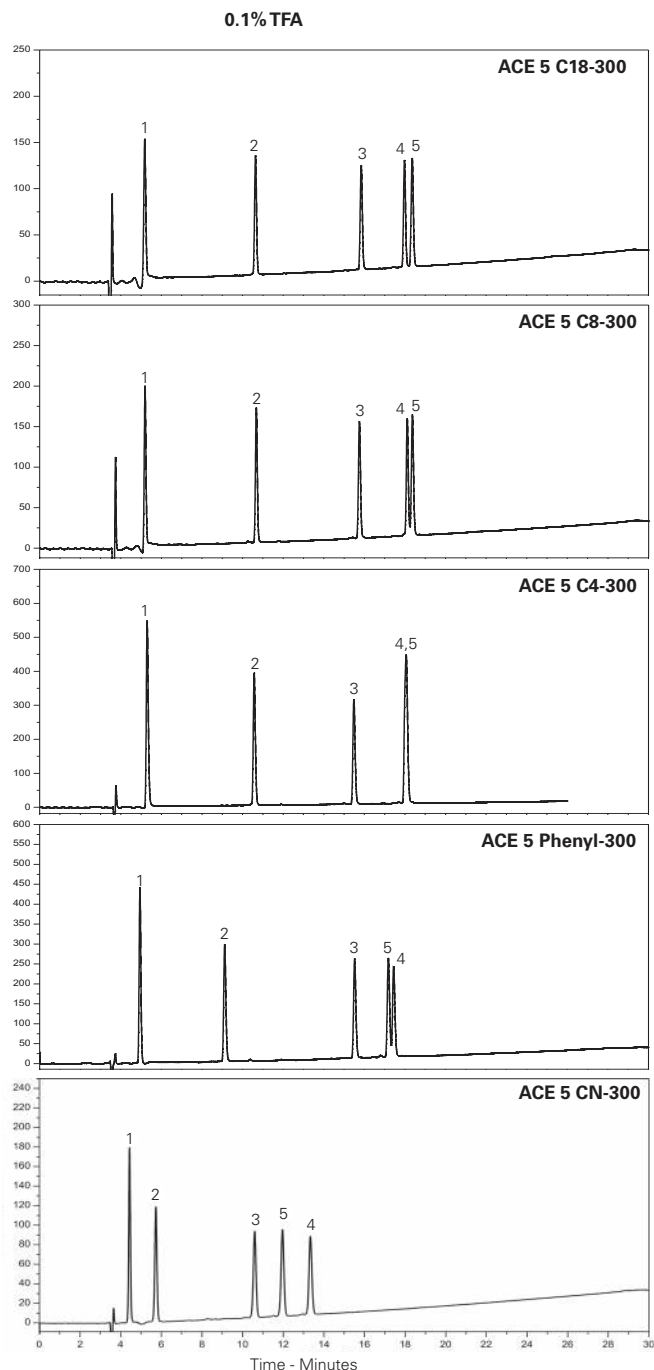
Flow Rate: 1 mL/min

Temperature: Ambient

Detection: UV, 220 nm

Analyses

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



Perfluoro Acids by LC-MS/MS

Application #AN1280

Conditions

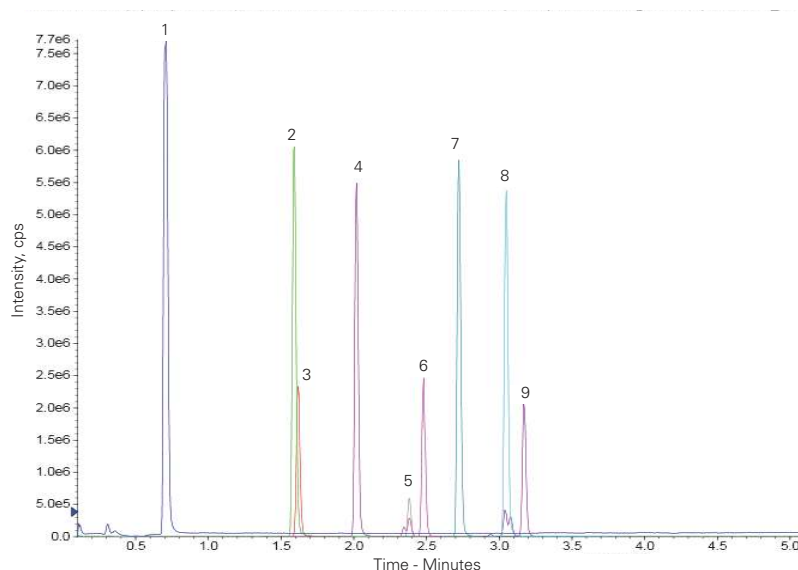
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% acetic acid/MeCN (95:5 v/v)
 B: 2 mM ammonium acetate, 0.1% acetic acid/MeCN (5:95 v/v)
Gradient:

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

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

Analytes

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



Reproduced with permission of Biotage GB Ltd, UK

Perfluoroalkyl Substances by Ion-Pairing LC-MS/MS

Application #AN2560

Conditions

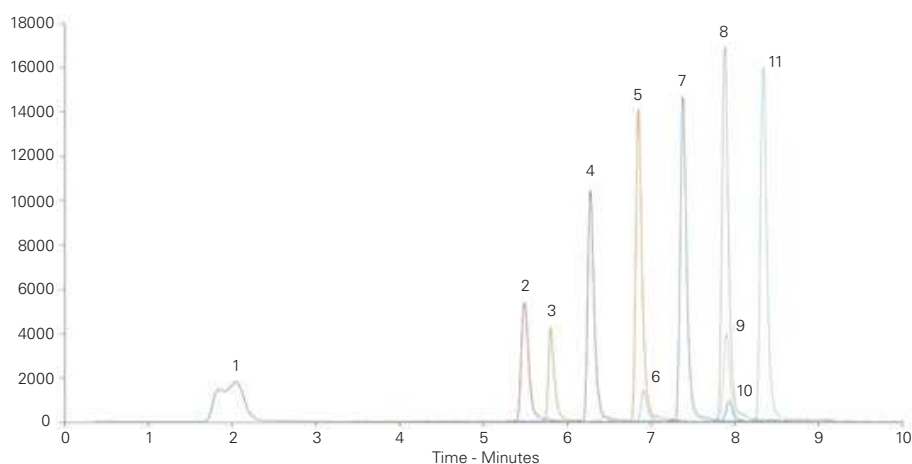
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 2 mM ammonium acetate + 5 mM 1-methylpiperidine in MeOH/H₂O (5:95 v/v)
 B: 2 mM ammonium acetate + 5 mM 1-methylpiperidine in MeOH/H₂O (95:5 v/v)
Gradient:

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

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

Analytes

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



Reproduced with permission of Department of Analytical Chemistry, Faculty of Science and Technology, University of the Basque Country, Spain



Perfluorinated Compounds in Water by LC-MS/MS

Application #AN2260

Conditions

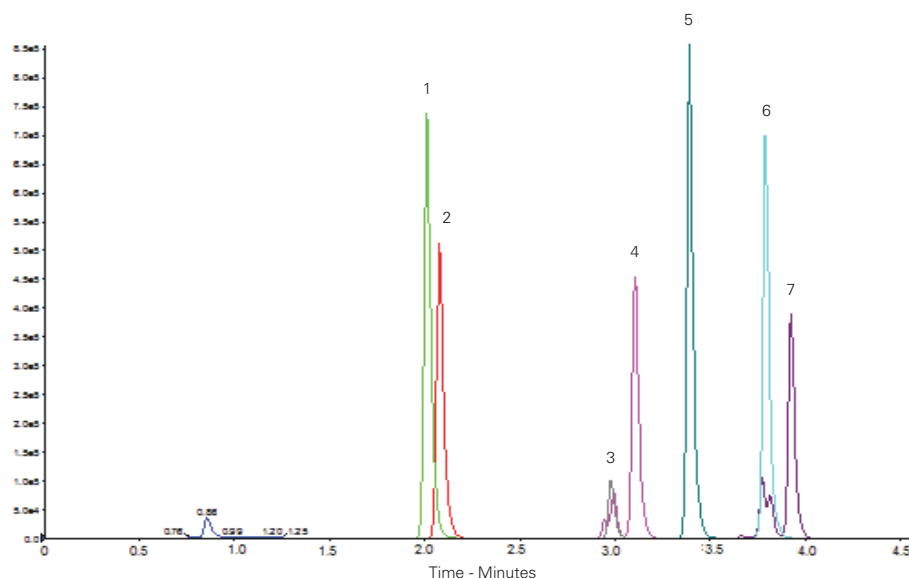
Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O/MeCN (90:10 v/v)
 B: 2 mM ammonium acetate, 0.1% formic acid in H₂O/MeCN (10:90 v/v)
Gradient:

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

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

Analytes

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



Reproduced with permission of Biotage GB Ltd, UK. For extraction conditions see Biotage Application Note AN839

ACE Method Development Kits

Intelligent Solutions for Method Development



- **Highly cost effective** - 2 and 3 column kits available for the same price as a single column
- **4 different Method Development Kits** available in dimensions from microbore (0.5 mm id) through to analytical (4.6 mm id) for rapid, systematic method development.
- Carefully selected ACE phases enabling the power of selectivity to be fully exploited
- Each ACE phase provides different selectivity due to differing interactions

FREE Application Support and FREE Method Development Service
 Learn more: www.ace-hplc.com or email: info@ace-hplc.com



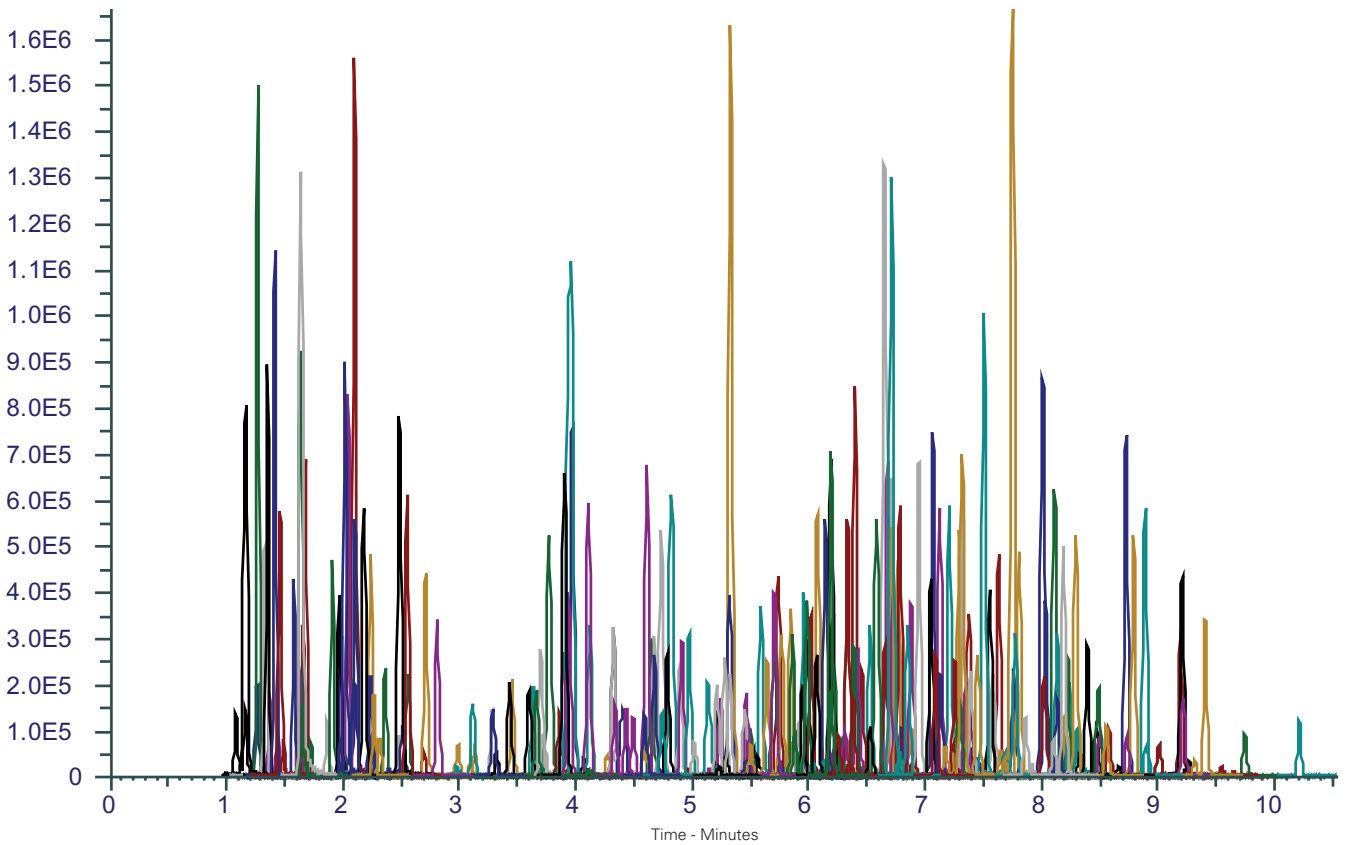
250 Pesticide Screen by LC-MS/MS

Conditions

Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 10 mM ammonium formate + 0.05% formic acid in H₂O
 B: 10 mM ammonium formate + 0.05% formic acid in MeOH
Gradient:

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

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



Reproduced with permission of Centre for Analytical Chemistry, California Department of Food and Agriculture, USA



250 Pesticide Screen by LC-MS/MS

Page 2 of 4

Application #AN3060

| Analyte | R _t (mins) | Adduct | Precursor Ion m/z | Quant Ion m/z | Conf Ion m/z | Analyte | R _t (mins) | Adduct | Precursor Ion m/z | Quant Ion m/z | Conf Ion m/z |
|---------------------|-----------------------|-----------------------------------|-------------------|---------------|--------------|------------------------|-----------------------|---|-------------------|---------------|--------------|
| 3-OH Carbofuran | 2.25 | [M+H] ⁺ | 238.1 | 181.2 | 163.1 | Cyprosulfamide | 3.30 | [M+H] ⁺ | 375.1 | 135.1 | 254.1 |
| 5-OH Thiabendazole | 1.66 | [M+H] ⁺ | 218.0 | 147.2 | 191.1 | Cyromazine | 1.15 | [M+H] ⁺ | 167.1 | 125.2 | 68.2 |
| Abamectin | 9.45 | [M+NH ₄] ⁺ | 890.5 | 305.3 | 567.5 | DEF | 9.20 | [M+H] ⁺ | 315.1 | 169.0 | 113.0 |
| Acephate | 1.26 | [M+H] ⁺ | 184.0 | 143.1 | 125.1 | Demeton-S sulfone | 2.55 | [M+H] ⁺ | 291.1 | 235.1 | 263.1 |
| Acetamiprid | 2.24 | [M+H] ⁺ | 223.1 | 126.1 | 90.1 | Dialifos | 7.46 | [M+H] ⁺ | 394.0 | 208.1 | 181.0 |
| Aldicarb | 2.95 | [M+NH ₄] ⁺ | 208.1 | 116.1 | 89.0 | Diazinon | 7.12 | [M+H] ⁺ | 305.1 | 169.1 | 153.2 |
| Aldicarb sulfone | 1.44 | [M+NH ₄] ⁺ | 240.1 | 148.0 | 86.0 | Diazinon OA | 5.32 | [M+H] ⁺ | 289.1 | 153.2 | 233.1 |
| Aldicarb sulfoxide | 1.37 | [M+NH ₄] ⁺ | 224.1 | 132.0 | 89.1 | Dichlormid | 3.85 | [M+H] ⁺ | 208.0 | 140.0 | 81.2 |
| Allethrin | 8.33 | [M+H] ⁺ | 303.2 | 135.1 | 123.1 | Dichlorvos | 3.63 | [M+H] ⁺ | 221.0 | 109.1 | 127.0 |
| Ametoctradin | 7.64 | [M+H] ⁺ | 276.2 | 149.1 | 176.2 | Dicrotophos | 1.87 | [M+H] ⁺ | 238.1 | 112.2 | 193.1 |
| Atrazine | 4.64 | [M+H] ⁺ | 216.1 | 174.0 | 104.0 | Diethofencarb | 5.53 | [M+H] ⁺ | 268.2 | 124.1 | 180.2 |
| Azinphos ethyl | 6.30 | [M+H] ⁺ | 346.0 | 132.1 | 223.0 | Diflubenzuron | 6.66 | [M+H] ⁺ | 311.0 | 158.0 | 141.0 |
| Azinphos methyl | 5.14 | [M+H] ⁺ | 318.0 | 132.0 | 124.9 | Dimethenamid | 5.70 | [M+H] ⁺ | 276.1 | 244.1 | 168.2 |
| Azinphos methyl OA | 2.98 | [M+H] ⁺ | 302.0 | 132.2 | 160.0 | Dimethoate | 2.23 | [M+H] ⁺ | 230.1 | 199.0 | 125.0 |
| Azoxystrobin | 5.59 | [M+H] ⁺ | 404.1 | 372.1 | 344.1 | Dimethomorph | 5.76, 6.07 | [M+H] ⁺ | 388.1 | 301.0 | 165.1 |
| Bendiocarb | 3.72 | [M+H] ⁺ | 224.1 | 167.1 | 109.1 | Dinotefuran | 1.36 | [M+H] ⁺ | 203.1 | 129.1 | 114.2 |
| Benoxacor | 5.23 | [M+H] ⁺ | 260.1 | 134.1 | 120.1 | Dioxacarb | 2.26 | [M+H] ⁺ | 224.1 | 123.1 | 167.1 |
| Bifenazate | 6.27 | [M+H] ⁺ | 301.1 | 198.0 | 170.1 | Dioxathion | 8.10 | [M-C ₄ H ₁₀ O ₂ PS ₂] ⁺ | 271.1 | 97.0 | 125.0 |
| Bitertanol | 7.41 | [M+H] ⁺ | 338.2 | 269.3 | 99.1 | Disulfoton sulfone | 4.59 | [M+H] ⁺ | 307.0 | 261.1 | 125.0 |
| Boscalid | 5.85 | [M+H] ⁺ | 343.0 | 307.0 | 140.0 | Disulfoton sulfoxide | 4.49 | [M+H] ⁺ | 291.0 | 185.1 | 213.1 |
| Bupirimate | 6.68 | [M+H] ⁺ | 317.2 | 210.2 | 237.3 | Diuron | 4.82 | [M+H] ⁺ | 233.0 | 72.1 | 160.0 |
| Buprofezin | 8.24 | [M+H] ⁺ | 306.1 | 201.1 | 106.1 | DMST | 3.90 | [M+H] ⁺ | 215.1 | 106.1 | 151.0 |
| Cadusafos | 7.58 | [M+H] ⁺ | 271.1 | 159.0 | 131.0 | Dodine | 7.56 | [M+H] ⁺ | 228.3 | 186.3 | 60.1 |
| Carbaryl | 4.07 | [M+NH ₄] ⁺ | 219.1 | 145.1 | 127.0 | Emamectin | 8.57 | [M+H] ⁺ | 886.5 | 158.1 | 126.1 |
| Carbendazim | 2.10 | [M+H] ⁺ | 192.1 | 160.1 | 132.1 | Ethiofencarb | 4.27 | [M+H] ⁺ | 226.1 | 107.1 | 169.1 |
| Carbofuran | 3.77 | [M+H] ⁺ | 222.1 | 165.2 | 123.2 | Ethiofencarb sulfone | 1.90 | [M+NH ₄] ⁺ | 275.1 | 107.1 | 201.1 |
| Carboxin | 3.97 | [M+H] ⁺ | 236.1 | 143.0 | 93.0 | Ethiofencarb sulfoxide | 1.98 | [M+H] ⁺ | 242.1 | 107.1 | 185.0 |
| Carfentrazone ethyl | 6.88 | [M+H] ⁺ | 412.0 | 346.1 | 366.0 | Ethion | 8.31 | [M+H] ⁺ | 385.0 | 199.1 | 143.0 |
| Chlorantraniliprole | 5.24 | [M+H] ⁺ | 484.0 | 286.0 | 194.0 | Ethion monoxon | 6.73 | [M+H] ⁺ | 369.0 | 199.0 | 143.0 |
| Chlorfenvinphos | 7.21 | [M+H] ⁺ | 359.0 | 170.0 | 99.1 | Ethiprole | 5.77 | [M+NH ₄] ⁺ | 413.9 | 351.0 | 255.0 |
| Chlorimuron ethyl | 5.73 | [M+H] ⁺ | 415.1 | 186.0 | 83.0 | Ethofumesate | 5.55 | [M+H] ⁺ | 287.1 | 121.1 | 241.1 |
| Chlorpyrifos | 8.47 | [M+H] ⁺ | 349.9 | 198.0 | 97.0 | Ethoprop | 6.46 | [M+H] ⁺ | 243.1 | 173.0 | 131.0 |
| Chlorpyrifos OA | 6.65 | [M+H] ⁺ | 334.0 | 278.0 | 197.9 | Etofenprox | 9.75 | [M+NH ₄] ⁺ | 394.2 | 177.2 | 107.1 |
| Clethodim | 7.71 | [M+H] ⁺ | 360.3 | 164.1 | 136.1 | Etozazole | 8.73 | [M+H] ⁺ | 360.2 | 141.0 | 304.2 |
| Clofentezine | 7.38 | [M+H] ⁺ | 303.0 | 138.1 | 102.0 | Famoxadone | 7.24 | [M+NH ₄] ⁺ | 392.2 | 331.1 | 238.0 |
| Cloransulam methyl | 4.13 | [M+H] ⁺ | 430.0 | 398.1 | 370.0 | Fenamidone | 5.76 | [M+H] ⁺ | 312.1 | 236.1 | 92.2 |
| Clothianidin | 1.99 | [M+H] ⁺ | 250.0 | 169.1 | 132.0 | Fenamiphos | 6.71 | [M+H] ⁺ | 304.1 | 217.1 | 202.0 |
| Coumaphos | 7.07 | [M+H] ⁺ | 363.0 | 227.1 | 307.1 | Fenamiphos sulfone | 4.10 | [M+H] ⁺ | 336.1 | 266.1 | 188.1 |
| Crotoxyphos | 5.86 | [M+NH ₄] ⁺ | 332.1 | 127.1 | 193.1 | Fenamiphos sulfoxide | 3.96 | [M+H] ⁺ | 320.1 | 233.1 | 171.1 |
| Crufomate | 6.77 | [M+H] ⁺ | 292.1 | 236.1 | 108.1 | Fenazaquin | 9.21 | [M+H] ⁺ | 307.2 | 161.2 | 57.2 |
| Cyantraniliprole | 4.33 | [M+2+H] ⁺ | 475.0 | 286.0 | 444.1 | Fenhexamid | 6.39 | [M+H] ⁺ | 302.1 | 178.0 | 97.2 |
| Cyazofamid | 6.52 | [M+H] ⁺ | 325.1 | 108.1 | 261.2 | Fenobucarb | 5.49 | [M+H] ⁺ | 208.1 | 95.0 | 152.0 |
| Cyflufenamid | 7.42 | [M+H] ⁺ | 413.1 | 295.1 | 203.0 | Fenoxaprop ethyl | 8.04 | [M+H] ⁺ | 362.1 | 288.1 | 91.1 |
| Cymoxanil | 2.48 | [M+H] ⁺ | 199.1 | 128.1 | 111.1 | Fenoxycarb | 6.80 | [M+H] ⁺ | 302.1 | 88.1 | 116.1 |
| Cyphenothrin | 9.27 | [M+NH ₄] ⁺ | 393.2 | 151.2 | 123.2 | Fenpropimorph | 6.42 | [M+H] ⁺ | 304.3 | 147.2 | 119.1 |





250 Pesticide Screen by LC-MS/MS Page 3 of 4
Application #AN3060

| Analyte | R _t (mins) | Adduct | Precursor Ion m/z | Quant Ion m/z | Conf Ion m/z | Analyte | R _t (mins) | Adduct | Precursor Ion m/z | Quant Ion m/z | Conf Ion m/z |
|--------------------|-----------------------|-----------------------------------|-------------------|---------------|--------------|---------------------------|-----------------------|-----------------------------------|-------------------|---------------|--------------|
| Fenpyroximate | 8.90 | [M+H] ⁺ | 422.2 | 366.1 | 214.2 | Mepanipyrim | 6.21 | [M+H] ⁺ | 224.1 | 106.2 | 77.1 |
| Fensulfothion | 4.89 | [M+H] ⁺ | 309.0 | 235.0 | 281.1 | Mesotrione | 2.01 | [M+H] ⁺ | 340.1 | 228.1 | 104.1 |
| Fenuron | 2.17 | [M+H] ⁺ | 165.1 | 72.1 | 77.1 | Metaflumizone | 8.30 | [M+H] ⁺ | 507.1 | 178.0 | 287.1 |
| Flonicamid | 1.66 | [M+H] ⁺ | 230.1 | 203.0 | 98.0 | Metalaxyl | 4.91 | [M+H] ⁺ | 280.1 | 220.1 | 192.1 |
| Fluazifop-p-butyl | 8.12 | [M+H] ⁺ | 384.1 | 282.2 | 328.2 | Metaldehyde | 2.02 | [M+NH ₄] ⁺ | 194.1 | 62.2 | 45.3 |
| Fludioxonil | 5.76 | [M+NH ₄] ⁺ | 266.1 | 158.1 | 131.0 | Metconazole | 7.32 | [M+H] ⁺ | 320.2 | 70.1 | 125.0 |
| Flufenoxuron | 8.79 | [M+H] ⁺ | 489.0 | 158.1 | 141.1 | Methamidophos | 1.16 | [M+H] ⁺ | 142.0 | 94.2 | 125.1 |
| Flufenpyr ethyl | 6.72 | [M+H] ⁺ | 409.1 | 335.0 | 307.0 | Methidathion | 4.97 | [M+NH ₄] ⁺ | 320.0 | 145.1 | 85.1 |
| Flumetsulam | 2.03 | [M+H] ⁺ | 326.1 | 129.1 | 109.0 | Methiocarb | 5.64 | [M+H] ⁺ | 226.1 | 169.2 | 121.1 |
| Flumiclorac pentyl | 8.13 | [M+NH ₄] ⁺ | 441.1 | 308.1 | 354.1 | Methiocarb sulfone | 2.35 | [M+NH ₄] ⁺ | 275.0 | 122.1 | 201.1 |
| Fluometuron | 4.31 | [M+H] ⁺ | 233.1 | 72.2 | 46.3 | Methiocarb sulfoxide | 2.10 | [M+H] ⁺ | 242.1 | 185.1 | 122.1 |
| Fluopicolide | 6.00 | [M+H] ⁺ | 383.0 | 173.0 | 145.0 | Methomyl | 1.61 | [M+H] ⁺ | 163.1 | 106.1 | 88.1 |
| Fluopyram | 6.33 | [M+H] ⁺ | 397.1 | 173.0 | 208.0 | Methoxyfenozide | 6.04 | [M+H] ⁺ | 369.2 | 149.1 | 313.1 |
| Fluoxastrobin | 6.40 | [M+H] ⁺ | 459.1 | 427.2 | 188.1 | Metolcarb | 3.28 | [M+H] ⁺ | 166.1 | 109.1 | 94.1 |
| Fluridone | 5.32 | [M+H] ⁺ | 330.1 | 309.1 | 290.0 | Metribuzin | 3.59 | [M+H] ⁺ | 215.1 | 187.1 | 131.1 |
| Flusilazole | 6.77 | [M+H] ⁺ | 316.1 | 247.2 | 165.1 | Mevinphos | 2.70 | [M+NH ₄] ⁺ | 242.1 | 193.1 | 127.1 |
| Fluthiacet methyl | 6.88 | [M+H] ⁺ | 404.0 | 344.0 | 273.9 | Monocrotophos | 1.71 | [M+H] ⁺ | 224.1 | 193.0 | 127.0 |
| Flutolanil | 5.95 | [M+H] ⁺ | 324.1 | 262.0 | 282.0 | Monolinuron | 4.16 | [M+H] ⁺ | 215.1 | 126.1 | 148.1 |
| Flutriafol | 4.74 | [M+H] ⁺ | 302.1 | 70.1 | 123.1 | Myclobutanil | 6.15 | [M+H] ⁺ | 289.1 | 125.0 | 70.1 |
| Fluxapyroxad | 6.02 | [M+H] ⁺ | 382.1 | 342.1 | 314.1 | Nicosulfuron | 3.45 | [M+H] ⁺ | 411.1 | 182.0 | 213.0 |
| Forchlorfenuron | 4.78 | [M+H] ⁺ | 248.1 | 129.1 | 93.1 | Norflurazon | 4.98 | [M+H] ⁺ | 304.0 | 160.0 | 140.0 |
| Formetanate HCl | 1.26 | [M+H] ⁺ | 222.0 | 165.1 | 120.0 | Norflurazon desmethyl | 4.43 | [M+H] ⁺ | 290.0 | 179.0 | 140.0 |
| Fosthiazate | 4.40 | [M+H] ⁺ | 284.1 | 104.1 | 228.1 | Omethoate | 1.33 | [M+H] ⁺ | 214.0 | 183.0 | 125.0 |
| Hexaconazole | 7.29 | [M+H] ⁺ | 314.1 | 158.9 | 70.0 | Oxamyl | 1.48 | [M+NH ₄] ⁺ | 237.1 | 72.0 | 90.0 |
| Hexythiazox | 8.51 | [M+H] ⁺ | 353.1 | 228.0 | 168.0 | Oxamyl oxime | 1.34 | [M+H] ⁺ | 163.1 | 72.1 | 90.1 |
| Imazalil | 5.14 | [M+H] ⁺ | 297.1 | 159.1 | 255.1 | Oxydemeton methyl | 1.57 | [M+H] ⁺ | 247.0 | 169.1 | 109.1 |
| Imazosulfuron | 5.28 | [M+H] ⁺ | 413.0 | 153.0 | 156.1 | Oxydemeton methyl sulfone | 1.62 | [M+H] ⁺ | 263.0 | 169.0 | 109.0 |
| Imidacloprid | 1.96 | [M+H] ⁺ | 256.1 | 209.1 | 175.0 | Parathion methyl OA | 3.10 | [M+H] ⁺ | 248.0 | 202.0 | 109.1 |
| Imiprothrin | 6.34 | [M+H] ⁺ | 319.2 | 151.1 | 123.1 | Parathion OA | 4.61 | [M+H] ⁺ | 276.1 | 220.1 | 248.1 |
| Indaziflam | 6.58 | [M+H] ⁺ | 302.2 | 158.1 | 145.1 | Pencycuron | 7.50 | [M+H] ⁺ | 329.1 | 125.1 | 89.1 |
| Indoxacarb | 7.75 | [M+H] ⁺ | 528.1 | 249.0 | 150.1 | Penflufen | 6.95 | [M+H] ⁺ | 318.2 | 234.1 | 141.0 |
| Ipconazole | 7.81 | [M+H] ⁺ | 334.2 | 70.1 | 125.0 | Penthiopyrad | 7.05 | [M+H] ⁺ | 360.1 | 177.1 | 276.1 |
| Iprovalicarb | 6.31 | [M+H] ⁺ | 321.2 | 119.1 | 186.2 | Phenothrin | 9.56 | [M+H] ⁺ | 351.2 | 183.1 | 168.0 |
| Isofenphos | 7.39 | [M+H] ⁺ | 346.1 | 217.0 | 245.1 | Phenthoate | 6.81 | [M+H] ⁺ | 321.0 | 247.1 | 79.1 |
| Isoprocarb | 4.67 | [M+H] ⁺ | 194.1 | 95.1 | 152.2 | Phorate OA | 5.10 | [M+H] ⁺ | 245.0 | 75.2 | 47.2 |
| Isoproturon | 4.79 | [M+H] ⁺ | 207.2 | 72.2 | 165.2 | Phorate OA Sulfone | 2.51 | [M+H] ⁺ | 277.0 | 155.0 | 127.0 |
| Kresoxim methyl | 6.90 | [M+H] ⁺ | 314.1 | 267.2 | 222.1 | Phorate OA Sulfoxide | 2.31 | [M+H] ⁺ | 261.0 | 153.0 | 81.0 |
| Lactofen | 8.22 | [M+NH ₄] ⁺ | 479.1 | 344.1 | 223.0 | Phorate Sulfone | 4.61 | [M+H] ⁺ | 293.0 | 114.9 | 171.0 |
| Lenacil | 4.67 | [M+H] ⁺ | 235.1 | 153.1 | 136.1 | Phorate Sulfoxide | 4.49 | [M+H] ⁺ | 277.0 | 170.9 | 199.0 |
| Leptophos OA | 7.75 | [M+2+H] ⁺ | 396.9 | 155.1 | 364.9 | Phosalone | 7.35 | [M+H] ⁺ | 368.0 | 182.0 | 111.1 |
| Linuron | 5.46 | [M+H] ⁺ | 249.0 | 182.1 | 160.1 | Phosmet | 5.21 | [M+H] ⁺ | 318.0 | 160.1 | 133.1 |
| Malathion | 5.92 | [M+H] ⁺ | 331.0 | 127.1 | 285.1 | Phosmet OA | 3.12 | [M+H] ⁺ | 302.0 | 160.0 | 133.0 |
| Malathion OA | 3.89 | [M+H] ⁺ | 315.1 | 127.1 | 99.0 | Phosphamidon | 3.43 | [M+H] ⁺ | 300.1 | 127.1 | 174.1 |
| Mandipropamid | 5.94 | [M+H] ⁺ | 412.1 | 328.2 | 356.2 | Phoxim | 7.25 | [M+H] ⁺ | 299.1 | 77.2 | 129.1 |
| Mefenpyr diethyl | 7.26 | [M+H] ⁺ | 373.1 | 327.1 | 160.0 | Picoxystrobin | 6.79 | [M+H] ⁺ | 368.1 | 145.0 | 115.0 |



250 Pesticide Screen by LC-MS/MS

Page 4 of 4

Application #AN3060

| Analyte | R _t (mins) | Adduct | Precursor Ion m/z | Quant Ion m/z | Conf Ion m/z | Analyte | R _t (mins) | Adduct | Precursor Ion m/z | Quant Ion m/z | Conf Ion m/z |
|----------------------|--------------------------|-----------------------------------|----------------------|------------------|-----------------|-----------------------|--------------------------|-----------------------------------|----------------------|------------------|-----------------|
| Pirimicarb | 4.24 | [M+H] ⁺ | 239.2 | 182.1 | 72.0 | Spiromesifen | 8.66 | [M+NH ₄] ⁺ | 388.1 | 273.1 | 187.0 |
| Pirimicarb Desmethyl | 2.71 | [M+H] ⁺ | 225.1 | 168.2 | 72.1 | Spiromesifen Alcohol | 5.01 | [M+H] ⁺ | 273.2 | 187.1 | 179.1 |
| Pirimiphos Methyl | 7.34 | [M+H] ⁺ | 306.1 | 164.2 | 108.1 | Spirotetramat | 6.38 | [M+H] ⁺ | 374.2 | 302.3 | 216.2 |
| Prallethrin | 7.69 | [M+H] ⁺ | 301.2 | 133.0 | 151.2 | Spiroxamine | 5.95 | [M+H] ⁺ | 298.3 | 144.2 | 100.2 |
| Prochloraz | 7.39 | [M+H] ⁺ | 376.0 | 308.1 | 70.1 | Sulfoxaflo | 2.39 | [M+NH ₄] ⁺ | 295.2 | 174.1 | 154.1 |
| Profoxydim | 7.71, 9.00 | [M+H] ⁺ | 466.2 | 280.0 | 180.0 | Sulprofos | 8.56 | [M+H] ⁺ | 323.0 | 219.1 | 139.1 |
| Promecarb | 5.88 | [M+H] ⁺ | 208.1 | 109.0 | 151.1 | TCMTB | 5.48 | [M+H] ⁺ | 239.0 | 180.0 | 136.0 |
| Propamocarb | 1.41 | [M+H] ⁺ | 189.1 | 102.0 | 144.0 | Tebufenozide | 6.78 | [M+H] ⁺ | 353.2 | 133.0 | 104.8 |
| Propaquizafop | 8.21 | [M+H] ⁺ | 444.1 | 299.2 | 371.2 | Tebufenpyrad | 8.19 | [M+H] ⁺ | 334.2 | 117.1 | 145.1 |
| Propargite | 8.74 | [M+NH ₄] ⁺ | 368.2 | 231.2 | 175.1 | Tebuthiuron | 3.89 | [M+H] ⁺ | 229.1 | 172.0 | 116.0 |
| Propetamphos | 6.13 | [M+H] ⁺ | 282.1 | 138.1 | 156.1 | Tepraloxymid | 4.10, 6.19 | [M+H] ⁺ | 342.2 | 250.1 | 166.1 |
| Propoxur(S) | 3.69 | [M+H] ⁺ | 210.1 | 168.2 | 111.1 | Terbufos Sulfone | 5.46 | [M+H] ⁺ | 321.0 | 115.0 | 143.0 |
| Prosulfuron | 5.29 | [M+H] ⁺ | 420.1 | 167.1 | 141.1 | Terbufos Sulfoxide | 5.49 | [M+H] ⁺ | 305.1 | 97.0 | 187.0 |
| Pymetrozine | 1.44 | [M+H] ⁺ | 218.1 | 105.1 | 78.1 | Terbutylazine | 5.71 | [M+H] ⁺ | 230.1 | 174.1 | 104.1 |
| Pyraclostrobin | 7.30 | [M+H] ⁺ | 388.1 | 163.1 | 194.1 | Tetrachlorvinphos | 6.86 | [M+2+H] ⁺ | 366.9 | 127.1 | 206.0 |
| Pyraflufen Ethyl | 7.13 | [M+H] ⁺ | 413.0 | 339.0 | 253.1 | Tetramethrin | 7.91, 8.10 | [M+H] ⁺ | 332.2 | 164.1 | 135.1 |
| Pyrazophos | 7.31 | [M+H] ⁺ | 374.1 | 222.2 | 194.1 | Thiabendazole | 2.48 | [M+H] ⁺ | 202.0 | 175.0 | 131.1 |
| Pyridaben | 9.22 | [M+H] ⁺ | 365.1 | 309.0 | 147.1 | Thiacloprid | 2.55 | [M+H] ⁺ | 253.0 | 126.1 | 99.1 |
| Pyridalyl | 10.21 | [M+2+H] ⁺ | 492.0 | 110.9 | 164.0 | Thiamethoxam | 1.65 | [M+H] ⁺ | 292.0 | 211.1 | 181.1 |
| Pyrimethanil | 5.45 | [M+H] ⁺ | 200.1 | 107.1 | 168.1 | Thifensulfuron Methyl | 3.28 | [M+H] ⁺ | 388.0 | 167.1 | 205.0 |
| Pyriproxyfen | 8.39 | [M+H] ⁺ | 322.1 | 96.0 | 227.1 | Thiobencarb | 7.46 | [M+H] ⁺ | 258.1 | 125.0 | 89.0 |
| Quinalphos | 6.78 | [M+H] ⁺ | 299.1 | 163.1 | 147.1 | Thiodicarb | 4.34 | [M+H] ⁺ | 355.1 | 163.2 | 88.1 |
| Quinoxifen | 8.50 | [M+H] ⁺ | 308.0 | 197.1 | 214.1 | Thionazin | 4.74 | [M+H] ⁺ | 249.1 | 193.1 | 97.0 |
| Quizalofop Ethyl | 8.01 | [M+H] ⁺ | 373.1 | 299.2 | 255.1 | Topramezone | 1.63 | [M+H] ⁺ | 364.1 | 334.1 | 125.1 |
| Resmethrin | 9.40 | [M+H] ⁺ | 339.2 | 128.1 | 171.1 | Triadimefon | 6.07 | [M+H] ⁺ | 294.1 | 197.0 | 225.0 |
| Rimsulfuron | 3.94 | [M+H] ⁺ | 432.1 | 182.1 | 139.0 | Triadimenol | 6.25 | [M+H] ⁺ | 296.1 | 70.2 | 99.0 |
| Rotenone | 6.71 | [M+H] ⁺ | 395.2 | 213.2 | 192.1 | Triazophos | 6.19 | [M+H] ⁺ | 314.1 | 162.1 | 119.1 |
| Saflufenacil | 5.32 | [M+H] ⁺ | 501.1 | 349.1 | 198.0 | Tribenuron Methyl | 4.59 | [M+H] ⁺ | 396.1 | 155.1 | 181.1 |
| Sedaxane | 6.20, 6.54 | [M+H] ⁺ | 332.2 | 159.0 | 139.0 | Trichlorfon | 2.26 | [M+H] ⁺ | 256.9 | 109.0 | 221.0 |
| Sethoxydim | 8.03 | [M+H] ⁺ | 328.2 | 178.0 | 220.1 | Tricyclazole | 2.80 | [M+H] ⁺ | 190.0 | 163.1 | 136.1 |
| Simazine | 3.66 | [M+H] ⁺ | 202.1 | 104.1 | 132.1 | Trifloxystrobin | 7.78 | [M+H] ⁺ | 409.1 | 186.2 | 206.2 |
| Spinetoram | 8.14 | [M+H] ⁺ | 748.5 | 142.1 | 203.1 | Triflumizole | 7.87 | [M+H] ⁺ | 346.1 | 278.0 | 73.0 |
| Spinosad A | 7.69 | [M+H] ⁺ | 732.5 | 142.1 | 98.0 | Triforine | 5.23 | [M+2+H] ⁺ | 434.9 | 213.0 | 98.2 |
| Spinosad D | 8.10 | [M+H] ⁺ | 746.5 | 142.1 | 98.0 | Zoxamide | 7.09 | [M+H] ⁺ | 336.0 | 187.0 | 159.0 |
| Spirodiclofen | 8.91 | [M+H] ⁺ | 411.1 | 313.1 | 71.1 | | | | | | |

300 Pesticide Screen by LC-MS/MS

Page 1 of 5

Application #AN3120

Conditions

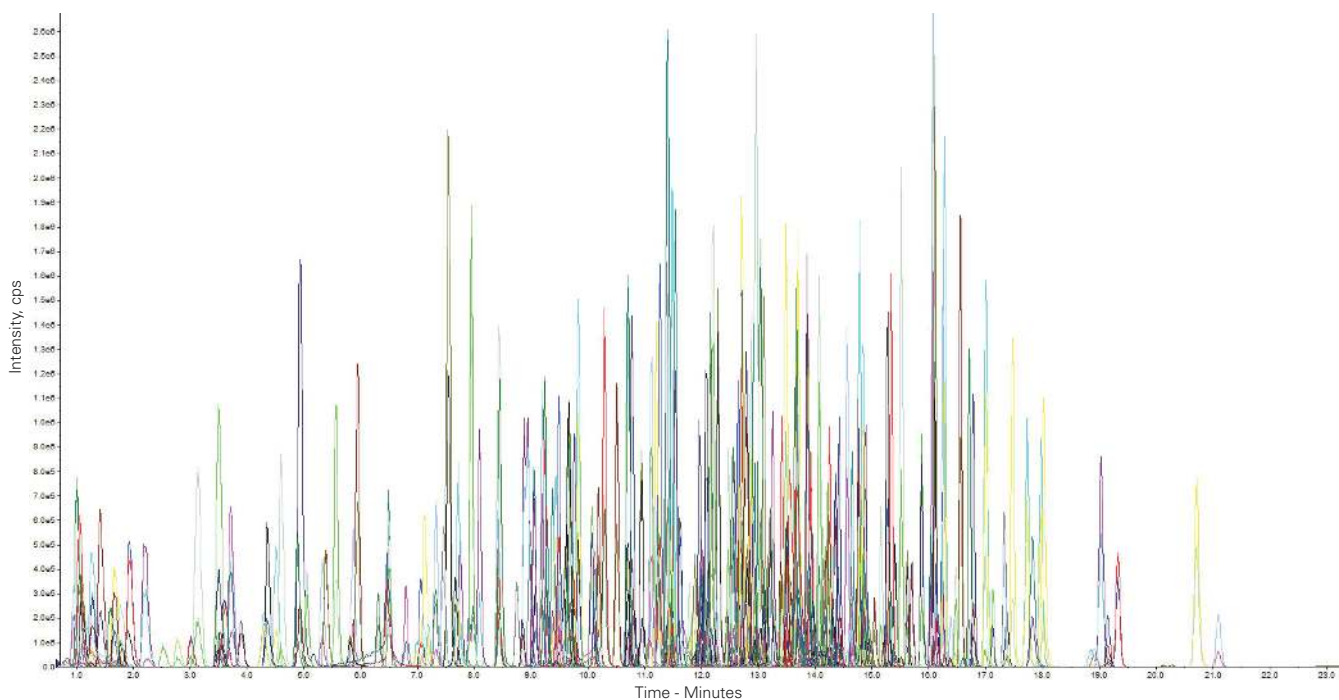
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 5 mM ammonium formate in H₂O/MeOH (9:1 v/v)
 B: 5 mM ammonium formate in H₂O/MeOH (1:9 v/v)

| Gradient: | Time (mins) | %B |
|-----------|-------------|-----|
| | 0.0 | 30 |
| | 0.5 | 30 |
| | 15.0 | 100 |
| | 22.0 | 100 |
| | 22.1 | 30 |
| | 27.0 | 30 |

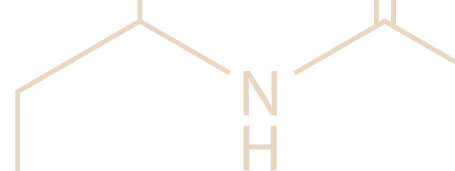
Flow Rate: 0.3 mL/min**Injection:** 6 µL**Temperature:** 24 °C

Detection: AB SCIEX 4000 QTRAP
 TurbolonSpray ESI positive mode
 Capillary voltage: 5000 V
 Heater gas temperature: 450 °C

Sample: Sample prepared using QuEChERS methodology
 Method validated using cucumber matrix spiked at
 0.01 mg/kg. 265 analytes successfully validated
 (Analytes in black)



Reproduced with permission of National Food Chain Safety Office, Directorate of Plant Protection, Soil Conservation and Agri-Environment, Hungary



300 Pesticide Screen by LC-MS/MS

Page 2 of 5

Application #AN3120


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

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





300 Pesticide Screen by LC-MS/MS

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



300 Pesticide Screen by LC-MS/MS

Page 4 of 5

Application #AN3120

| Analyte | Retention Time (mins) | MRM transitions (m/z) |
|---|-----------------------|------------------------------|
| Mevinfos A | 4.9 | 225.0 → 193.0, 225.0 → 127.0 |
| Mevinfos B | 3.4 | 225.0 → 193.0, 225.0 → 127.0 |
| Molinate | 12.0 | 188.2 → 126.2, 188.2 → 55.1 |
| Monocrotofos | 1.8 | 224.2 → 192.9, 224.2 → 126.9 |
| Monolinuron | 8.7 | 215.1 → 126.1, 215.1 → 148.1 |
| Myclobutanil | 12.2 | 289.2 → 70.0, 289.2 → 125.0 |
| Napropamide | 12.9 | 272.2 → 129.1, 272.2 → 171.1 |
| Nitenpyram | 1.3 | 271.1 → 189.2, 271.1 → 126.0 |
| Novaluron | 15.6 | 493.0 → 158.1, 493.0 → 141.1 |
| Nuarimol | 11.2 | 315.0 → 252.0, 315.0 → 81.0 |
| Ofurace | 7.6 | 282.0 → 160.1, 282.0 → 236.3 |
| Omethoate | 1.0 | 214.0 → 183.0, 214.0 → 125.0 |
| Oxadiazon | 16.2 | 345.0 → 220.0, 345.0 → 303.0 |
| Oxadixyl | 6.4 | 279.0 → 219.0, 279.0 → 133.0 |
| Oxamyl NH ₄ ⁺ | 1.2 | 237.1 → 72.0, 220.2 → 72.0 |
| Oxycarboxin | 4.5 | 268.1 → 174.9, 268.1 → 147.0 |
| Oxydemeton-methyl | 1.4 | 247.0 → 108.9, 247.0 → 168.9 |
| Paclobutrazol | 11.8 | 294.0 → 70.0, 294.0 → 125.0 |
| Paraoxon | 9.4 | 275.9 → 219.9, 275.9 → 248.0 |
| Paraoxon-methyl | 6.1 | 248.1 → 202.1, 248.1 → 90.0 |
| Parathion | 13.8 | 292.0 → 236.0, 292.0 → 264.1 |
| Penconazole | 13.7 | 248.1 → 70.0, 284.1 → 159.0 |
| Pencycuron | 14.8 | 329.3 → 125.1, 331.3 → 127.0 |
| Pendimethalin | 16.9 | 282.2 → 212.1, 282.2 → 194.1 |
| Pethoxamid | 12.7 | 296.2 → 131.0, 296.2 → 250.0 |
| Phenmedipham | 10.8 | 301.2 → 168.0, 301.2 → 136.0 |
| Phenthoate | 13.9 | 321.0 → 247.0, 321.0 → 275.1 |
| Phorate sulfone | 9.6 | 293.0 → 170.8, 293.0 → 96.7 |
| Phorate sulfoxide | 9.2 | 277.0 → 199.0, 277.0 → 171.0 |
| Phosalone | 14.6 | 368.0 → 182.0, 369.9 → 183.9 |
| Phosphamidon | 6.4 | 300.2 → 127.1, 300.2 → 226.8 |
| Phoxim | 14.7 | 299.2 → 129.2, 299.2 → 77.1 |
| Picloram | 1.2 | 243.0 → 224.9, 241.0 → 222.9 |
| Picolinafen | 16.2 | 377.1 → 238.0, 377.1 → 359.0 |
| Picoxystrobin | 13.6 | 368.0 → 205.0, 368.0 → 145.0 |
| Piperonyl butoxide | 16.2 | 356.2 → 177.2, 356.2 → 119.0 |
| Pirimicarb | 9.0 | 239.2 → 72.0, 239.2 → 182.3 |
| Pirimiphos-ethyl | 16.3 | 334.1 → 198.0, 334.1 → 182.3 |
| Pirimiphos-methyl | 14.8 | 306.2 → 108.0, 306.2 → 164.3 |
| Prochloraz | 14.4 | 376.0 → 308.0, 376.0 → 70.0 |
| Profenofos | 15.6 | 375.0 → 304.9, 373.0 → 302.9 |
| Prometryn | 12.6 | 242.2 → 158.1, 242.2 → 200.0 |
| Propachlor | 9.6 | 212.0 → 170.0, 212.0 → 94.1 |
| Propamocarb | 1.1 | 189.0 → 102.0, 189.0 → 144.0 |
| Propaquizafop | 16.0 | 444.2 → 100.0, 444.2 → 371.0 |
| Propargite NH ₄ ⁺ | 17.0 | 368.2 → 231.1, 368.2 → 175.0 |

| Analyte | Retention Time (mins) | MRM transitions (m/z) |
|--------------------------------------|-----------------------|------------------------------|
| Propazine | 11.0 | 230.2 → 188.1, 230.2 → 146.1 |
| Propetamfos | 12.4 | 282.1 → 138.0, 282.1 → 156.1 |
| Propham | 9.4 | 180.1 → 138.1, 180.1 → 120.1 |
| Propiconazole | 14.0 | 342.1 → 159.0, 342.1 → 69.0 |
| Propisochlor | 14.0 | 284.2 → 224.0, 284.2 → 148.0 |
| Propoxur | 7.2 | 210.1 → 111.1, 210.1 → 168.0 |
| Propyzamide | 11.9 | 256.1 → 190.0, 256.1 → 173.0 |
| Proquinazid | 17.7 | 373.2 → 330.9, 373.2 → 289.0 |
| Prosulfocarb | 15.5 | 252.2 → 91.0, 252.2 → 128.1 |
| Prosulfuron | 9.0 | 420.1 → 141.0, 420.1 → 167.1 |
| Prothioconazole | 14.1 | 344.1 → 326.0, 346.1 → 328.1 |
| Prothioconazole-desthio | 13.0 | 312.0 → 70.0, 312.0 → 125.0 |
| Pymetrozine | 1.5 | 218.0 → 105.0, 218.0 → 78.0 |
| Pyraclostrobin | 14.5 | 388.1 → 194.0, 388.1 → 163.0 |
| Pyrazophos | 14.8 | 374.0 → 222.0, 374.0 → 194.0 |
| Pyridaben | 18.0 | 365.0 → 309.0, 365.0 → 147.0 |
| Pyridapenthion | 12.4 | 341.0 → 189.0, 341.0 → 205.0 |
| Pyridate | 19.1 | 379.1 → 206.9, 379.1 → 350.9 |
| Pyrifenoxy | 13.0 | 295.1 → 93.0, 297.1 → 93.0 |
| Pyrimethanil | 11.3 | 200.0 → 82.0, 200.0 → 107.0 |
| Pyriproxyfen | 16.7 | 322.0 → 96.0, 322.0 → 185.0 |
| Pyroxsulam | 5.6 | 435.0 → 195.1, 435.0 → 194.0 |
| Quinalfos | 13.9 | 299.0 → 271.0, 299.0 → 243.0 |
| Quinoclamine | 6.8 | 208.0 → 105.0, 208.0 → 77.0 |
| Quinoxyfen | 16.4 | 308.0 → 197.0, 308.0 → 162.0 |
| Rotenone | 13.4 | 395.1 → 213.1, 395.1 → 192.0 |
| Secbumeton | 10.6 | 226.2 → 170.1, 226.2 → 100.0 |
| Silthiofam | 13.5 | 268.0 → 252.0, 268.0 → 73.0 |
| Simazine | 7.2 | 202.2 → 132.1, 202.2 → 104.0 |
| Simetryn | 9.4 | 214.1 → 124.1, 214.1 → 144.0 |
| Spinosyn A | 17.3 | 732.5 → 142.0, 732.5 → 98.0 |
| Spinosyn D | 18.3 | 746.5 → 142.0, 746.5 → 98.0 |
| Spirodiclofen | 17.4 | 313.1 → 295.0, 313.1 → 213.0 |
| Spiromesifen | 16.8 | 371.2 → 273.1, 371.2 → 255.2 |
| Spirotetramat | 12.8 | 374.2 → 302.2, 374.2 → 330.2 |
| Spiroxamine | 13.3 | 298.3 → 100.1, 298.3 → 144.1 |
| Sulfotep | 14.0 | 323.0 → 97.0, 323.0 → 115.0 |
| Tau-fluvalinate | 18.9 | 503.0 → 208.0, 503.0 → 181.0 |
| Tebuconazole | 13.9 | 308.1 → 70.0, 308.1 → 125.0 |
| Tebufenozide | 13.5 | 353.2 → 297.2, 353.2 → 133.0 |
| Tebufenpyrad | 15.9 | 334.0 → 145.0, 334.0 → 117.0 |
| Teflubenzuron | 16.3 | 381.1 → 158.2, 381.1 → 141.2 |
| Tembotrione (NH ₄ adduct) | 5.9 | 458.0 → 340.9, 458.0 → 441.0 |
| Terbufos | 16.1 | 289.1 → 103.1, 289.1 → 232.9 |
| Terbufos sulfone | 11.1 | 321.1 → 171.0, 321.1 → 115.0 |
| Terbufos sulfoxide | 11.0 | 305.1 → 187.2, 305.1 → 131.1 |



300 Pesticide Screen by LC-MS/MS

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

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





Pesticides by LC-MS/MS

Application #AN1290

Conditions

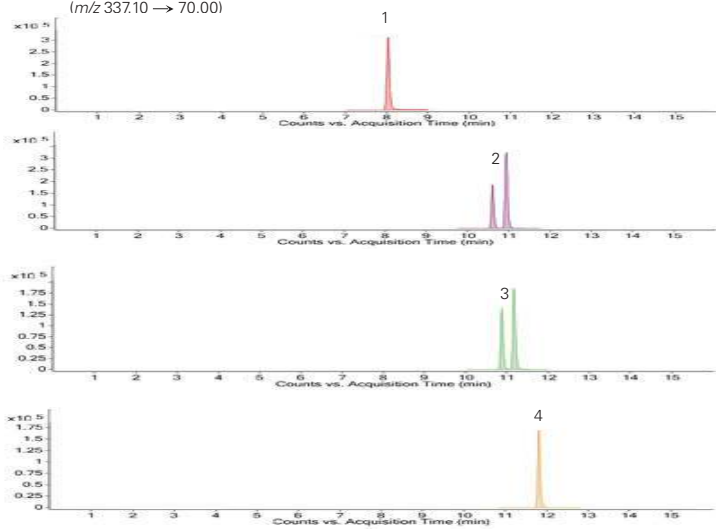
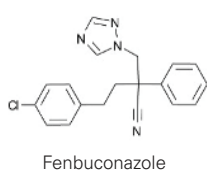
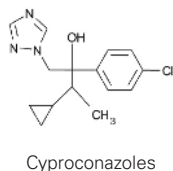
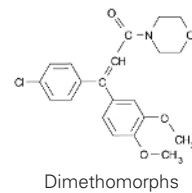
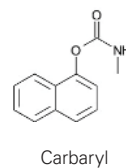
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 0.1% formic acid + 5 mM ammonium formate in H₂O/MeOH (90:10 v/v)
 B: 0.1% formic acid + 5 mM ammonium formate in H₂O/MeOH (10:90 v/v)
Gradient:

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

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

Analytes

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



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

Reproduced with permission of Kent Scientific Services

Pesticides in Water

Application #AN3020

Conditions

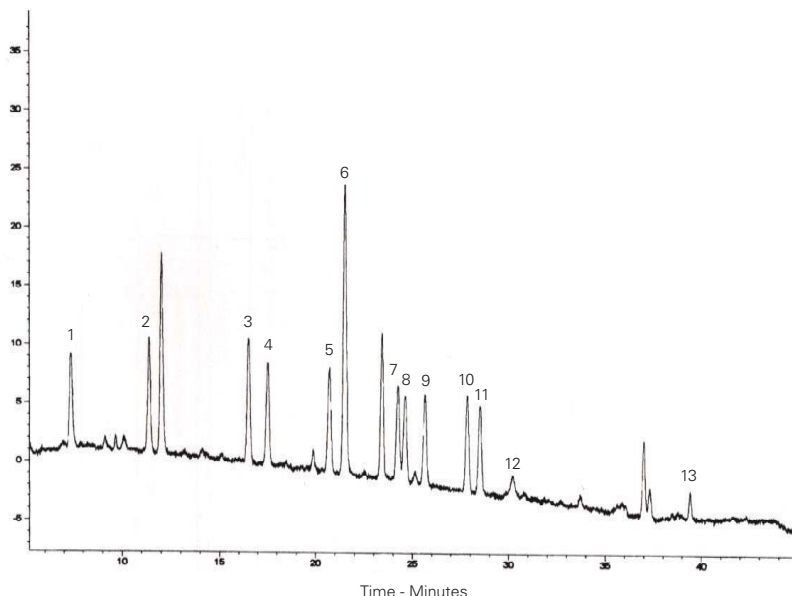
Column: ACE 3 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-111-1502
Mobile Phase: A: 0.1 M ammonium acetate in H₂O
 B: MeCN
Gradient:

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

Flow Rate: 0.3 mL/min
Injection: 25 µL
Temperature: 40 °C
Detection: UV, 220 nm (Pendimethalin at 245 nm)
Sample: 0.05 µg/L standards in MeCN/H₂O (10:90 v/v)

Analytes

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



Reproduced with permission of Amt der Tiroler Landesregierung, Chemisch-technische Umweltschutzanstalt, Innsbruck, Austria

Pharmaceutically Relevant Compounds (II) Application #AN1630

Conditions

Column: ACE Excel 3 CN-ES
ACE Excel 3 C18-Amide
ACE Excel 3 C18-PFP

Dimensions: 100 x 3.0 mm

Part Numbers: EXL-1113-1003U, EXL-1112-1003U, EXL-1110-1003U

Mobile Phase: A: 20 mM ammonium formate in H₂O
B: 20 mM ammonium formate in MeOH

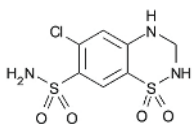
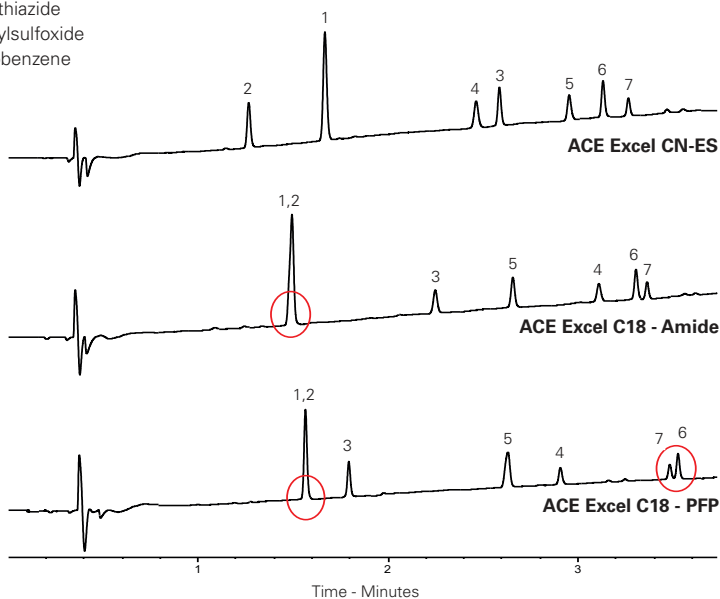
Gradient:

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

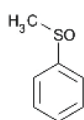
Flow Rate: 0.6 mL/min
Temperature: 40 °C
Detection: UV

Analytes

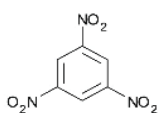
1. Hydrochlorothiazide
2. Methylphenylsulfonide
3. 1,3,5-Trinitrobenzene
4. Myricetin
5. p-Cresol
6. Sulindac
7. Toluene



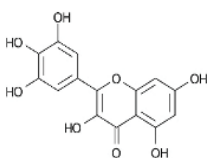
Hydrochlorothiazide



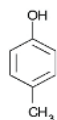
Methylphenylsulfonide



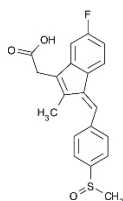
1,3,5-Trinitrobenzene



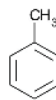
Myricetin



p-Cresol



Sulindac



Toluene

Pharmaceutically Relevant Compounds (III) Application #AN2400

Conditions

Column: ACE 5 C18-PFP

Dimensions: 150 x 4.6 mm

Part Number: ACE-1210-1546

Mobile Phase: A: 5 mM formic acid in H₂O
B: 5 mM formic acid in MeOH

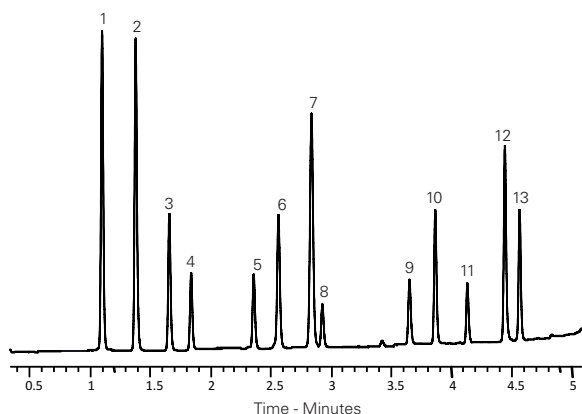
Gradient:

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

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

Analytes

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



Pharmaceutically Relevant Compounds (IV) Application #AN2460

Conditions

Column: ACE Excel 3 CN-ES

Dimensions: 100 x 2.1 mm

Part Number: EXL-1113-1002U

Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeCN

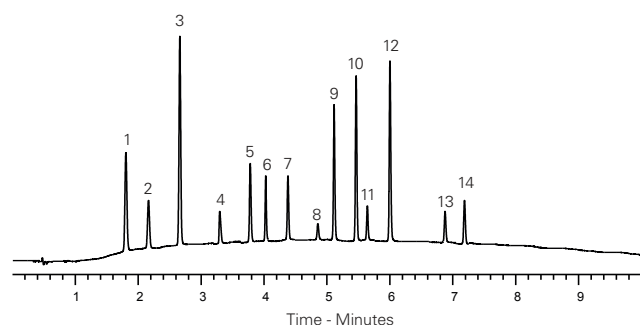
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 3 |
| 10 | 100 |

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

Analytes

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





Pharmaceutically Relevant Compounds (V)
Application #AN2500

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

Conditions

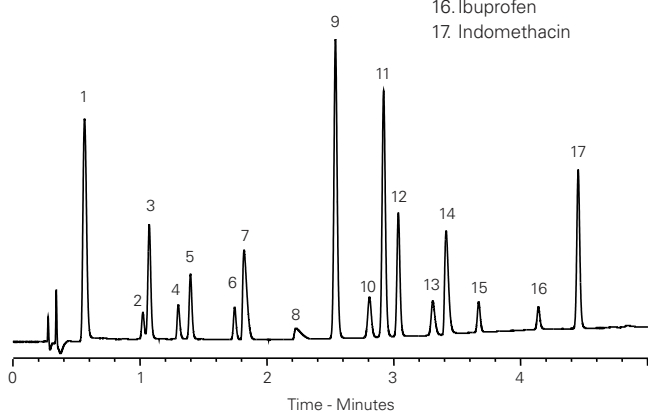
Column: ACE 3 C18-PFP
Dimensions: 50 x 2.1 mm
Part Number: ACE-1110-0502
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 3 |
| 5 | 100 |

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

Analytes

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



Pharmaceutically Relevant Mixture (I) – Different Selectivity Using pH
Application #AN1310

Conditions

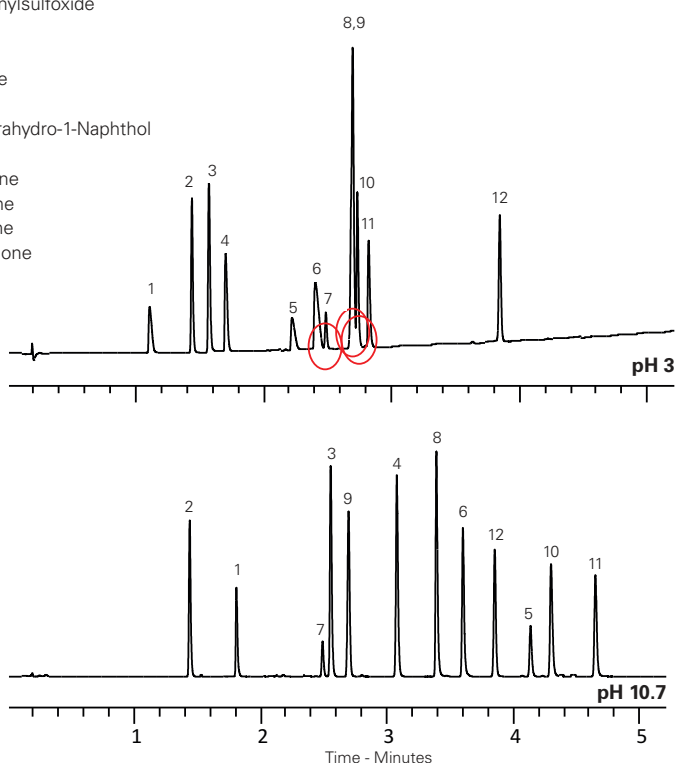
Column: ACE Ultracore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A1: 10 mM ammonium formate pH 3 in H₂O
 A2: 0.1% ammonia pH 10.7 in H₂O
 B1: 10 mM ammonium formate pH 3 in MeCN/H₂O (90:10 v/v)
 B2: 0.1% ammonia pH 10.7 in MeCN/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 3 |
| 5 | 100 |
| 6 | 100 |

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

Analytes

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



Pharmaceutically Relevant Mixture (II) – Different Selectivity Using pH

Application #AN1300

Conditions

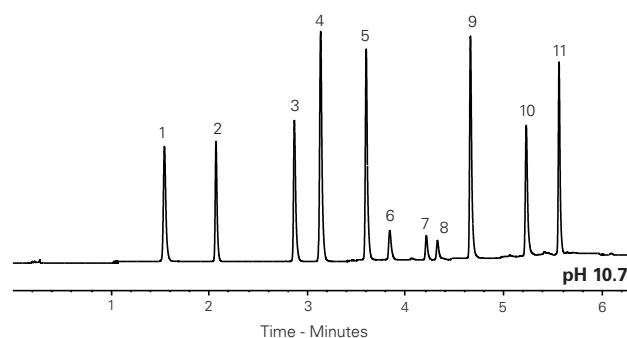
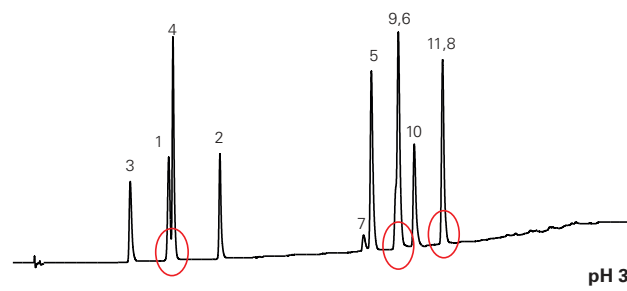
Column: ACE Ultracore 2.5 SuperPhenylHexyl
Dimensions: 50 x 2.1 mm
Part Number: CORE-25B-0502U
Mobile Phase: A1: 10 mM ammonium formate pH 3 in H₂O
 A2: 0.1% ammonia pH 10.7 in H₂O
 B1: 10 mM ammonium formate pH 3 in MeCN/H₂O (90:10 v/v)
 B2: 0.1% ammonia pH 10.7 in MeCN/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 3 |
| 5 | 100 |
| 6 | 100 |

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

Analytes

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



Phenelzine in Human Plasma by LC-MS/MS

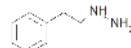
Application #AN4200

Conditions

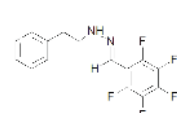
Column: ACE 5 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-121-1046
Mobile Phase: 10 mM ammonium acetate in H₂O, pH 4.0/MeOH (20:80 v/v)
Flow Rate: 1 mL/min with 70% split flow into MS
Injection: 10 µL
Temperature: 45 °C
Detection: AB Sciex API-4000 MS
 MRM using ESI in positive ion mode
 TurbolonSpray Interface Temperature: 600 °C
 IonSpray Voltage: 5500 V
Sample: Phenelzine derivatised with pentafluorobenzaldehyde, followed by SPE extraction of derivative and hydroxyzine (I.S.) from 200 µL human plasma.

Analytes

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



Phenelzine

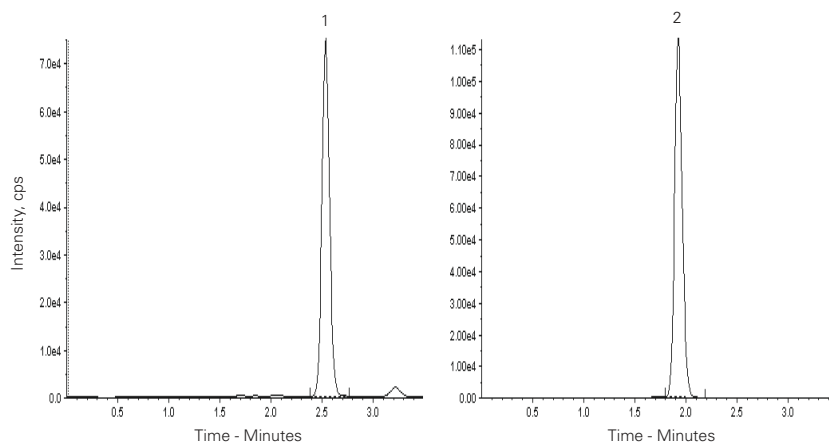


Phenelzine derivative



Hydroxyzine

Spiked human plasma





Phenol and Phenoxy Acid Herbicides

Application #AN2290

Conditions

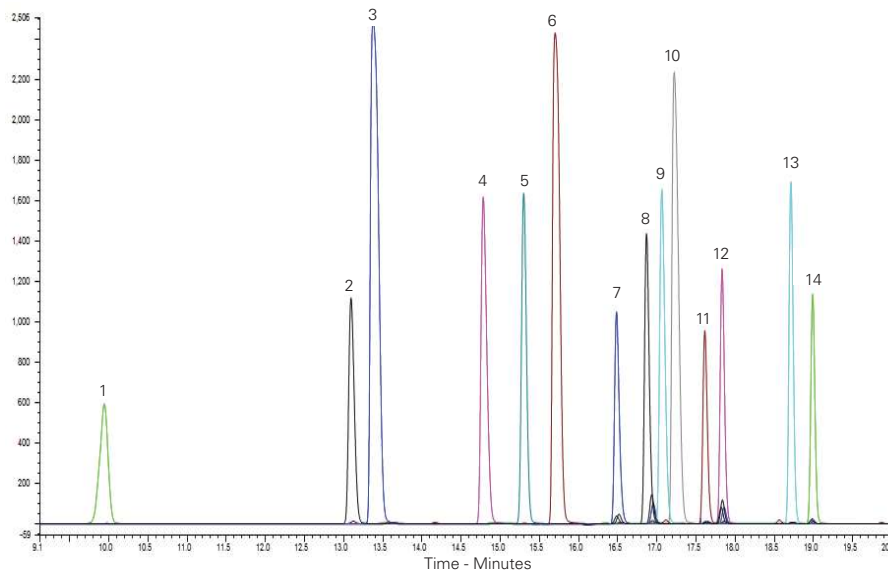
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: MeOH
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0.0 | 10 |
| 20.0 | 100 |

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

Analytes

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



Reproduced with permission of Nufarm UK Ltd

Phenolic Acids

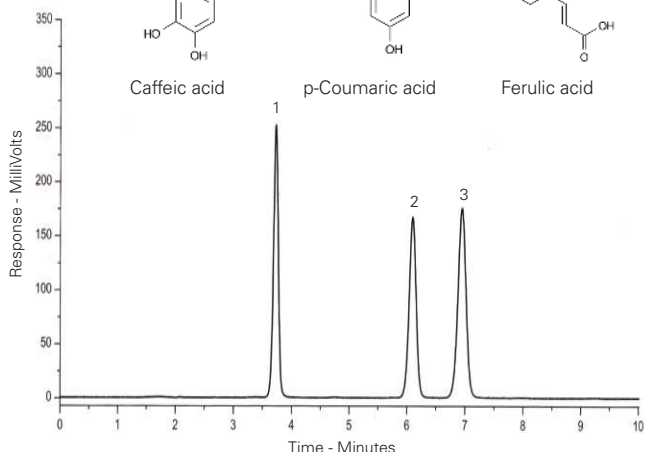
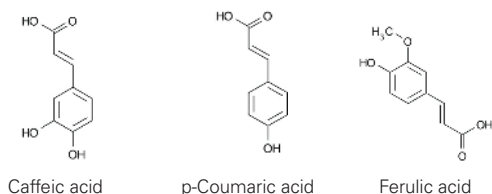
Application #AN3030

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/0.1% formic acid in H₂O (20:80 v/v)
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: Ambient
Detection: UV, 254 nm

Analytes

- Caffeic acid
- p-Coumaric acid
- Ferulic acid



Phenolic Compounds in Ground Water & Landfill Leachates

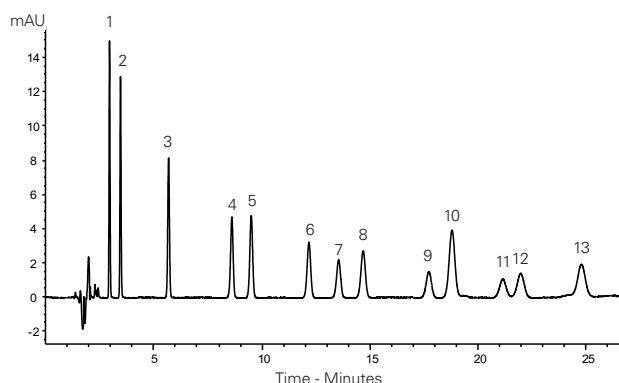
Application #AN3070

Conditions

Column: ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: EXL-1112-1546U
Mobile Phase: 0.1% formic acid v/v in H₂O
 MeCN (65:35 v/v)
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 30 °C
Detection: UV, 274 nm

Analytes

- Pyrocatechol
- Resorcinol
- Phenol
- m-Cresol
- o-Cresol
- 2,4-Dimethylphenol
- 3,4-Dimethylphenol
- 3,5-Dimethylphenol
- 1-Naphthol
- 3,4,5-Trimethylphenol
- 2,3,6-Trimethylphenol
- 2,4,6-Trimethylphenol
- 2-Naphthol



Reproduced with permission of Environmental Scientific Group Ltd, UK

Phenolic Compounds from Red Grape Seed Extract

Application #AN3790

Conditions

Column: ACE 3 C18-AR
Dimensions: 200 x 4.6 mm
Part Number: ACE-119-2046
Mobile Phase: A: 2% acetic acid in H₂O
 B: 2% acetic acid in MeCN
Gradient:

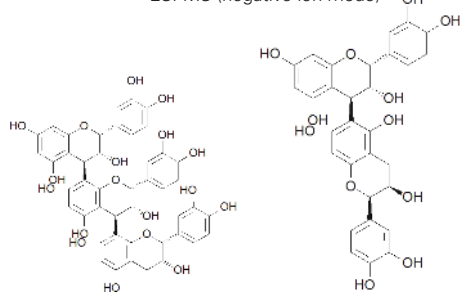
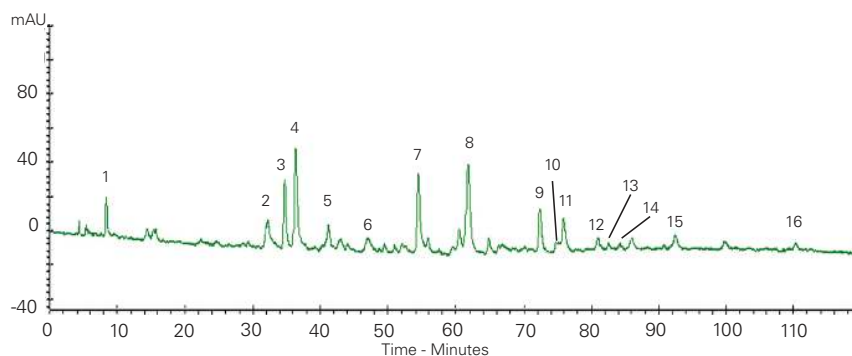
| Times (mins) | %B |
|--------------|-----|
| 0 | 0 |
| 80 | 20 |
| 115 | 28 |
| 120 | 100 |
| 130 | 100 |

Flow Rate: 0.6 mL/min

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

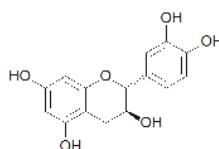
Analytes

- Gallic acid
- Procyanidin B3 (dimer) + procyanidin C2 (trimer)
- Procyanidin B1 (dimer)
- (+)-Catechin
- Procyanidin C3 (trimer)
- Procyanidin B4 (dimer)
- Procyanidin B2 (dimer)
- (-)-Epicatechin
- Procyanidin B3 gallate (dimer)
- Procyanidin B7 (dimer)
- Procyanidin C1 (trimer)
- Procyanidin tetramer
- Procyanidin pentamer
- Procyanidin hexamer
- (-)-Epigallocatechin
- Procyanidin B5 (dimer)

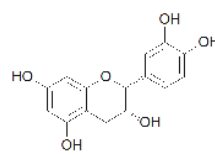


Procyanidin C1

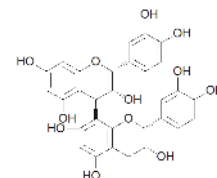
Procyanidin B5



(±)-Catechin



(±)-Epicatechin



Procyanidin B2

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

Phenols in Purple Coneflower (*Echinacea Purpurea*)

Application #AN2920

Conditions

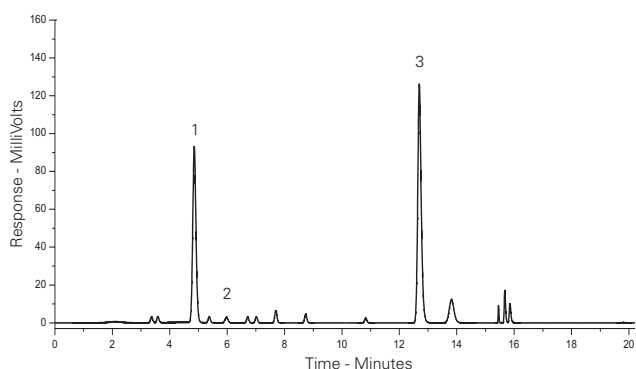
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% H₃PO₄ in H₂O
 B: MeCN
Gradient:

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

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

Analytes

- Caftaric acid
- Chlorogenic acid
- Cichoric acid

*Echinacea Purpurea*

Reproduced with permission of Bionorica Extracts SL, Spain



Phosphatidylethanol Biomarker Analysis by UHPLC-MS/MS

Application #AN3400

Conditions

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

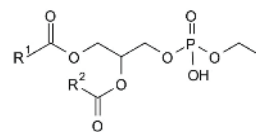
| Gradient: | Time (mins) | %B |
|-----------|-------------|-----|
| | 0.00 | 10 |
| | 1.00 | 10 |
| | 3.00 | 60 |
| | 3.01 | 100 |
| | 5.00 | 100 |
| | 5.10 | 10 |

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

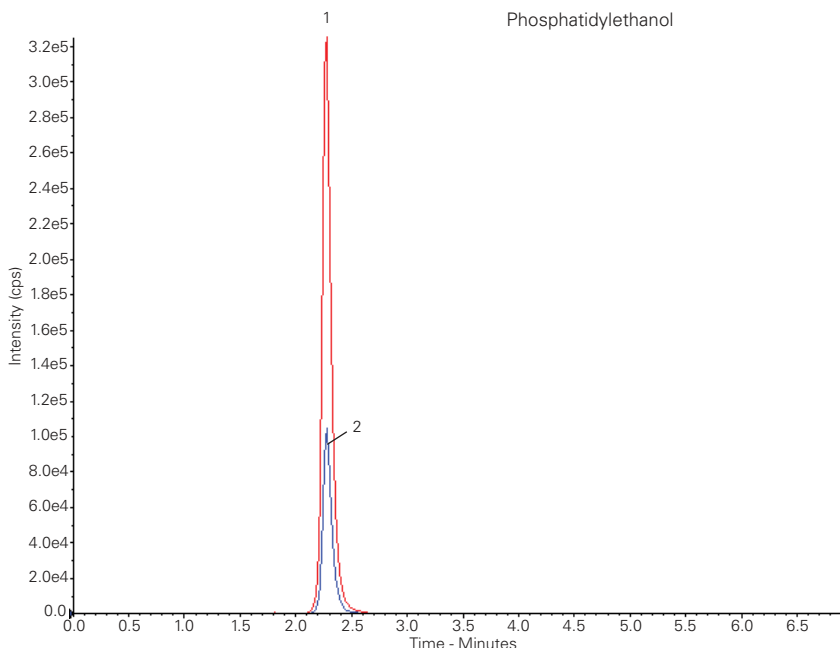
Phosphatidylethanol (PEth) measurement in blood is used as a biomarker of chronic alcohol use/abuse.

Analytes

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



Phosphatidylethanol



Reproduced with permission of Biotage GB Ltd, UK

Phytoestrogens from Hop Extract by LC-MS/MS

Application #AN1160

Conditions

Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: A: 1% formic acid in MeCN
 B: 1% formic acid in MeOH
 C: 1% formic acid in H₂O
 D: MeOH

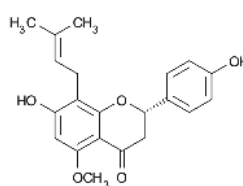
| Gradient: | Time (mins) | %A | %B | %C | %D |
|-----------|-------------|----|----|----|----|
| | 0 | 56 | 0 | 44 | 0 |
| | 8 | 51 | 5 | 44 | 0 |
| | 10 | 51 | 5 | 44 | 0 |
| | 17 | 95 | 5 | 0 | 0 |
| | 22 | 95 | 0 | 0 | 5 |

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

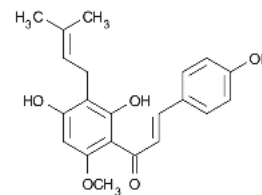


Analytes

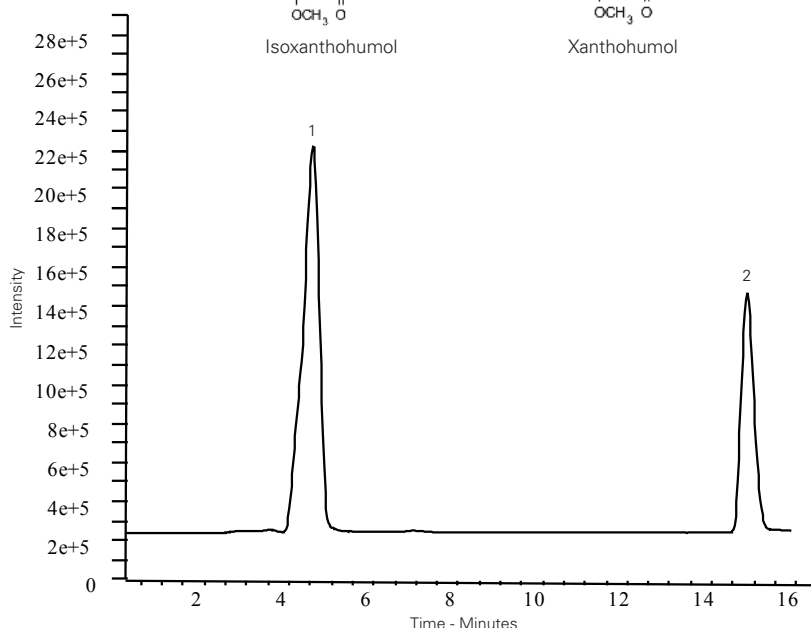
1. Isoxanthohumol
 LOQ 0.07 µg/mL
2. Xanthohumol
 LOQ 0.01 µg/mL



Isoxanthohumol



Xanthohumol



Reproduced with permission of Institute of Food Science Research, University of Madrid, Spain

Pilocarpine

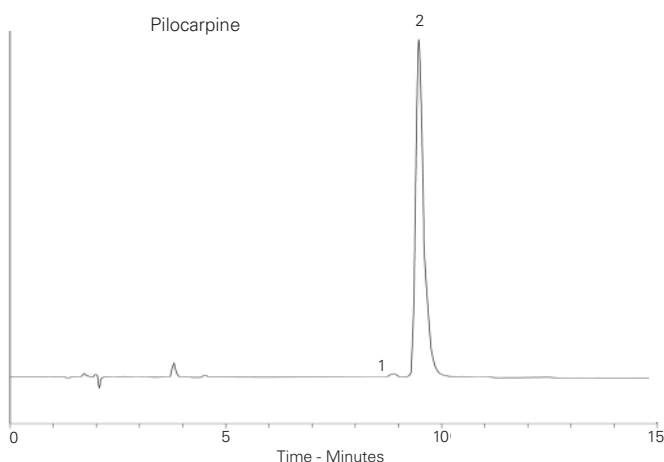
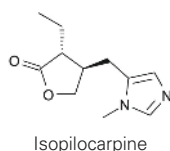
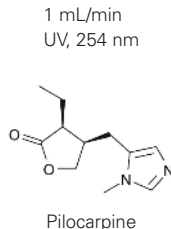
Application #AN3720

Conditions

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

Analytes

1. Isopilocarpine
2. Pilocarpine



Reproduced with permission of Controlled Therapeutics, Scotland, 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

Plant Hormones Involved in Abiotic Stresses

Application #AN4010

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: CORE-25A-1546U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: MeCN
Gradient:

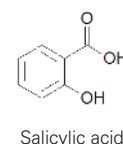
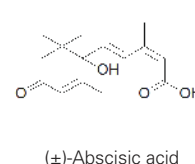
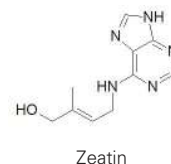
| Time (mins) | %B |
|-------------|-----|
| 0 | 0 |
| 2 | 40 |
| 5 | 60 |
| 13 | 100 |
| 15 | 20 |

Flow Rate: 0.5 mL/min
Temperature: 40 °C
Detection: Shimadzu LCMS-8040 triple quad MS
 ESI positive and negative mode

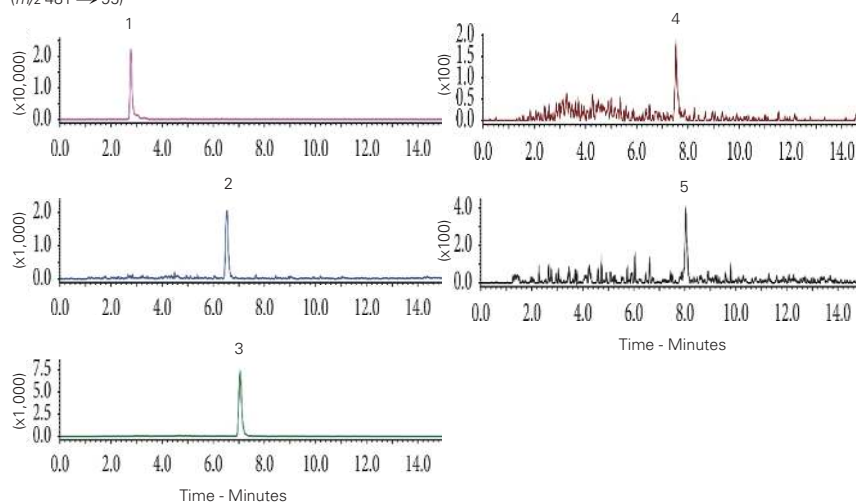
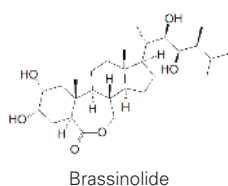
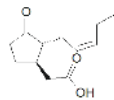
Sample: Crude extract of *Arabidopsis thaliana* rosette leaves

Analytes

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



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



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



Polar Compounds Separation

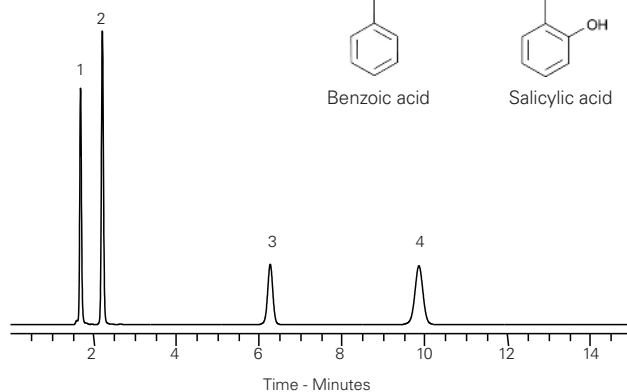
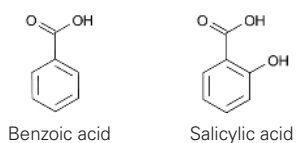
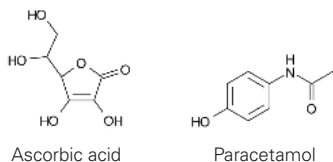
Application #AN1590

Conditions

Column: ACE Excel 5 CN-ES
Dimensions: 150 x 4.6 mm
Part Number: EXL-1213-1546U
Mobile Phase: MeOH/H₂O (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 20 °C
Detection: UV, 254 nm

Analytes

1. Ascorbic acid
2. Paracetamol
3. Benzoic acid
4. Salicylic acid



Polyamines

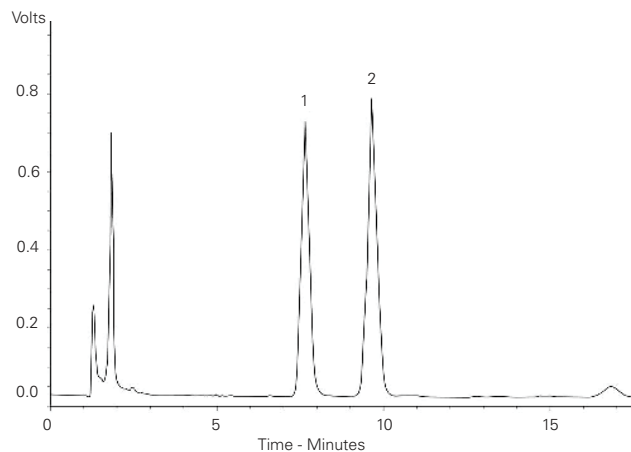
Application #AN3740

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: TRIS buffer pH 7.0/MeOH (10:90 v/v)
Flow Rate: 1.2 mL/min
Detection: Fluorescence – λ_{ex} 340 nm, λ_{em} 450 nm

Analytes

1. Putrescine
2. Cadaverine (as OPA derivatives)



Reproduced with permission of Centre for Chemical Sciences, Royal Holloway University of London, UK

Polycyclic Tetracarboxylic Acids

Application #AN1340

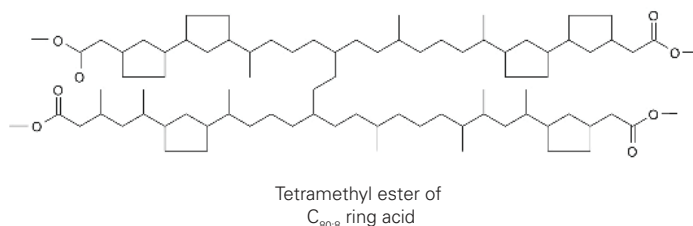
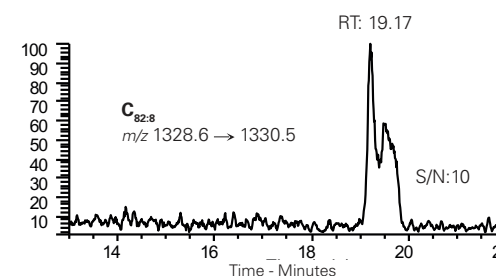
Conditions

Column: ACE UltraCore 2.5 SuperPhenylHexyl
Dimensions: 100 x 2.1 mm
Part Number: CORE-25B-1002U
Mobile Phase: A: 10 mM ammonium acetate in MeOH/H₂O (98:2 v/v)
 B: 10 mM ammonium acetate in IPA/H₂O (98:2 v/v)
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0.0 | 0 |
| 1.0 | 0 |
| 15.0 | 100 |
| 25.0 | 100 |

Flow Rate: 0.15 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: LCQ Ion trap MS
 LC-ESI-MS extracted ion chromatograms
 Compounds detected as ammoniated quasimolecular ions [M+NH₄]⁺
 Detection limit ~ 0.1 ppm

C₈₀₋₈₂ polycyclic tetracarboxylic acids isolated from oilfield deposits



Reproduced with permission of Petroleum & Environmental Geochemistry Group, Plymouth University, UK

Polyethylene Glycol 1000

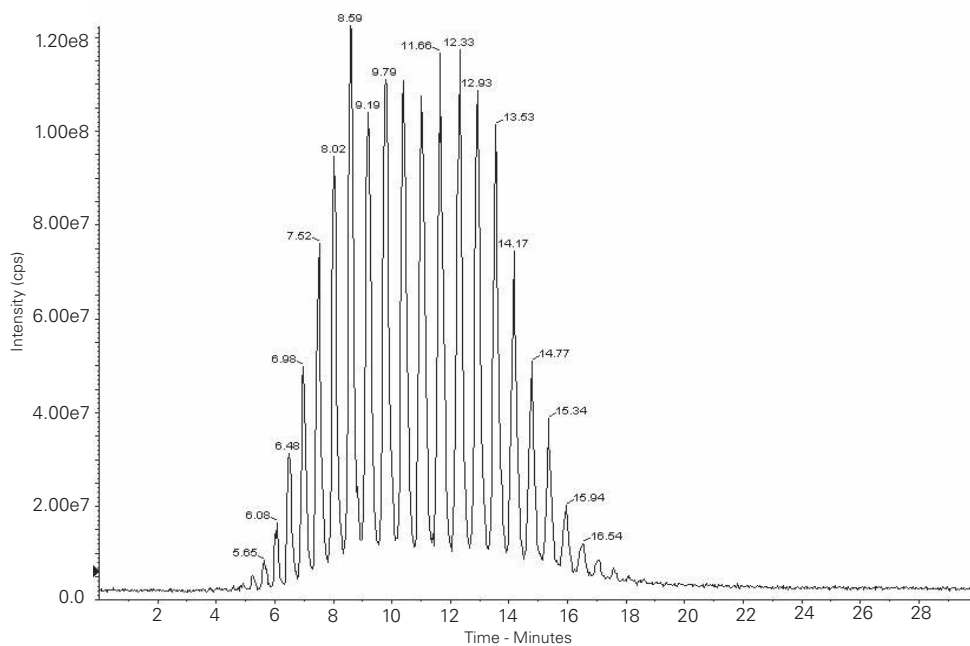
Application #AN3900

Conditions

Column: ACE 3 C8
Dimensions: 150 x 4.6 mm
Part Number: ACE-112-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 50 |
| 45 | 85 |
| 50 | 50 |
| 60 | 50 |

Flow Rate: 1 mL/min
Detection: APCI (negative ion)



Reproduced with permission of Wickham Laboratories, UK

[¹⁴C]Pomalidomide and Metabolites in Human Plasma and Urine

Application #AN4240

Conditions

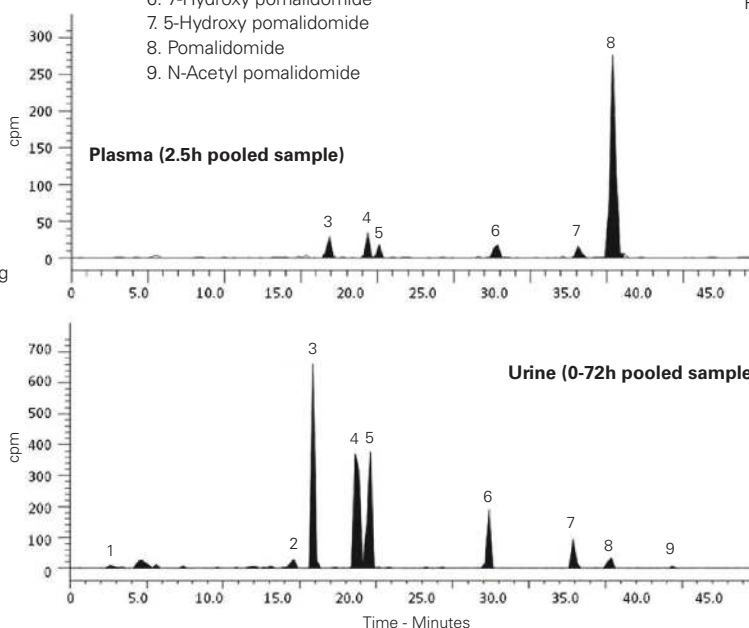
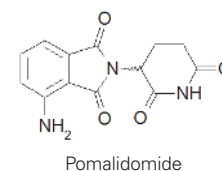
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: A: 25 mM ammonium acetate pH 5.5 in H₂O
 B: MeOH
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 0 |
| 2 | 0 |
| 38 | 36 |
| 44 | 100 |
| 48 | 100 |
| 50 | 0 |

Flow Rate: 0.7 mL/min
Temperature: 30 °C
Detection: Radiometric
 Metabolites characterised using LC-MS/MS (positive ion mode)

Analytes

- 3-Aminophthalic acid
- Hydrolysis product of pomalidomide
- Hydrolysis product of pomalidomide
- Glucuronide conjugate of 5-hydroxy pomalidomide
- Glucuronide conjugate of 5-hydroxy pomalidomide
- 7-Hydroxy pomalidomide
- 5-Hydroxy pomalidomide
- Pomalidomide
- N-Acetyl pomalidomide



Hoffmann M, Kasserra C, Reyes J, Schafer P, Kosek J, Capone L, Parton A, Kim-Kang H, Surapaneni S, Kumar G. Absorption, Metabolism and Excretion of [¹⁴C] Pomalidomide in Humans following Oral Administration. *Cancer Chemotherapy and Pharmacology* 71, 489-501 (2013) doi 10.1007/s00280-012-2040-6



Porphyrins in Oral Bacteria by LC-MS/MS

Application #AN3080

Conditions

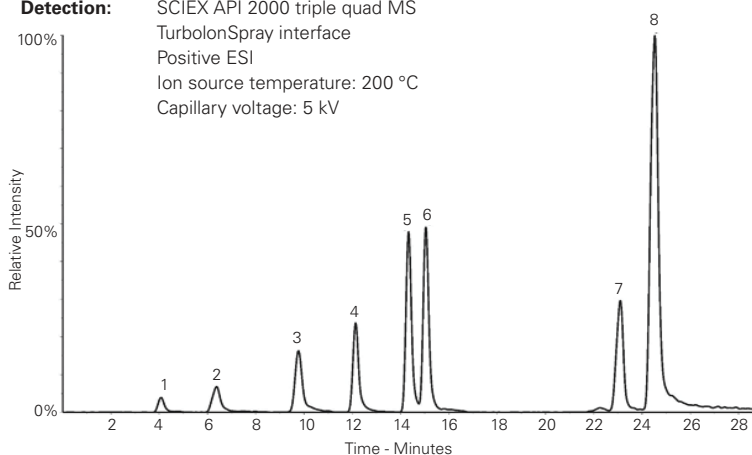
Column: ACE 3 C18-PFP
Dimensions: 75 x 2.1 mm
Part Number: ACE-1110-7502
Mobile Phase: A: 0.1% formic acid in H₂O/MeCN (95:5 v/v)
 B: 0.1% formic acid in H₂O/MeCN (5:95 v/v)
Gradient:

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

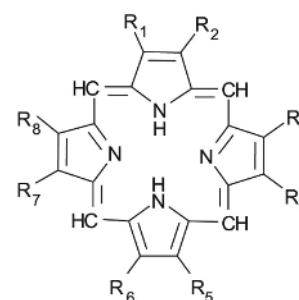
Flow Rate: 0.1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: SCIEX API 2000 triple quad MS
 TurbolonSpray interface
 Positive ESI
 Ion source temperature: 200 °C
 Capillary voltage: 5 kV

Analytes

1. Uroporphyrin I
(R₁:A, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:A, R₈:P)
(m/z 831 → 727, 623, 655)
2. 7-Carboxyporphyrin I
(R₁:A, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(m/z 787 → 683, 670, 623)
3. 6-Carboxyporphyrin I
(R₁:M, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(m/z 743 → 639, 507, 521)
4. 5-Carboxyporphyrin I
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(m/z 699 → 463, 595, 640)
5. Coproporphyrin I
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:M, R₆:P, R₇:M, R₈:P)
(m/z 655 → 537, 596, 523)
6. Coproporphyrin III
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:M, R₆:P, R₇:P, R₈:M)
(m/z 655 → 537, 596, 523)
7. Mesoporphyrin IX
(R₁:M, R₂:E, R₃:M, R₄:E, R₅:M, R₆:P, R₇:M, R₈:P)
(m/z 567 → 449, 479, 508)
8. Protoporphyrin IX
(R₁:M, R₂:V, R₃:M, R₄:V, R₅:M, R₆:P, R₇:P, R₈:M)
(m/z 563 → 445, 504, 489)



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



Reproduced with permission of Department of Environmental Science and Analytical Chemistry, Stockholm University, Sweden

Pravastatin and Isomers by LC-MS/MS

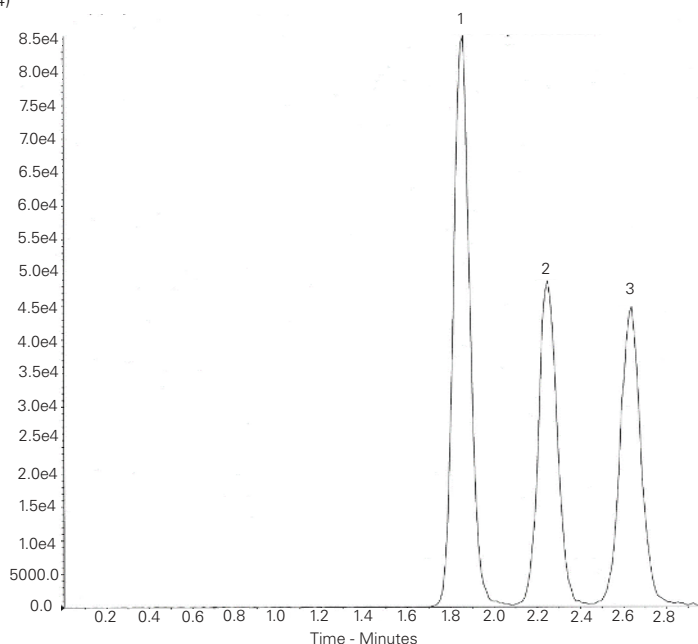
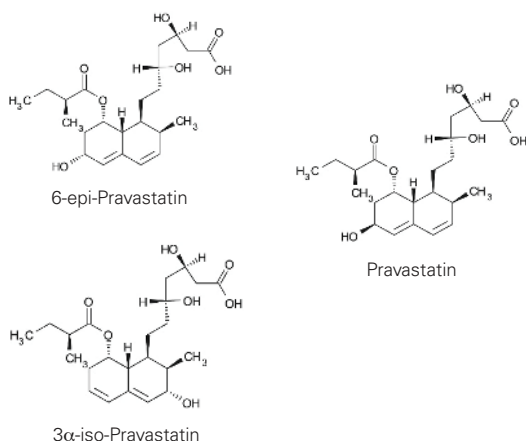
Application #AN1350

Conditions

Column: ACE 3 C18
Dimensions: 50 x 3.0 mm
Part Number: ACE-111-0503
Mobile Phase: MeCN/MeOH/THF/H₂O/Acetic Acid
 (15:20:5:60:0.1 v/v/v/v/v)
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: API 3000 triple quad MS
 TurbolonSpray – negative mode
 Extracted ion chromatogram
 of MRM m/z 423.3 → 321.1

Analytes

1. 6-epi-Pravastatin
(MW 424)
2. Pravastatin
(MW 424)
3. 3α-iso-Pravastatin
(MW 424)



Reproduced with permission of Biotrial Bioanalytical Services, Laval, QC, Canada

Pravastatin in Cell Lysate Samples by LC-MS/MS

Application #AN4350

Conditions

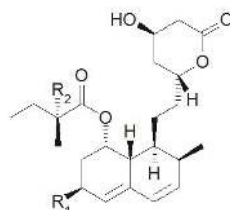
Column: ACE Excel 3 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1111-1003U
Mobile Phase: A: 5 mM ammonium acetate pH 4.5 in H₂O
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 65 |
| 4 | 65 |
| 5 | 75 |
| 7 | 75 |
| 8 | 65 |

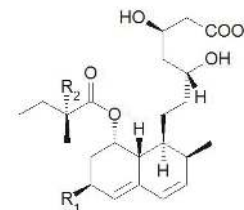
Flow Rate: 0.3 mL/min
Temperature: 40 °C
Detection: Quattro Ultima triple quad MS
 ESI MRM mode: +ve (lactones)
 -ve (hydroxy acids)
 Source temperature: 125 °C
 Desolvation temperature: 350 °C

Analytes

1. Lactone form (pharmacologically inactive)
2. Hydroxy acid form (pharmacologically active)



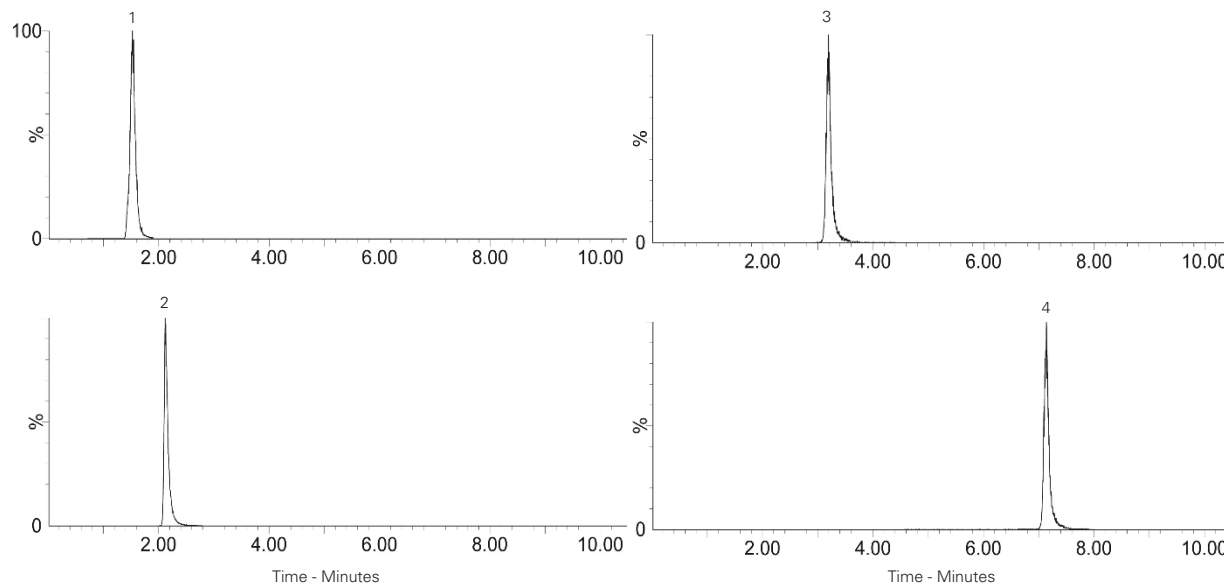
Lactone form
(pharmacologically inactive)



Hydroxy acid form
(pharmacologically active)

| Peak | Analyte | Precursor ion | MRM transition (<i>m/z</i>) | LLOQ (ng/mL) |
|------|------------------------------|---------------------|-------------------------------|--------------|
| 1 | Pravastatin hydroxy acid | [M-H] ⁻ | 423.23 → 321.37 | 2.23 |
| 2 | Pravastatin lactone | [M+H] ⁺ | 407.46 → 183.22 | 2.03 |
| 3 | Lovastatin hydroxy acid (IS) | [M-H] ⁻ | 421.08 → 319.54 | n/a |
| 4 | Lovastatin lactone (IS) | [M+Na] ⁺ | 427.15 → 325.36 | n/a |

Pravastatin: R₁ = OH, R₂ = H
Lovastatin (IS): R₁ = CH₃, R₂ = H



Taha DA, de Moor CH, Barrett DA, Lee JB, Gandhi RD, Hoo CW, Gershkovich P. (2016) The role of acid-base imbalance in statin-induced myotoxicity. Translational Research, The Journal of Laboratory and Clinical Medicine. <http://dx.doi.org/10.1016/j.trsl.2016.03.015>

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

Application #AN2690

Conditions

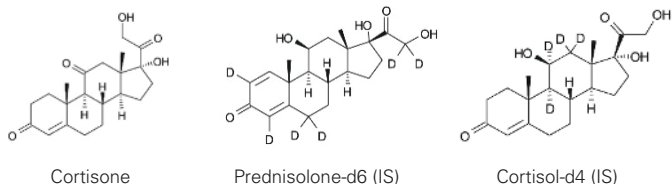
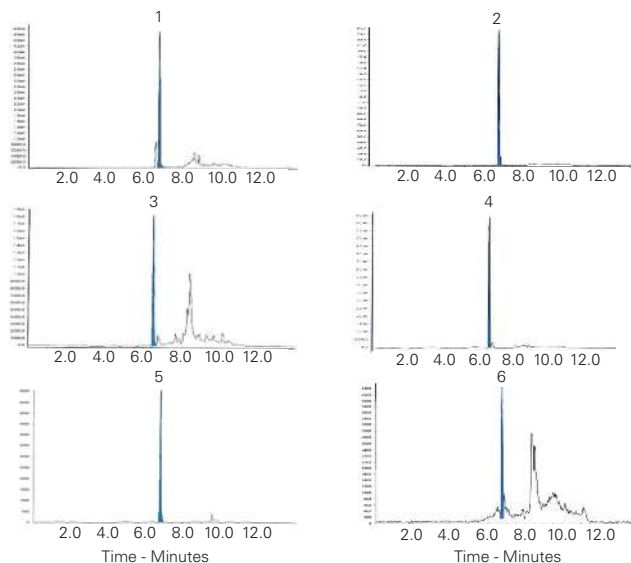
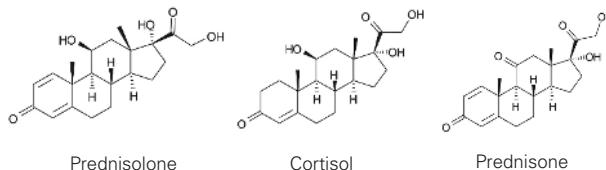
Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 4 mM ammonium acetate in H₂O
 B: 0.2% (v/v) formic acid in MeOH
Gradient:

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

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

Analytes

1. Prednisolone (*m/z* 361.5 → 147.1)
2. Cortisol (*m/z* 363.5 → 121.3)
3. Prednisone (*m/z* 359.4 → 147.1)
4. Cortisone (*m/z* 361.5 → 163.3)
5. Prednisolone-d6 (IS) (*m/z* 367.4 → 150.3)
6. Cortisol-d4 (IS) (*m/z* 367.3 → 331.3)



Reproduced with permission of Department of Pathology and Laboratory Medicine, Heartlands Hospital, Birmingham, UK

Preservatives (I)

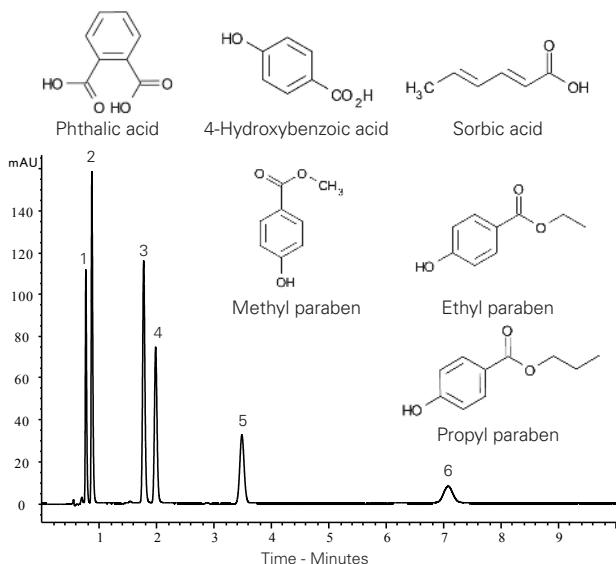
Application #AN2230

Conditions

Column: ACE Excel 1.7 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-171-0503U
Mobile Phase: 20 mM potassium phosphate
 pH 2.5 in MeCN/H₂O (30:70 v/v)
Flow Rate: 0.43 mL/min
Injection: 0.7 µL
Temperature: 20 °C
Detection: UV, 230 nm

Analytes

1. Phthalic acid
2. 4-Hydroxybenzoic acid
3. Sorbic acid
4. Methyl paraben
5. Ethyl paraben
6. Propyl paraben



Preservatives (II)

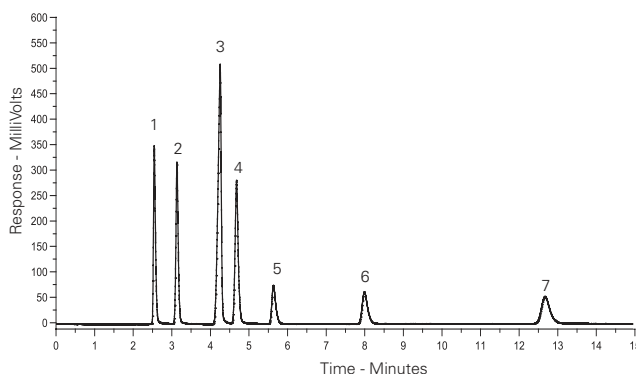
Application #AN3040

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/50 mM KH₂PO₄
 pH 4.4 in H₂O (40:60 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 230 nm

Analytes

1. Phthalic acid
2. p-Hydroxybenzoic acid
3. Benzoic acid
4. Sorbic acid
5. Methyl paraben
6. Ethyl paraben
7. Propyl paraben



Pristinamycin Components in Plasma by LC-MS/MS Application #AN1360

Conditions

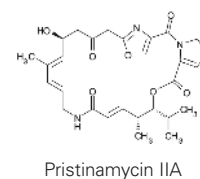
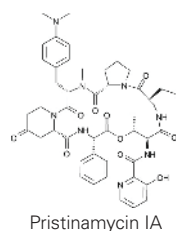
Column: ACE 3 C18
Dimensions: 30 x 3.0 mm
Part Number: ACE-111-0303
Mobile Phase: A: 1 mM ammonium formate + 0.1% formic acid in MeCN/H₂O (35:65 v/v)
 B: MeCN
Gradient:

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

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

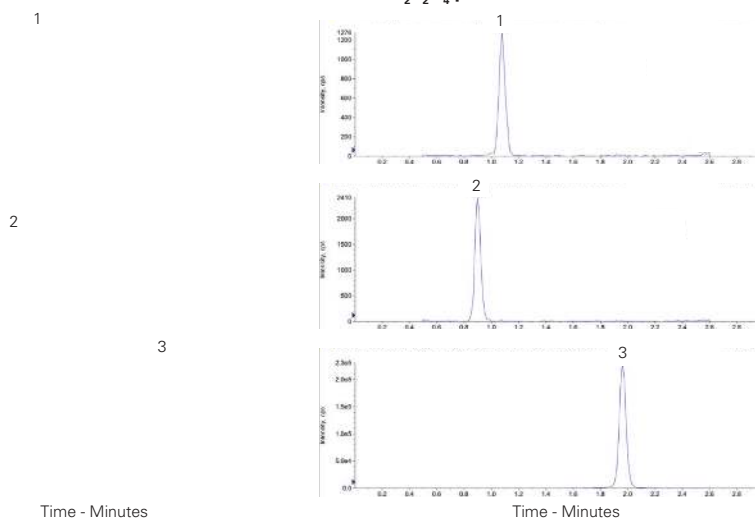
Analytes

1. Pristinamycin IA
(*m/z* 8675 → 134.2)
2. Pristinamycin IIA
(*m/z* 526.3 → 355.1)
3. Virginiamycin (IS)
(*m/z* 824.6 → 134.0)



Processed study sample containing pristinamycin IA and IIA

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



Reproduced with permission of inVentiv Health Clinical, Quebec, Canada

Proanthocyanidins from Cinnamon Bark Extract Application #AN3510

Conditions

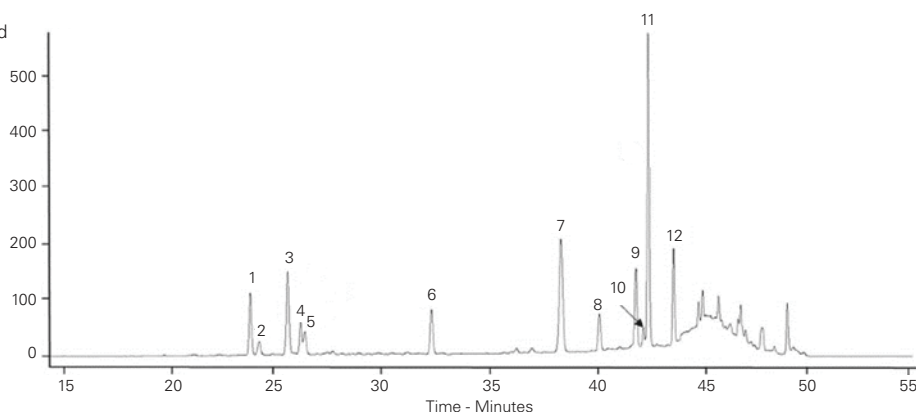
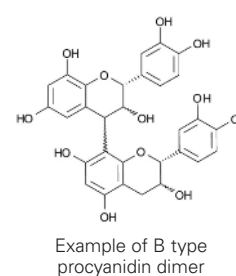
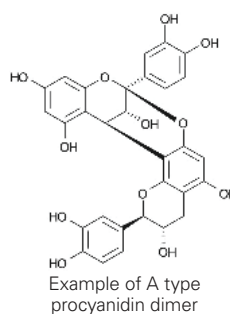
Column: ACE 3 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-111-2546
Mobile Phase: A: 1% acetic acid in H₂O
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 36 |
| 35 | 36 |
| 40 | 50 |
| 45 | 100 |
| 55 | 0 |
| 60 | 0 |

Flow Rate: 0.75 mL/min
Temperature: Ambient
Detection: UV, 280 nm
Sample: Cinnamon bark extract thiolysed with benzyl mercaptan

Analytes

1. Catechin
 2. A-type PC dimer
 3. A-type PC trimer
 4. Epicatechin
 5. A-type PC trimer
 6. IS
 7. cis-Cinnamic acid
 8. A-type PC-BM trimer
 9. trans-Cinnamic acid
 10. cis-Catechin-BM
 11. Epicatechin-BM
 12. A-type PC-BM dimer
- PC = Procyanidin
 BM = Benzyl mercaptan adduct



Williams, A. R. et al. Anthelmintic activity of trans-cinnamaldehyde and A and B-type proanthocyanidins derived from cinnamon (*Cinnamomum verum*). *Sci. Rep.* 5, 14791; doi:10.1038/srep14791 (2015).



Procaine and p-Aminobenzoic Acid Separation

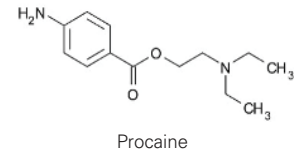
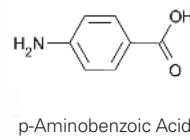
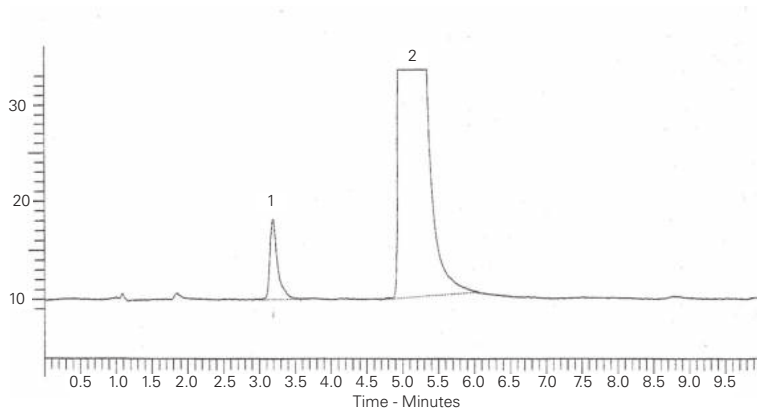
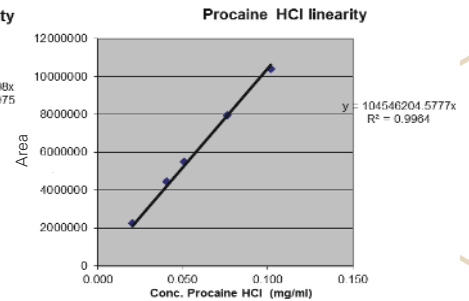
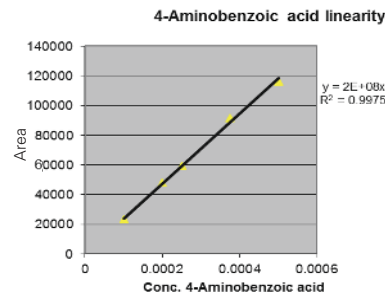
Application #AN1660

Conditions

Column: ACE 3 C18-PFP
Dimensions: 100 x 4.6 mm
Part Number: ACE-1110-1046
Mobile Phase: 0.6% acetic acid in H₂O/MeOH (81:19 v/v), adjusted to pH 4.7 with 20% NaOH
Flow Rate: 1 mL/min
Detection: UV, 279 nm
 S/N limit: 10
Sample: Procaine 0.0002 mg/mL, p-Aminobenzoic acid 0.00005 mg/mL

Analytes

1. p-Aminobenzoic acid (4-Aminobenzoic acid)
2. Procaine



Reproduced with permission of Huddersfield Royal Infirmary, UK

Propolis Phenolic Acids Applied to Human Skin

Application #AN4230

Conditions

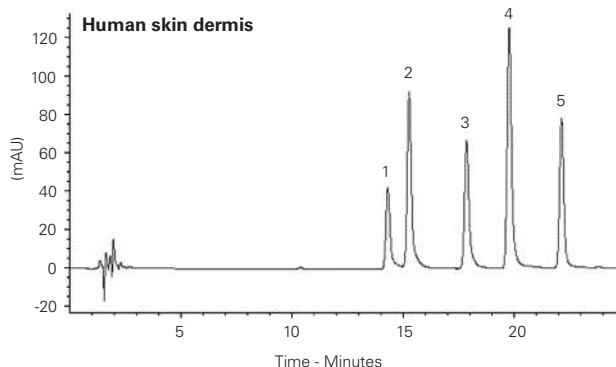
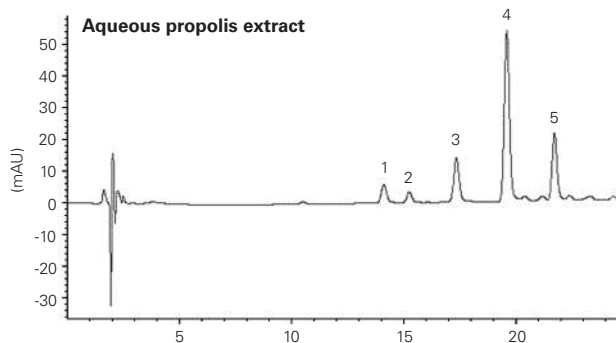
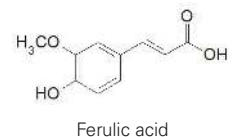
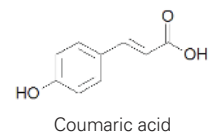
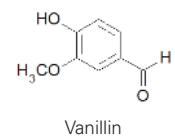
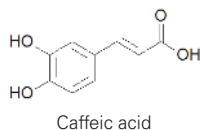
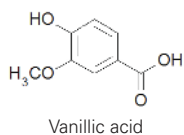
Column: ACE 5 C18
Dimensions: 150 x 0.5 mm
Part Number: ACE-121-15005
Mobile Phase: A: 0.5% acetic acid in H₂O
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 1 |
| 25 | 21 |

Flow Rate: 20 µL/min
Injection: 0.2 µL
Temperature: 25 °C
Detection: UV, 290 nm

Analytes

1. Vanillic acid
2. Caffeic acid
3. Vanillin
4. Coumaric acid
5. Ferulic acid



Zilius M, Ramanauskienė K, Briedis V. Release of Propolis Phenolic Acids from Semisolid Formulations and their Penetration into the Human Skin in vitro. Evidence-based Complementary and Alternative Medicine (2013) <http://dx.doi.org/10.1155/2013/958717>

Prostaglandins using LC-MS/MS

Application #AN3260

Conditions

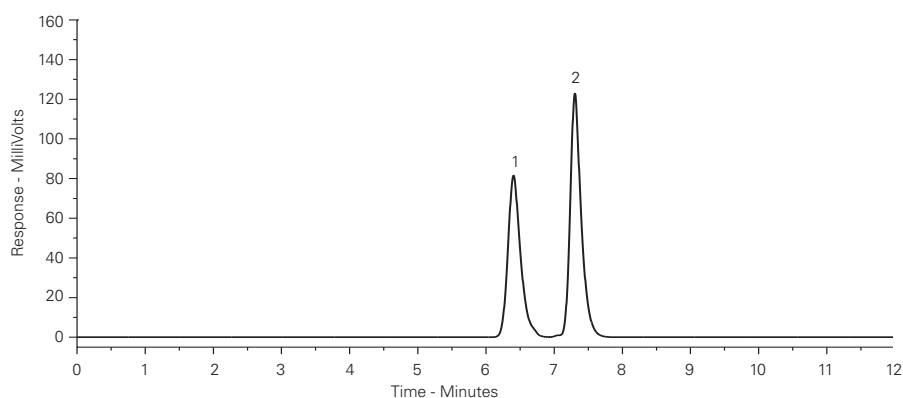
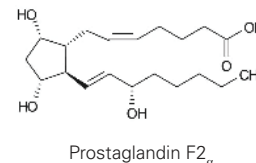
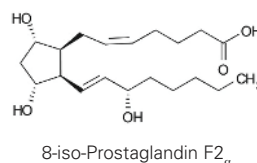
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: H₂O
 B: MeOH
 C: MeCN
Gradient:

| Time (mins) | %A | %B | %C |
|-------------|------|------|------|
| 0 | 70.0 | 20.0 | 10.0 |
| 9 | 10.0 | 60.0 | 30.0 |
| 10 | 0.1 | 66.6 | 33.3 |

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

Analytes

- 8-iso-Prostaglandin F_{2α}
- Prostaglandin F_{2α}



Reproduced with permission of Department of Internal Medicine, Fukuoka University, Japan

Protein Test Mix

Application #AN3730

Conditions

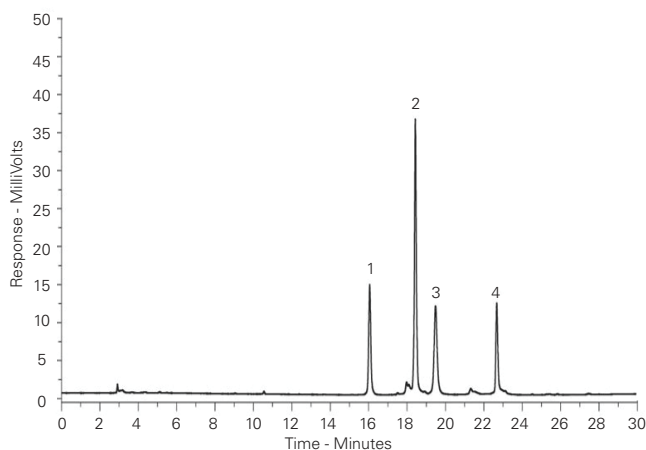
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 5 |
| 30 | 70 |

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 280 nm

Analytes

- Ribonuclease A (MW ~14 kDa)
- Cytochrome C (MW ~12 kDa)
- Holo-transferrin (MW ~77 kDa)
- Apomyoglobin (MW ~17 kDa)



Proton Pump Inhibitors (PPIs)

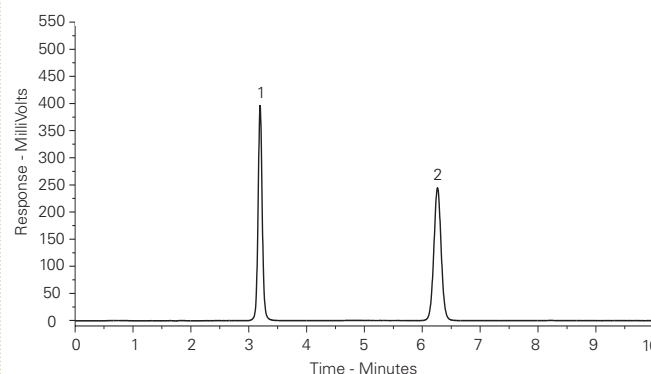
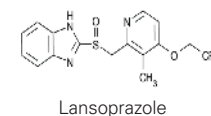
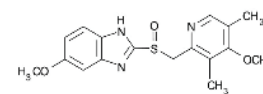
Application #AN3710

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM ammonium formate
 pH 3.0/MeCN (65:35 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

- Omeprazole
- Lansoprazole





Psychoactive Substances in 'Synthacaine' by LC-UV

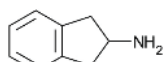
Application #AN3440

Conditions

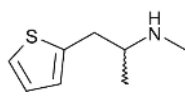
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: 10 mM ammonium formate pH 3.5/MeCN (90:10 v/v)
Flow Rate: 1.2 mL/min
Temperature: 22 °C
Detection: UV, 207 nm (2-Aminoindane) and 233 nm (Methiopropamine)
Sample: Synthacaine 40 µg/mL

Analytes

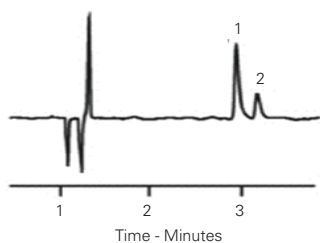
1. 2-Aminoindane
LOD 0.83 µg/mL
2. Methiopropamine
LOD 0.31 µg/mL



2-Aminoindane



Methiopropamine



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

Quinidine, Quinine and their Hydroderivatives Separation

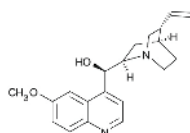
Application #AN1600

Conditions

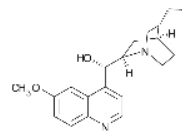
Column: ACE 3 C18-AR
Dimensions: 50 x 4.6 mm
Part Number: ACE-119-0546
Mobile Phase: 20 mM ammonium formate pH 3.0 in MeOH/H₂O (30:70 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 254 nm

Analytes

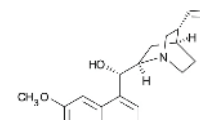
1. Quinidine
2. Quinine
3. Hydroquinidine
4. Hydroquinine



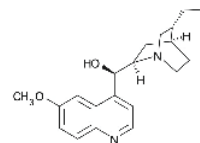
Quinine



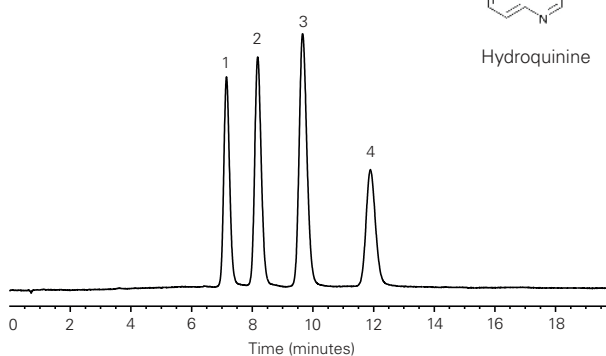
Hydroquinidine



Quinidine



Hydroquinine



Need a custom column for your application?

Please enquire
 email: info@ace-hplc.com

Ranitidine Hydrochloride and Related Impurities

Application #AN3450

Conditions

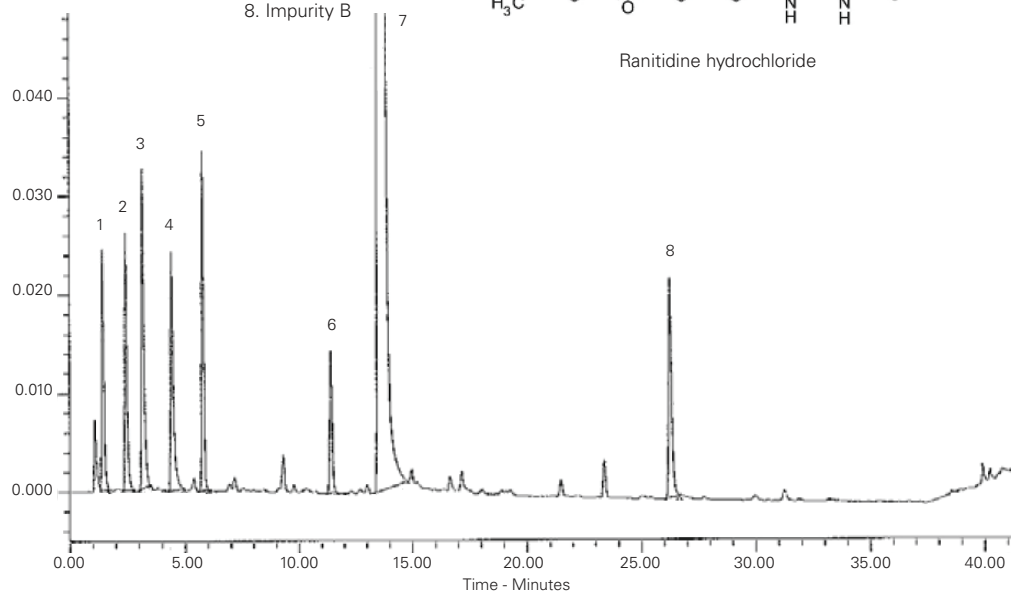
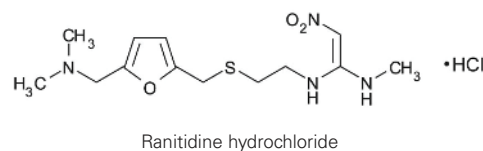
Column: ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-111-1046
Mobile Phase: A: 0.05 M KH_2PO_4 pH 6.5 in $\text{H}_2\text{O}/\text{MeCN}$ (98:2 v/v)
 B: $\text{H}_2\text{O}/\text{MeCN}$ (5:95 v/v)

| Gradient: | Time (mins) | %B |
|-----------|-------------|----|
| | 0 | 0 |
| | 10 | 5 |
| | 25 | 15 |
| | 35 | 20 |
| | 40 | 55 |
| | 55 | 0 |

Flow Rate: 1 mL/min
Injection: 40 μL
Temperature: 40 $^\circ\text{C}$
Detection: UV, 230 nm

Analytes

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



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

Recombinant hGMCSF Purified from *Escherichia Coli*

Application #AN3840

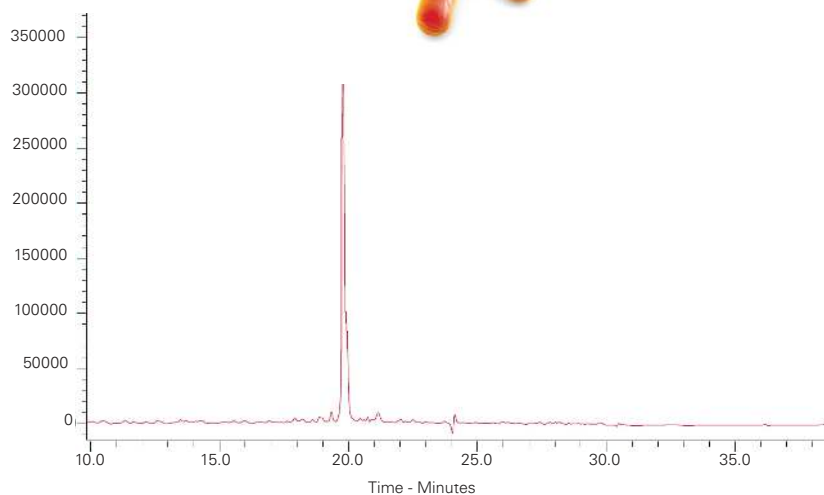
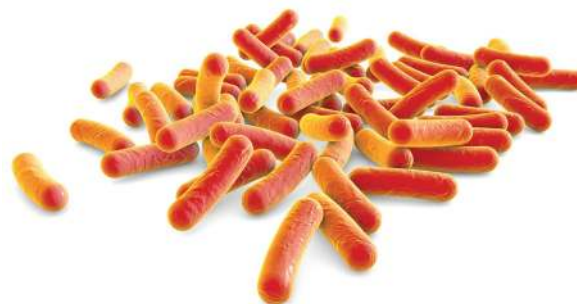
Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: A: 0.1% TFA in $\text{H}_2\text{O}/\text{MeCN}$ (90:10 v/v)
 B: 0.1% TFA in $\text{H}_2\text{O}/\text{MeCN}$ (10:90 v/v)

| Gradient: | Time (mins) | %B |
|-----------|-------------|-----|
| | 0 | 10 |
| | 20 | 65 |
| | 23 | 100 |

Flow Rate: 1 mL/min
Temperature: 30 $^\circ\text{C}$
Detection: UV, 215 nm

hGMCSF = human Granulocyte Macrophage Colony Stimulating Factor, a 127 amino acid residue cytokine with a molecular weight of 14,477 Da



Das KMP, Banerjee S, Shekhar N, Damodaran K, Nair R, Somani S, Raiker VP, Jain S, Padmanabhan S. Cloning, Soluble Expression and Purification of High Yield Recombinant hGMCSF in *Escherichia coli*. *Int. J. Mol. Sci.* 2011, 12, 2064-2076; doi:10.3390/ijms12032064



Rifamycin Anti-tubercular Antibiotics in Human Plasma

Application #AN4090

Conditions

Column: ACE 3 C18
Dimensions: 100 x 3.0 mm
Part Number: ACE-111-1003
Mobile Phase: A: 15 mM ammonium formate pH 5.0 with formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

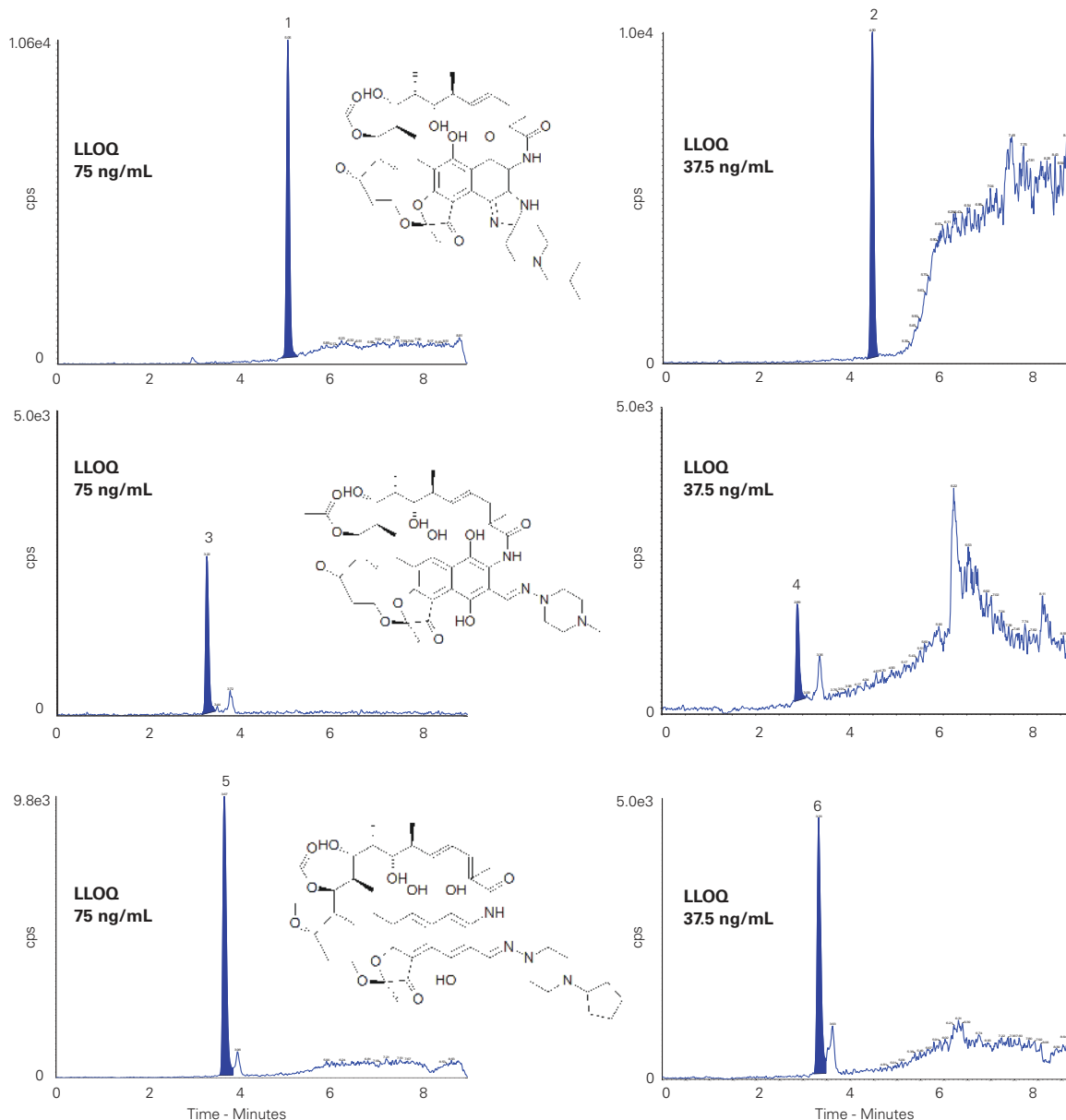
| Time (mins) | %B |
|-------------|----|
| 0.0 | 60 |
| 4.0 | 95 |
| 7.0 | 95 |
| 7.2 | 60 |
| 9.0 | 60 |

Flow Rate: 0.35 mL/min
Injection: 2 µL
Temperature: 30 °C
Detection: API 5000 triple quad MS
 ESI in positive ion mode

Analytes

1. Rifabutin
(*m/z* 847.5 → 815.5)
2. Desacetyl rifabutin
(*m/z* 805.5 → 773.4)
3. Rifampicin
(*m/z* 823.5 → 791.4)
4. Desacetyl rifampicin
(*m/z* 781.5 → 749.4)
5. Rifapentine
(*m/z* 877.5 → 845.4)
6. Desacetyl rifapentine
(*m/z* 835.5 → 803.5)

Assay for simultaneous quantification of rifamycin antibiotics and their corresponding active desacetyl metabolites



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

Sennosides in Traditional Chinese Medicine

Application #AN1390

Conditions

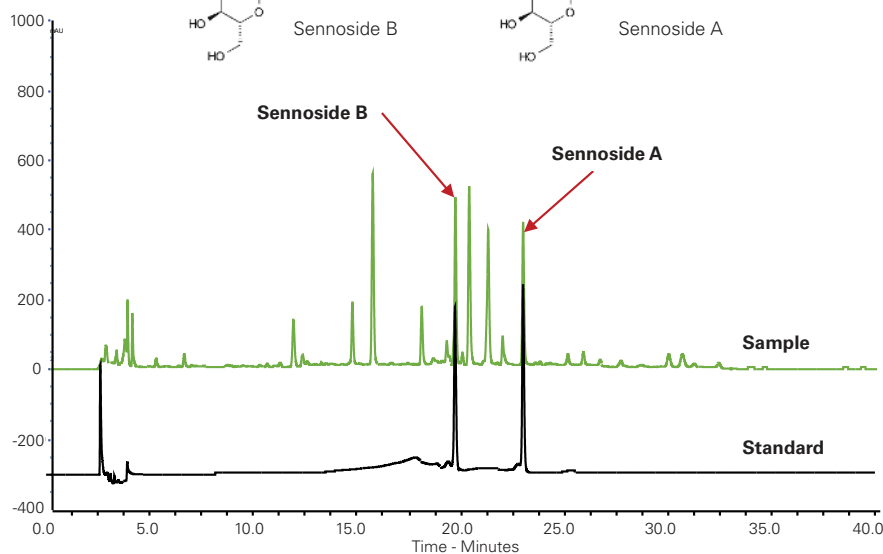
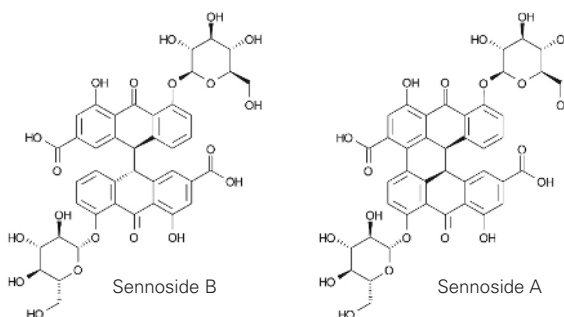
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: A: 0.75% acetic acid in H₂O
 B: MeCN/MeOH (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 9 |
| 23 | 28 |
| 40 | 28 |

Flow Rate: 0.6 mL/min
Temperature: 35 °C
Detection: UV, 271 nm
Sample: Herbal tea bag containing Folium Sennae, Peppermint, Folium Mori, Folium Nelumbinis, Glycyrrhiza Uralensis and Lalang Grass Rhizome

Analytes

Sennoside A
 Sennoside B



Reproduced with permission of Vercotech Inc., Taiwan

Sotalol

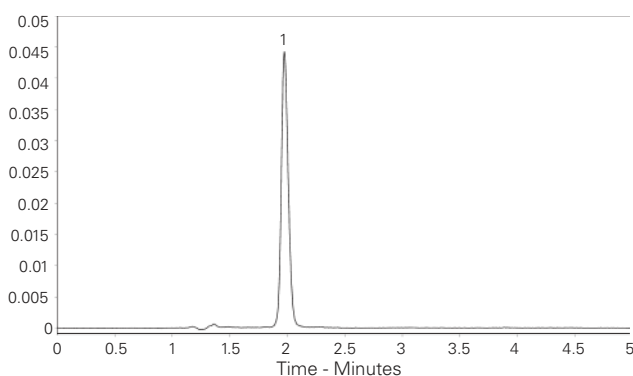
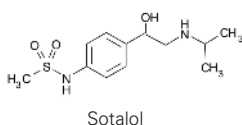
Application #AN3700

Conditions

Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: 20 mM ammonium formate pH 3.0/MeOH (85:15 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL (0.2mg/mL solution)
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Sotalol



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

Snake Venom from *Crotalus Durissus Terrificus*

Application #AN4190

Conditions

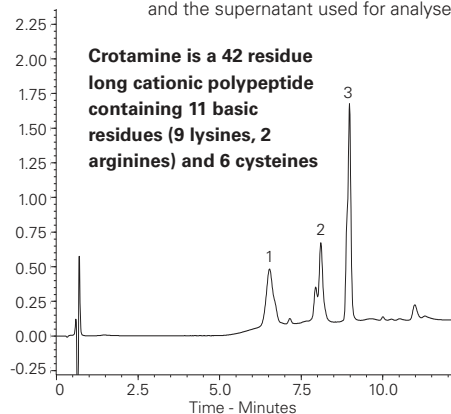
Column: ACE 3 C8-300
Dimensions: 50 x 4.6 mm
Part Number: ACE-212-0546
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in MeCN/H₂O (90:10 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 20 |
| 2 | 20 |
| 27 | 70 |

Analytes

1. Crota mine
 2. Crota potin
 3. Phospholipase A2 (PLA₂)

Flow Rate: 1.2 mL/min
Injection: 20 µL
Detection: UV, 214 nm
Sample: Lyophilised crude venom powder was solubilised (1 mg/mL) in 0.1% TFA. Resulting solutions were centrifuged and the supernatant used for analyses.



Crota mine is a 42 residue long cationic polypeptide containing 11 basic residues (9 lysines, 2 arginines) and 6 cysteines



Reproduced with permission of Center for the Study of Venoms and Venomous Animals, (CEVAP), UNESP, Sao Paulo State University, Brazil



Stability Indicating Method for HIV Injection Treatment

Application #AN4170

Conditions

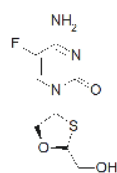
Column: ACE Excel 2 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-101-0503U
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 10 |
| 3.0 | 90 |
| 6.0 | 90 |
| 6.1 | 10 |
| 8.0 | 10 |

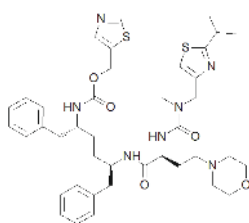
Flow Rate: 0.4 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 240 nm

Analytes

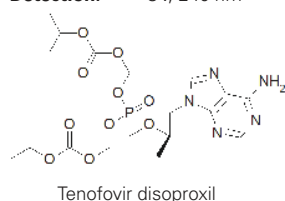
1. Emtricitabine (LLOQ 0.10 µg/mL)
2. Tenofovir disoproxil (LLOQ 0.10 µg/mL)
3. Cobicistat (LLOQ 0.20 µg/mL)
4. Elvitegravir (LLOQ 0.02 µg/mL)



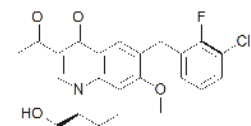
Emtricitabine



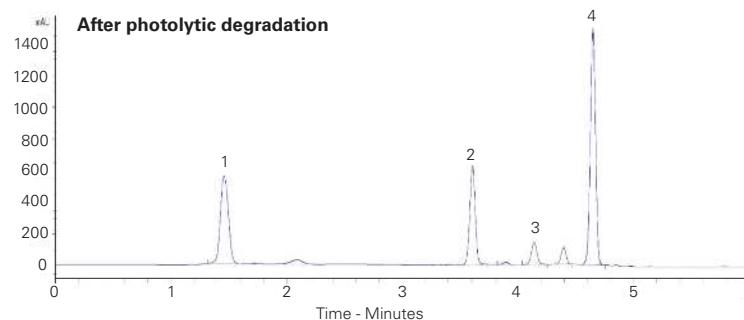
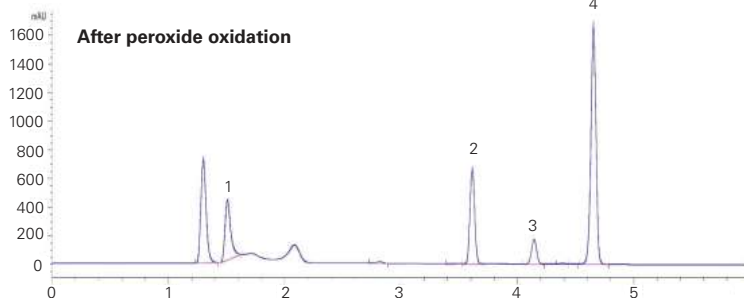
Cobicistat



Tenofovir disoproxil



Elvitegravir



Revath Naga Lakshmi P, Prahlad P, Mastananna SK., Ravindra N., Venkata Basaveswara Rao M, UPLC Separation Analysis of Emtricitabine, Tenofovir, Cobicistat and Elvitegravir from their Degradation products, Int. J. Pharm & Pharm Sci, 8(4), 362- 369 (2016)



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

Statins in Lactone and Hydroxy Acid Forms by HPLC-UV

Application #AN4360

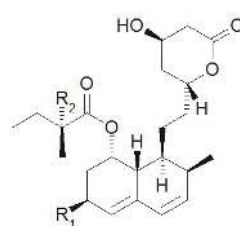
Conditions

Column: ACE Excel 3 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1111-1003U
Mobile Phase: A: MeCN
 B: 5 mM ammonium acetate pH 4.5 in H₂O
 A/B (I) 73:27 v/v (II) 55:45 v/v
Flow Rate: (I) 0.4 mL/min (II) 0.3 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: UV, 238 nm

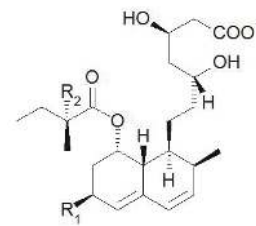
Analytes

1. Simvastatin hydroxy acid
2. 4,4-Dichlorodiphenyl trichloroethane (I.S.)
3. Simvastatin lactone
4. Pravastatin hydroxy acid
5. Griseofulvin (I.S.)
6. Pravastatin lactone

Simvastatin: R₁, R₂ = CH₃
Pravastatin: R₁ = OH, R₂ = H

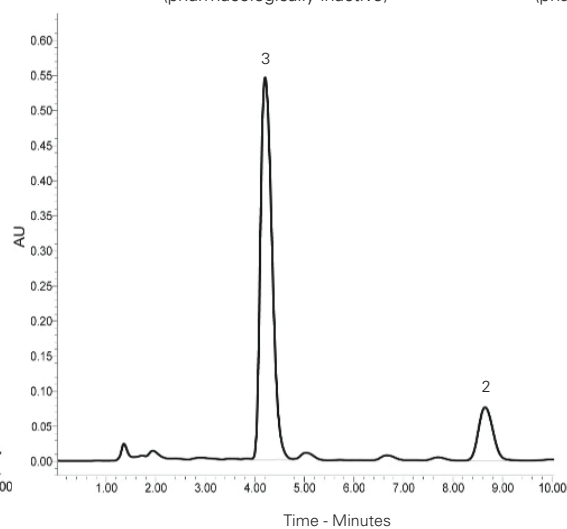
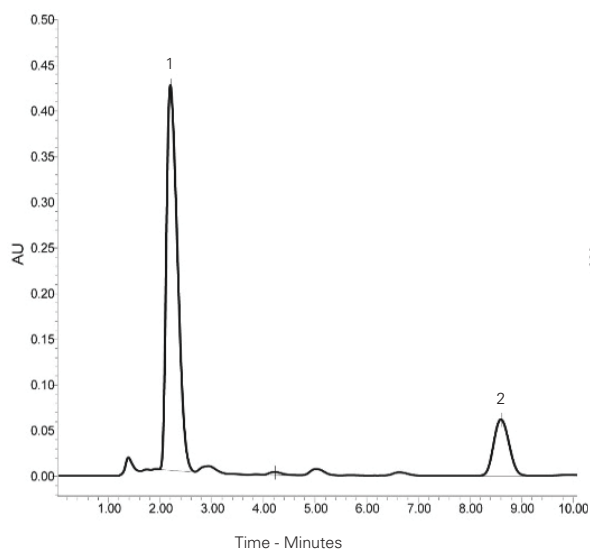


Lactone form
(pharmacologically inactive)

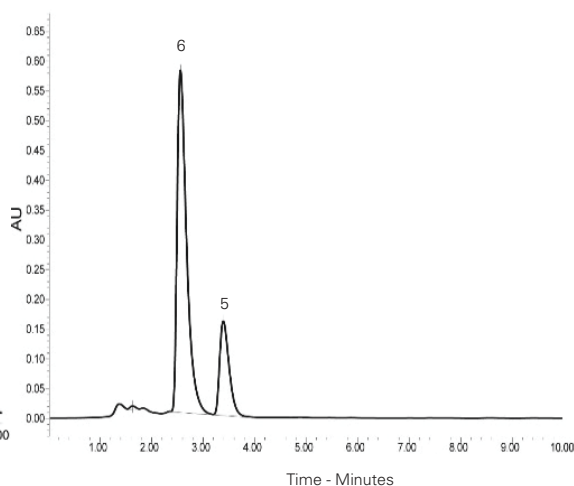
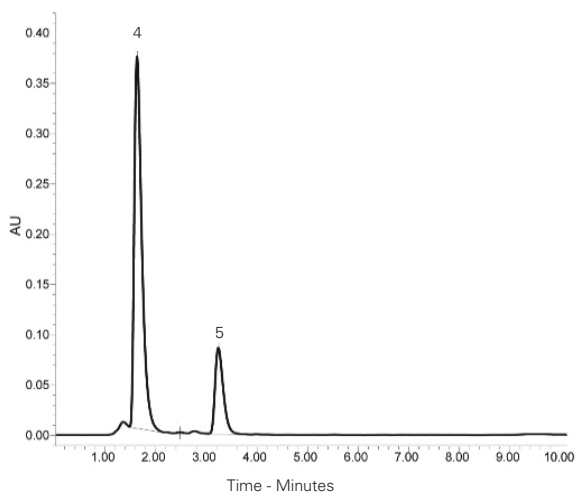


Hydroxy acid form
(pharmacologically active)

Conditions (I)



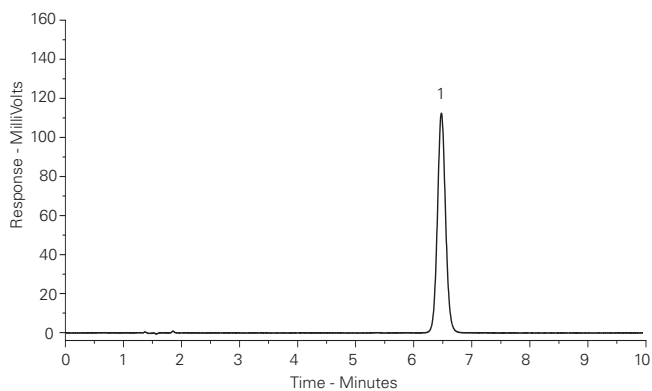
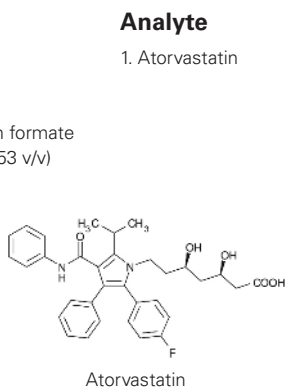
Conditions (II)





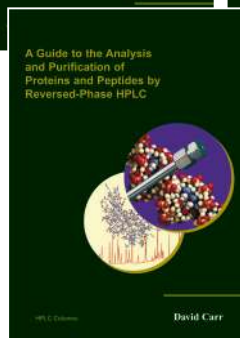
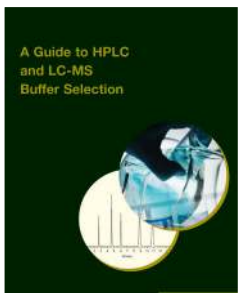
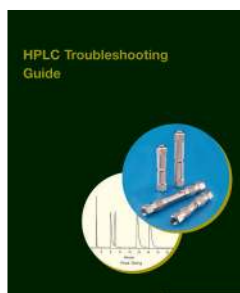
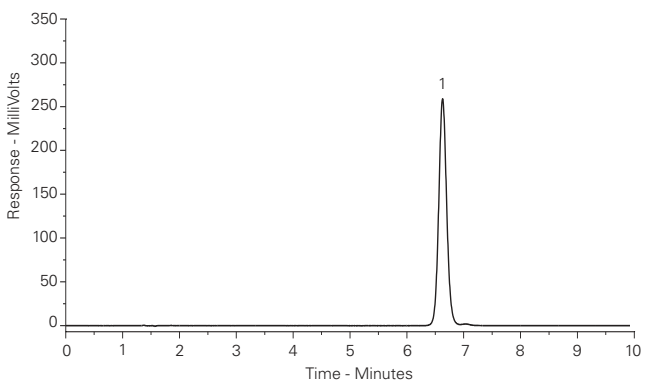
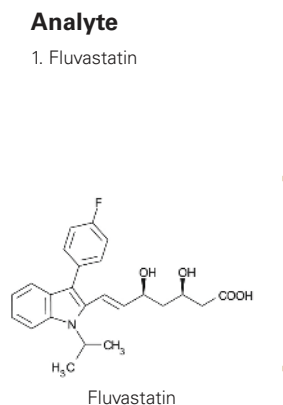
Statins – Atorvastatin
Application #AN3310

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



Statins – Fluvastatin
Application #AN3320

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



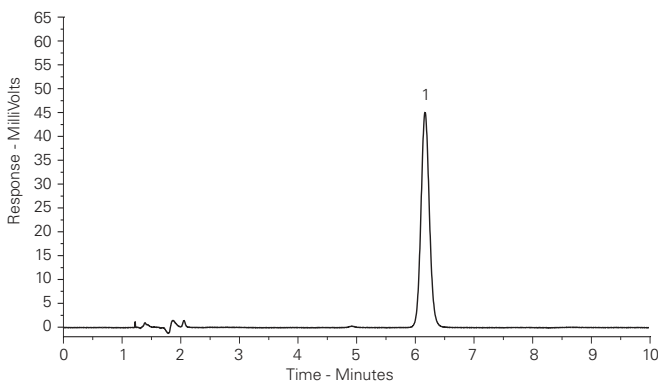
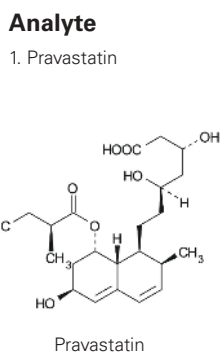
FREE HPLC Technical Guides

- HPLC Column Comparison Guide
- HPLC Protein and Peptide Guide
- HPLC & LC-MS Buffer Selection Guide
- HPLC Troubleshooting Guide

To receive your FREE copies of these guides or the latest ACE HPLC Columns Catalogue contact your local distributor or email: info@ace-hplc.com

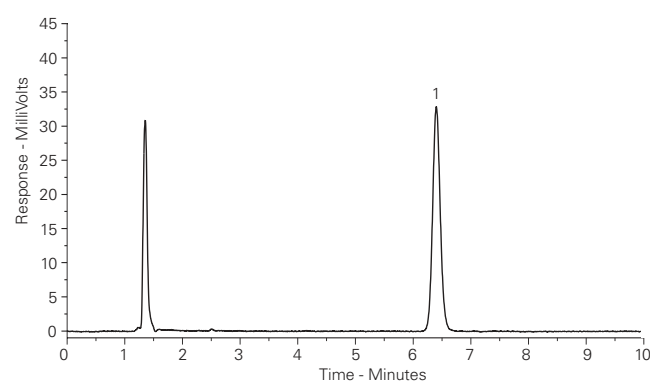
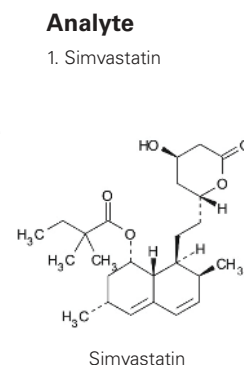
Statins – Pravastatin
Application #AN3330

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



Statins – Simvastatin
Application #AN3340

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



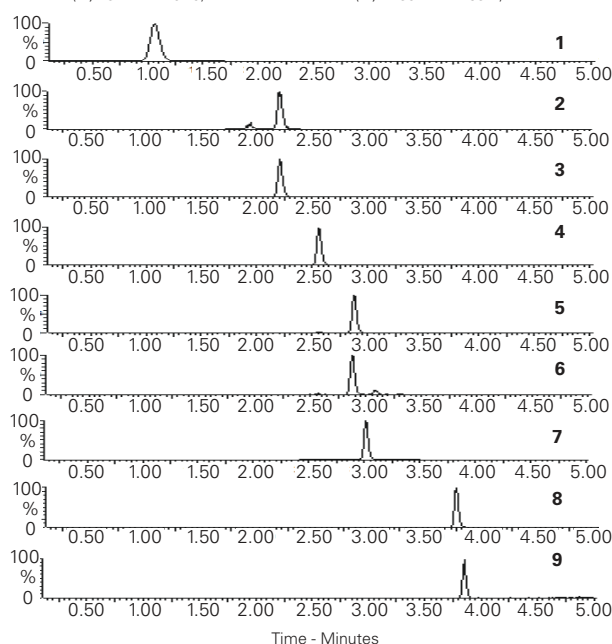
Steroid Hormones (Endogenous) by LC-MS/MS
Application #AN2640

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

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

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

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





Steroid Mixture Separation

Application #AN1060

Conditions

Column: ACE 3 C18
ACE 3 Phenyl
ACE 3 C18-AR

Dimensions: 150 x 4.6 mm

Part Number: ACE-111-1546, ACE-115-1546, ACE-119-1546

Mobile Phase: A: H₂O
B: MeCN

Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 25 |
| 24 | 46 |
| 26 | 46 |
| 27 | 25 |

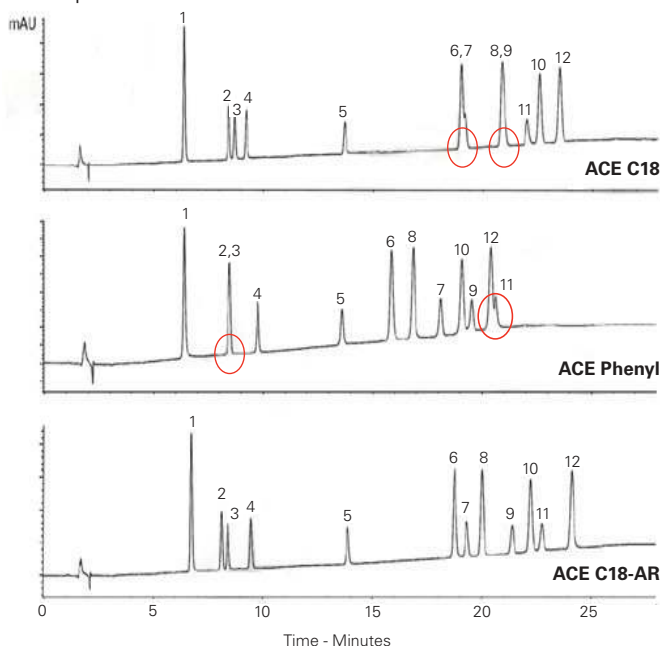
Flow Rate: 1 mL/min

Temperature: 20 °C

Detection: UV, 214 nm

Analytes

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



Steroids UHPLC-UV Analysis and Comparison

Application #AN1640

Conditions

Column: ACE Excel 2 CN-ES
ACE Excel 2 C18
ACE Excel 2 CN

Dimensions: 50 x 2.1 mm

Part Number: EXL-1013-0502U,
EXL-101-0502U,
EXL-104-0502U

Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeCN

Gradient:

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

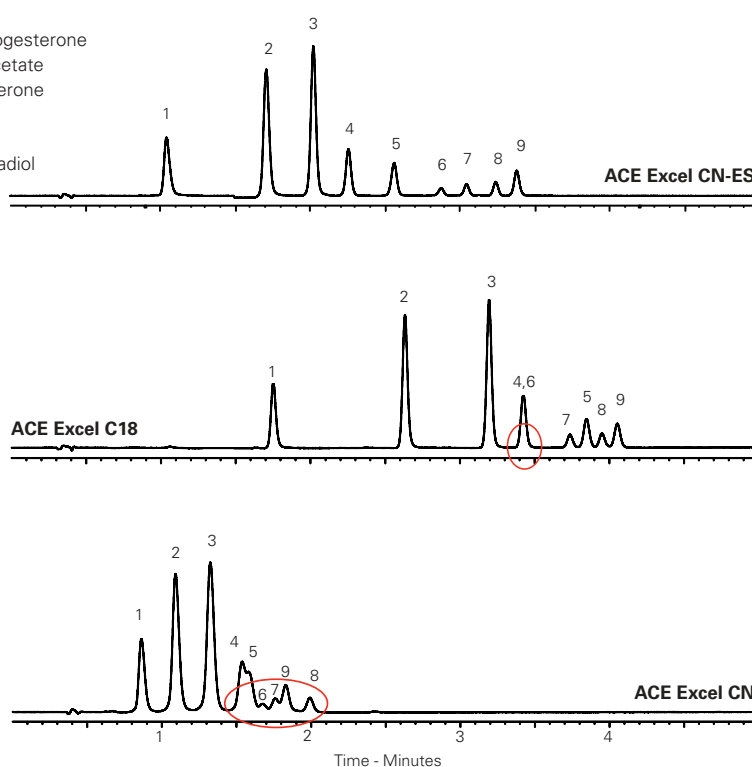
Flow Rate: 0.4 mL/min

Temperature: 40 °C

Detection: UV, 260 nm

Analytes

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



Steroids Separation using Enhanced Polar Selectivity

Application #AN2470

Conditions

Column: ACE Excel 3 C18-Amide
Dimensions: 50 x 2.1 mm
Part Number: EXL-1112-0502U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 25 |
| 10 | 80 |

Flow Rate: 0.4 mL/min
Temperature: 20 °C
Detection: UV, 260 nm

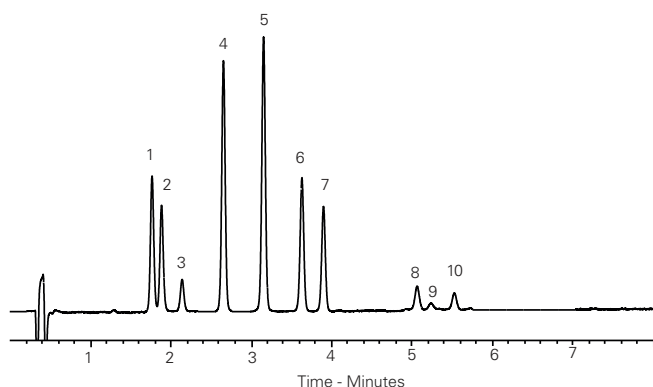
Analytes

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

Explore Selectivity

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

See page 5 for details



Steroids (Veterinary) by LC-MS/MS

Application #AN1830

Conditions

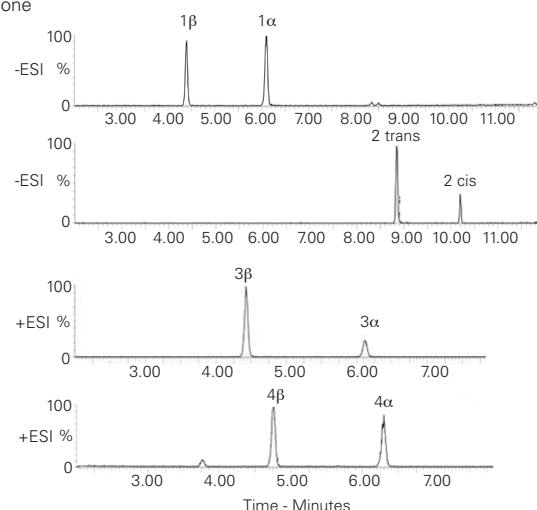
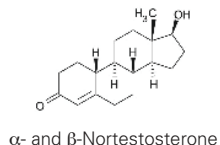
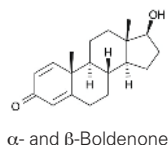
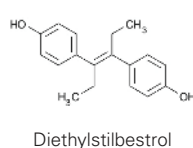
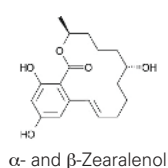
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 0.01 mM ammonium fluoride + 0.001% formic acid
 B: MeCN
Gradient:

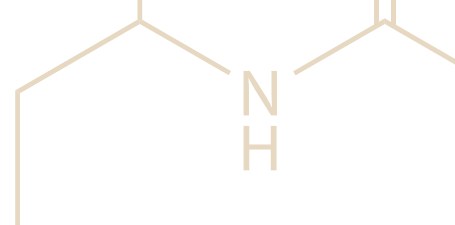
| Time (mins) | %B |
|-------------|----|
| 0.0 | 25 |
| 0.5 | 25 |
| 7.0 | 35 |
| 7.5 | 35 |
| 10.5 | 60 |
| 12.5 | 90 |

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

Analytes

1. α - and β -Zearalenol
(*m/z* 319.17 \rightarrow 275.12)
2. Diethylstilbestrol-d8
(*m/z* 275.23 \rightarrow 245.09)
Also analysed in -ESI:
Talaranol and zeranol-d4
Talaranol and zeranol
Zearalenone
Hexestrol
Diethylstilbestrol
Dienestrol
3. α - and β -Boldenone
(*m/z* 287.17 \rightarrow 121.12)
4. α - and β -Nortestosterone
(*m/z* 275.23 \rightarrow 109.09)
Also analysed in +ESI:
Hydroxystanozolol
Hydroxystanozolol-d3
Methyltestosterone
Methyltestosterone-d3
 β -Nortestosterone-d3
 β -Trenbolone
 α -Trenbolone





St John's Wort

Application #AN4300

Conditions

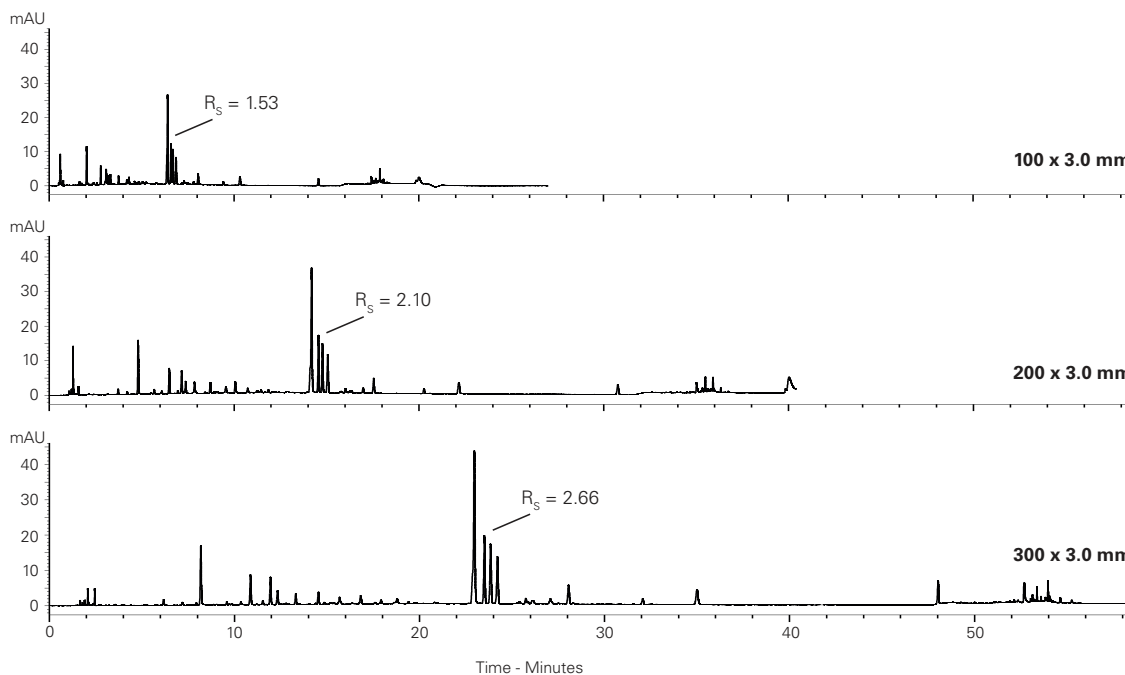
Column: ACE Excel 1.7 SuperC18
Dimensions: 100 x 3.0 mm; 2 x 100 x 3.0 mm (coupled); 3 x 100 x 3.0 mm (coupled)
Part Number: EXL-1711-1003U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN

| Gradient: | Time (mins) | | | |
|-----------|--------------|--------------|--------------|-----|
| | 100 x 3.0 mm | 200 x 3.0 mm | 300 x 3.0 mm | %B |
| - | 0.00 | 0.00 | 0.00 | 5 |
| 0.00 | 0.35 | 0.71 | 0.71 | 5 |
| 15.00 | 30.35 | 45.71 | 45.71 | 30 |
| 17.00 | 34.35 | 51.71 | 51.71 | 100 |
| 19.00 | 38.35 | 57.71 | 57.71 | 100 |
| 20.00 | 39.35 | 58.71 | 58.71 | 5 |
| 27.00 | 53.35 | 79.71 | 79.71 | 5 |

Flow Rate: 0.8 mL/min
Injection: 2 µL (100 x 3.0 mm); 4 µL (200 x 3.0 mm); 6 µL (300 x 3.0 mm)
Temperature: 80 °C
Detection: UV, 280 nm
Sample: Tablet ground to fine powder and extracted with MeCN/H₂O (1:1 v/v) with ultrasonication. Supernatant diluted with H₂O and filtered using Whatman Mini-Uniprep syringeless filter
System: Chromaster Ultra Rs



Hypericum perforatum



Substituted Methoxybenzene Isomers

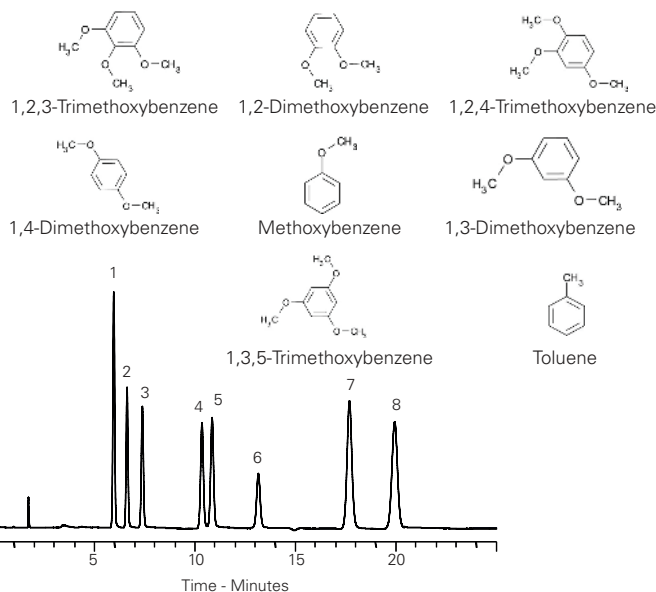
Application #AN2430

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: H₂O/MeOH (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 40 °C
Detection: UV, 214 nm

Analytes

- 1,2,3-Trimethoxybenzene
- 1,2-Dimethoxybenzene
- 1,2,4-Trimethoxybenzene
- 1,4-Dimethoxybenzene
- Methoxybenzene
- 1,3-Dimethoxybenzene
- 1,3,5-Trimethoxybenzene
- Toluene



Sugars – Cola vs Diet Cola

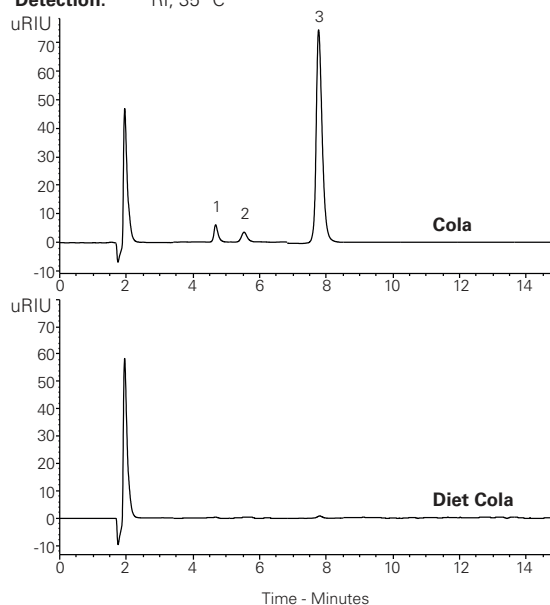
Application #AN4150

Conditions

Column: ACE Excel 3 NH₂
Dimensions: 150 x 4.6 mm
Part Number: EXL-1114-1546U
Mobile Phase: MeCN/H₂O (75:25 v/v)
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 35 °C
Detection: RI, 35 °C

Analytes

1. Fructose
2. Glucose
3. Sucrose



Sugars – Disaccharides

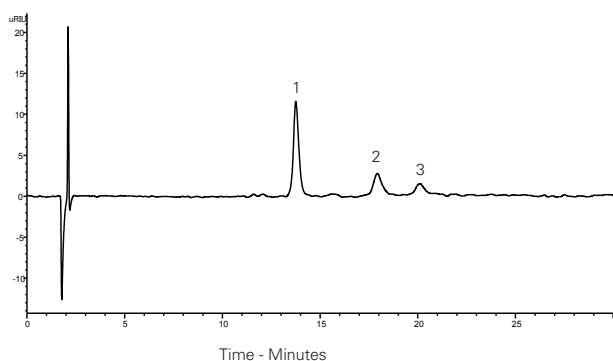
Application #AN4320

Conditions

Column: ACE Excel 3 NH₂
Dimensions: 150 x 4.6 mm
Part Number: EXL-1114-1546U
Mobile Phase: MeCN/H₂O (80:20 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 35 °C
Detection: RI, 35 °C
Sample: 2 mg/mL each disaccharide in MeCN/H₂O (80:20 v/v)
System: Chromaster 600

Analytes

1. Sucrose
2. Maltose
3. Lactose



Sugars – Lactulose

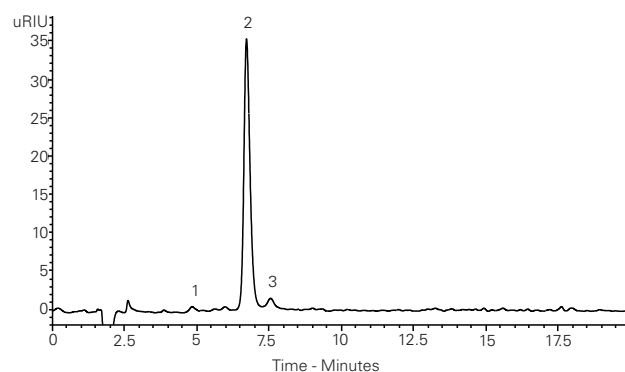
Application #AN4020

Conditions

Column: ACE Excel 5 NH₂
Dimensions: 150 x 4.6 mm
Part Number: EXL-1214-1546U
Mobile Phase: MeCN/H₂O (70:30 v/v)
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 35 °C
Detection: RI, 35 °C

Analytes

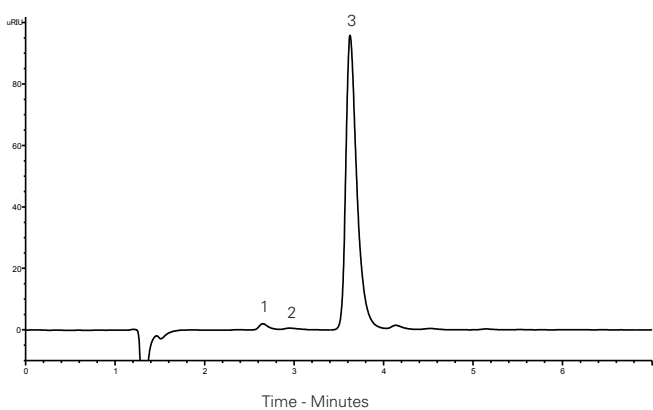
1. Galactose
2. Lactulose
3. Lactose





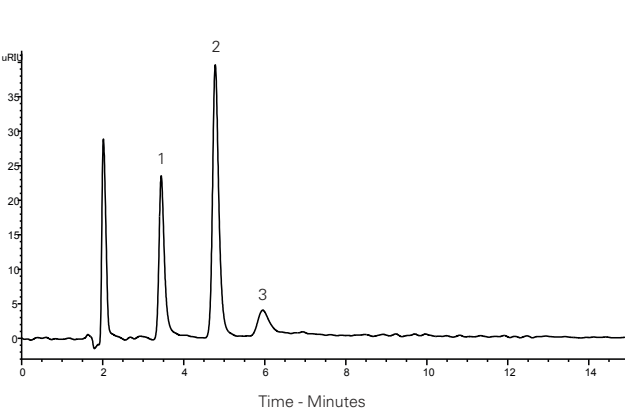
Sugars – Maple Syrup Application #AN4310

| Conditions | Analytes |
|---|-------------|
| Column: ACE Excel 1.7 NH ₂ | 1. Fructose |
| Dimensions: 100 x 3.0 mm | 2. Glucose |
| Part Number: EXL-1714-1003U | 3. Sucrose |
| Mobile Phase: MeCN/H ₂ O (70:30 v/v) | |
| Flow Rate: 0.43 mL/min | |
| Injection: 10 µL | |
| Temperature: 35 °C | |
| Detection: RI, 35 °C | |
| Sample: 100 µL maple syrup in 9900 µL mobile phase | |
| System: Chromaster 600 | |



Sugars – Monosaccharides Application #AN4330

| Conditions | Analytes |
|--|--------------|
| Column: ACE Excel 5 NH ₂ | 1. Fructose |
| Dimensions: 150 x 4.6 mm | 2. Galactose |
| Part Number: EXL-1214-1546U | 3. Rhamnose |
| Mobile Phase: MeCN/H ₂ O (75:25 v/v) | |
| Flow Rate: 1 mL/min | |
| Injection: 10 µL | |
| Temperature: 35 °C | |
| Detection: RI, 35 °C | |
| Sample: 5 mg/mL per monosaccharide in MeCN/H ₂ O (70:30 v/v) | |
| System: Chromaster 600 | |



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

Sugars – Orange Juice

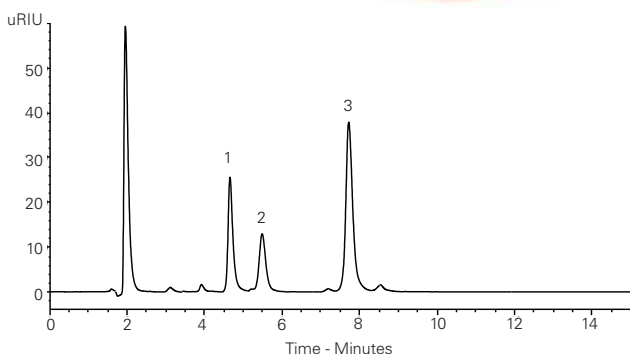
Application #AN4160

Conditions

Column: ACE Excel 3 NH₂
Dimensions: 150 x 4.6 mm
Part Number: EXL-1114-1546U
Mobile Phase: MeCN/H₂O (75:25 v/v)
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 35 °C
Detection: RI, 35 °C

Analytes

1. Fructose
2. Glucose
3. Sucrose



Sugars Separation

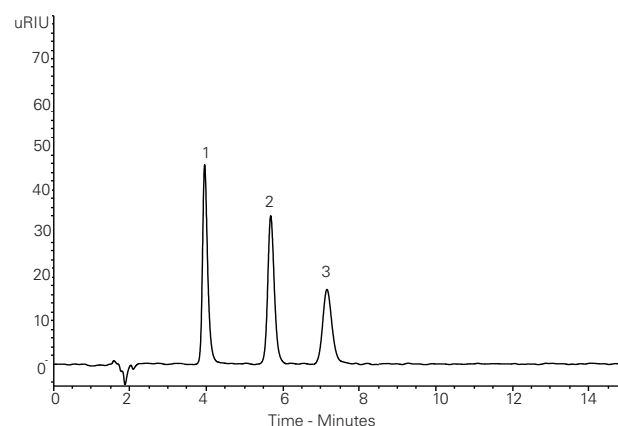
Application #AN4030

Conditions

Column: ACE Excel 5 NH₂
Dimensions: 150 x 4.6 mm
Part Number: EXL-1214-1546U
Mobile Phase: MeCN/H₂O (70:30 v/v)
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 35 °C
Detection: RI, 35 °C

Analytes

1. Fructose
2. Sucrose
3. Lactose



Sulfonamides

Application #AN1610

Conditions

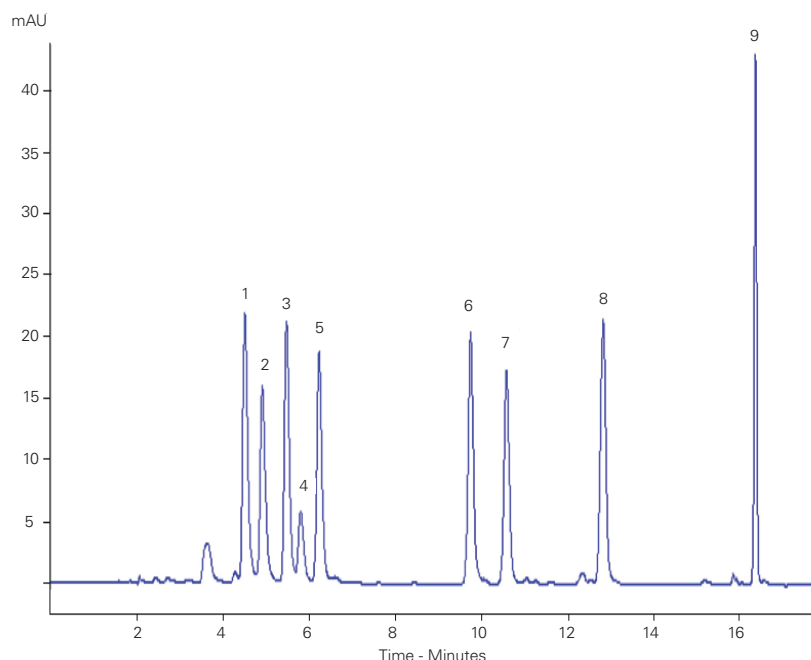
Column: ACE Excel 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: EXL-1110-1546U
Mobile Phase: A: H₂O
 B: MeCN
 C: 10% formic acid
Gradient:

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

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

Analytes

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





Sulfurous Analytes Separation Comparison

Application #AN1320

Conditions

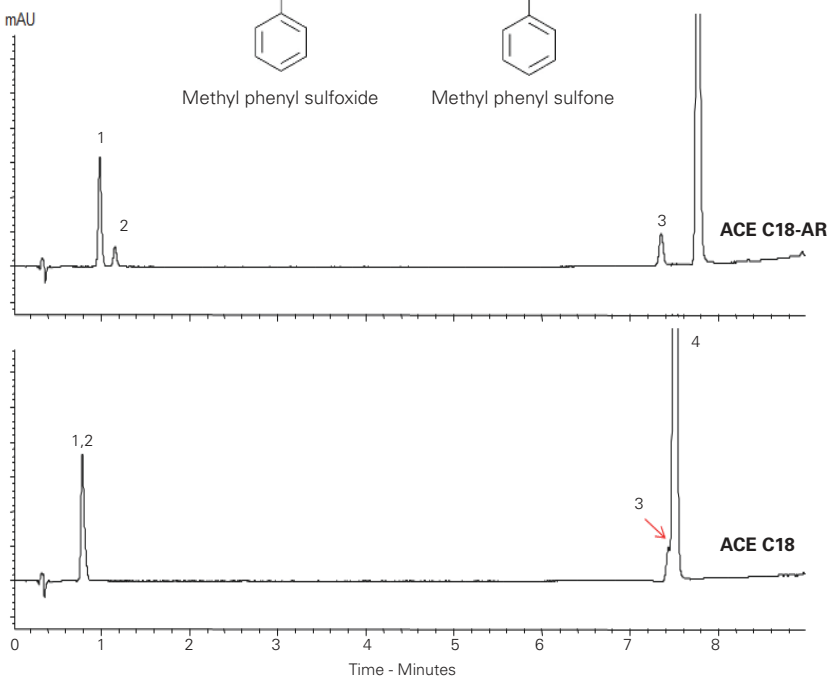
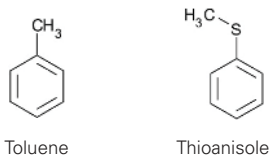
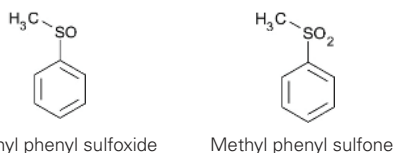
Column: ACE 3 C18-AR, ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-119-0502, ACE-111-0502
Mobile Phase: A: H₂O
 B: MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 30 |
| 5.0 | 30 |
| 9.0 | 95 |
| 9.5 | 30 |
| 13.5 | 30 |

Flow Rate: 0.5 mL/min
Injection: 1 µL
Temperature: 22 °C
Detection: UV, 254 nm

Analytes

1. Methyl phenyl sulfoxide
2. Methyl phenyl sulfone
3. Toluene
4. Thioanisole



Sumatriptan and Promethazine by LC-MS/MS

Application #AN2530

Conditions

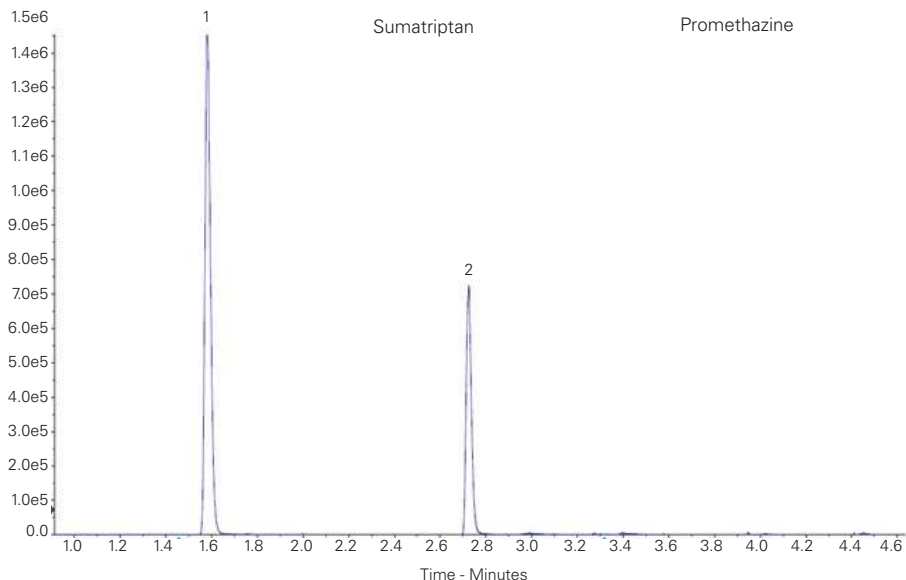
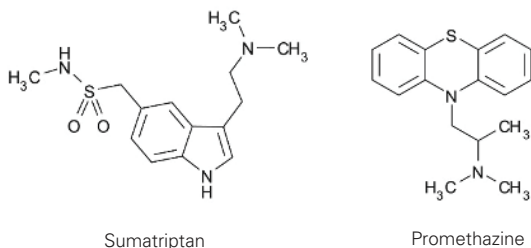
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 15 |
| 0.5 | 15 |
| 2.5 | 90 |
| 3.5 | 90 |
| 5.5 | 15 |

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

Analytes

1. Sumatriptan
(*m/z* 296 → 58)
2. Promethazine
(*m/z* 286 → 86)



Sunscreen Agents

Application #AN4370

Conditions

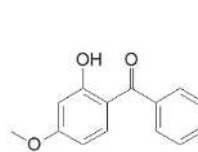
Column: ACE 3 C18
Dimensions: 150 x 4.0 mm
Part Number: ACE-111-1504
Mobile Phase: A: MeOH/H₂O (85:15 v/v)
 B: THF
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 0 |
| 7 | 0 |
| 10 | 50 |
| 14 | 50 |
| 16 | 0 |

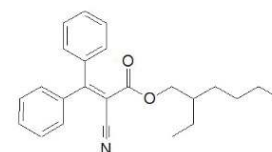
Flow Rate: 0.85 mL/min
Temperature: 30 °C
Detection: UV, 310 nm
Sample: 40 µg/mL each standard

Analytes

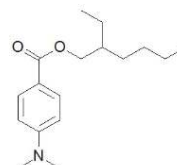
1. Benzophenone-3
2. Octocrylene
3. Octyl dimethyl PABA
4. Octyl methoxycinnamate
5. Avobenzene
6. Ethylhexyl salicylate
7. Homosalate
8. Ethylhexyl triazone
9. Tinosorb® M
10. Tinosorb® S



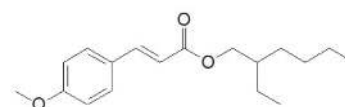
Benzophenone-3



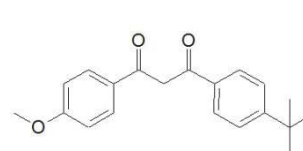
Octocrylene



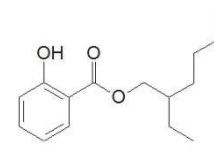
Octyl dimethyl PABA



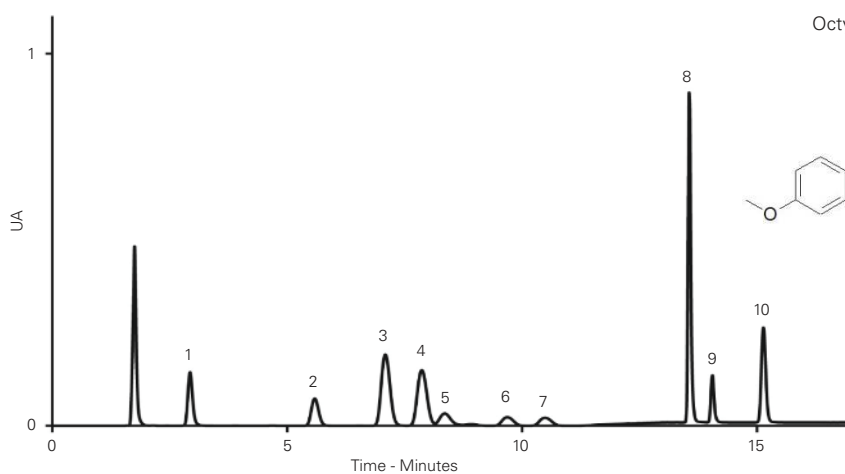
Octyl methoxycinnamate



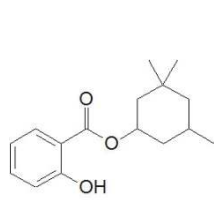
Avobenzene



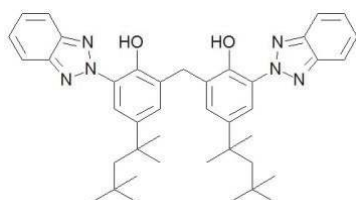
Ethylhexyl salicylate



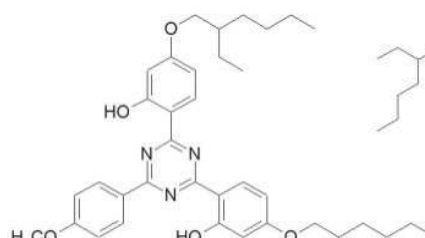
Reproduced with permission of Department of Analytical Chemistry, Institute of Chemistry, University of Campinas, Brazil



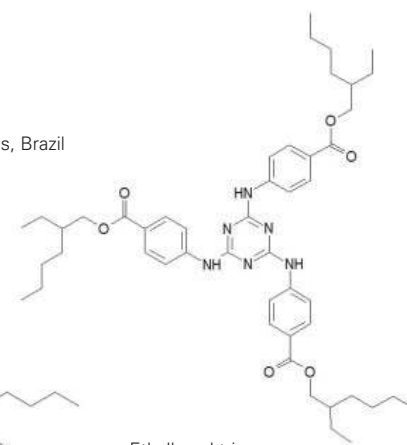
Homosalate



Tinosorb® M



Tinosorb® S



Ethylhexyl triazone

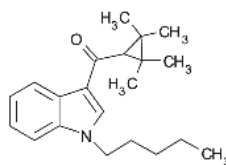


Synthetic Cannabinoids (SPICE) from Oral Fluid

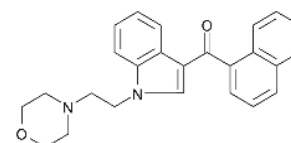
Application #AN1650

Conditions

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



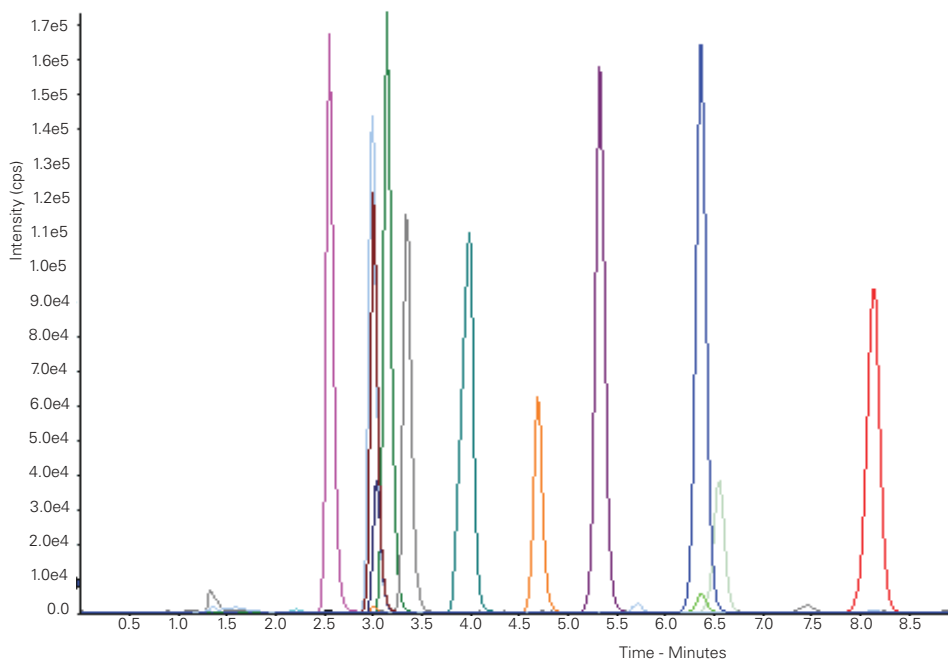
UR - 144



JWH - 200

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

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



Reproduced with permission of Biotage®, Charlotte, NC, USA. See Biotage Application note AN791 for further details of extraction & analysis.

Taxol in Fungal Extract by LC-MS/MS

Application #AN1670

Conditions

Column: ACE UltraCore 2.5 SuperC18**Dimensions:** 150 x 2.1 mm**Part Number:** CORE-25A-1502U**Mobile Phase:** A: 0.5% formic acid in H₂O
B: 0.5% formic acid in MeCN**Gradient:**

| Time (mins) | %B |
|-------------|----|
| 0.0 | 10 |
| 1.0 | 10 |
| 3.0 | 40 |
| 22.0 | 60 |
| 25.0 | 95 |

0.0 10

1.0 10

3.0 40

22.0 60

25.0 95

Flow Rate: 0.35 mL/min**Detection:** Orbitrap Elite MS

FT positive ion mode

Collision induced dissociation isolation width 5 Da

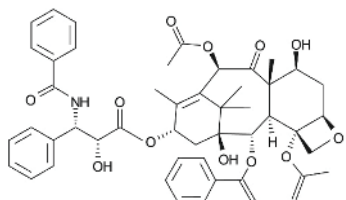
Normalised collision energy 32 eV

Activation Q 0.25

Activation times 10 ms

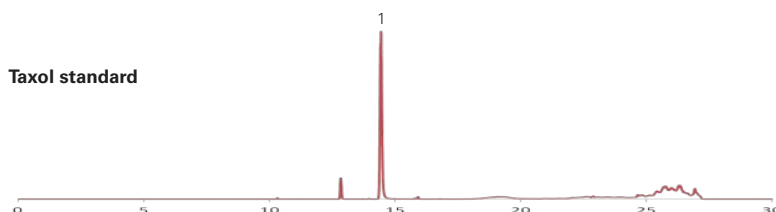
Analyte

1. Taxol (Paclitaxel)

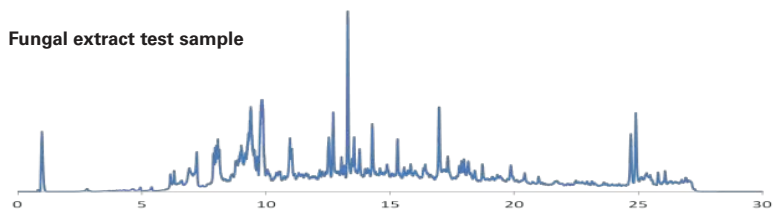
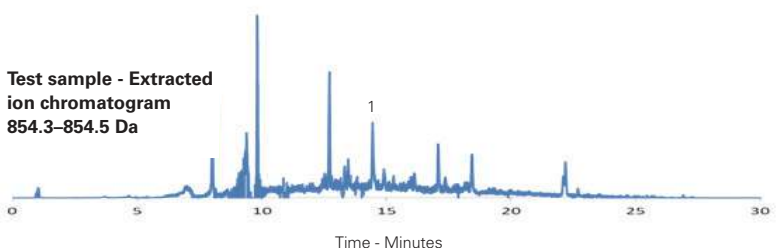


Taxol (Paclitaxel)

Taxol standard



Fungal extract test sample

Test sample - Extracted ion chromatogram
854.3–854.5 Da

Time - Minutes

Reproduced with permission of University of Bristol, UK

Telithromycin Analysis

Application #AN3280

Conditions

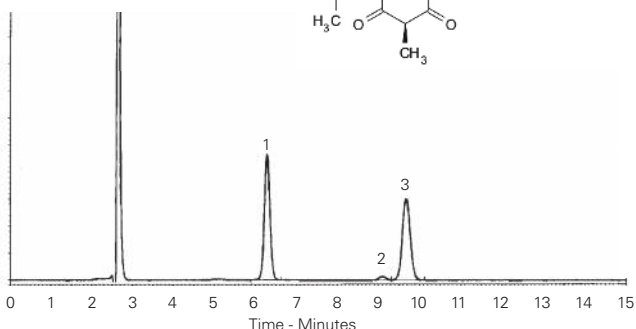
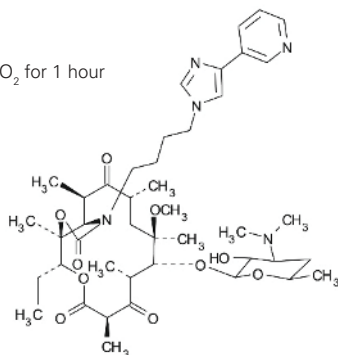
Column: ACE 5 C18**Dimensions:** 250 x 4.6 mm**Part Number:** ACE-121-2546**Mobile Phase:** 0.05 M phosphate buffer pH
4.0/MeOH (45:55 v/v)**Flow Rate:** 1 mL/min**Injection:** 20 µL**Temperature:** 50 °C**Detection:** UV, 265 nm**Sample:** Exposed to 3% H₂O₂ for 1 hour

Analytes

1. Telithromycin

2. Degradant 1

3. Degradant 2



Reproduced with permission of Brazilian Pharmacopoeia

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

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



Terfenadine and Fexofenadine in Rat Plasma

Application #AN3290

Conditions

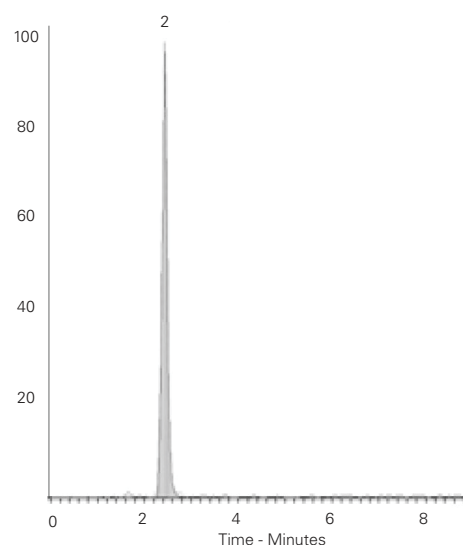
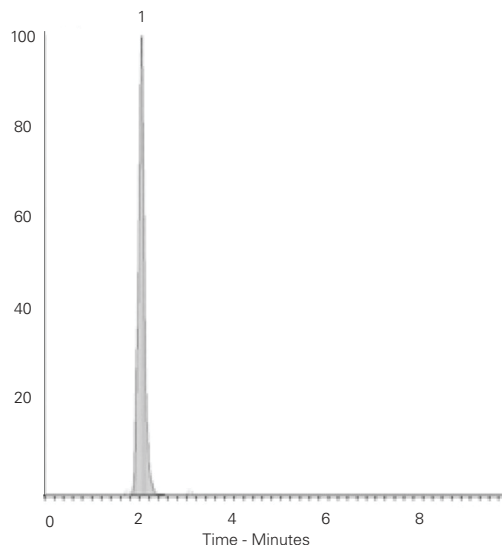
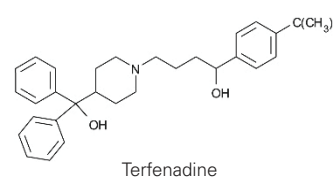
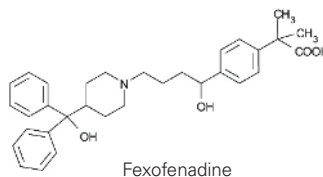
Column: ACE 5 AQ
Dimensions: 50 x 3.0 mm
Part Number: ACE-126-0503
Mobile Phase: A: 0.1% formic acid in H₂O
 B: MeOH
Gradient:

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

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

Analytes

1. Fexofenadine
(*m/z* 502.3 → 466.3)
2. Terfenadine
(*m/z* 472.3 → 436.3)



Reproduced with permission of Aptuit, Edinburgh, UK

Testosterone

Application #AN3300

Conditions

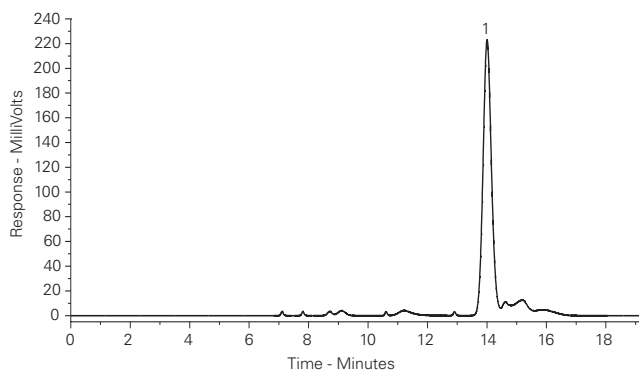
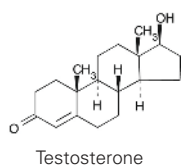
Column: ACE 5 C18
Dimensions: 150 x 0.075 mm
Part Number: ACE-121-1500075
Mobile Phase: A: 0.1% formic acid in MeCN/0.1% formic acid in H₂O (10:90 v/v)
 B: 0.1% formic acid in MeCN/0.1% formic acid in H₂O (90:10 v/v)
Gradient:

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

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

Analyte

1. Testosterone



Reproduced with permission of University of London, UK

Tetracyclines

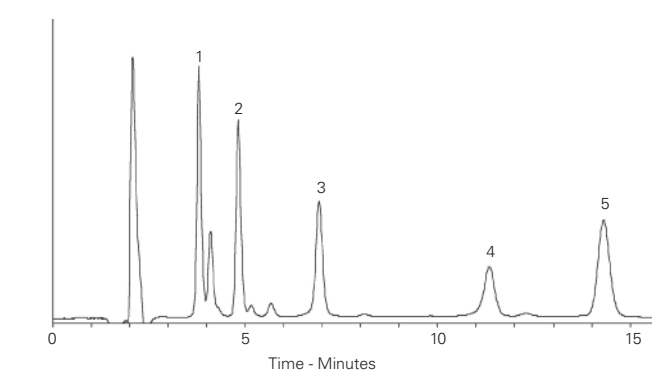
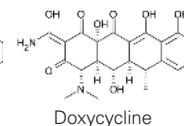
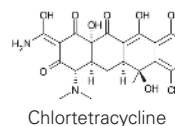
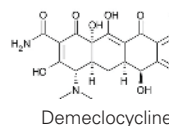
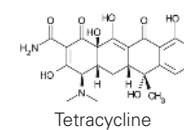
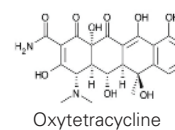
Application #AN3680

Conditions

Column: ACE 5 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-121-1503
Mobile Phase: 10 mM oxalic acid pH 2.9/MeCN (80:20 v/v)
Flow Rate: 0.5 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV-Vis, 350 nm

Analytes

1. Oxytetracycline
2. Tetracycline
3. Demeclocycline
4. Chlortetracycline
5. Doxycycline



Reproduced with permission of Fera Science Ltd, York, UK

Thyroid Hormones by LC-MS/MS (I)

Application #AN2170

Conditions

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

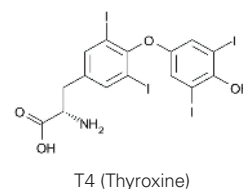
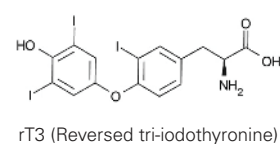
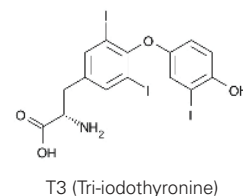
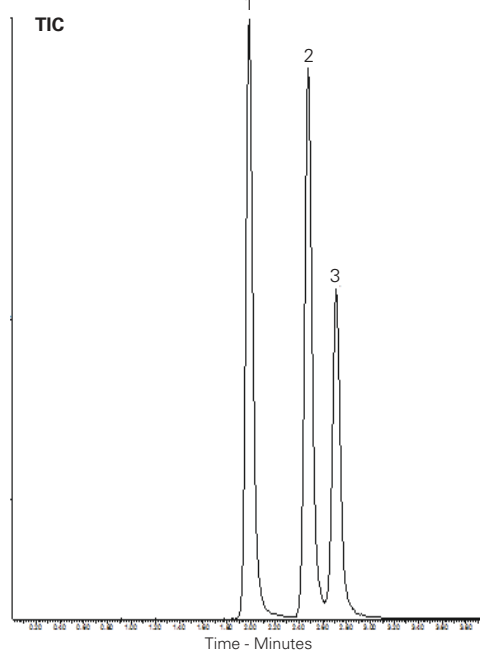
| Time (mins) | %B |
|-------------|----|
| 0.0 | 60 |
| 3.0 | 77 |
| 3.1 | 60 |

Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: XEVO TQS triple quad MS
 Desolvation temperature: 500 °C
 Ion source temperature: 150 °C
 Positive mode ESI, MRM
Sample: Serum samples extracted using Biotage EVOLUTE EXPRESS AX methodology

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

Analytes

1. T3 (Tri-iodothyronine)
2. rT3 (Reversed tri-iodothyronine)
3. T4 (Thyroxine)



Reproduced with permission of Biotage GB Ltd, UK

Tocopherols Mixture Separation

Application #AN3390

Conditions

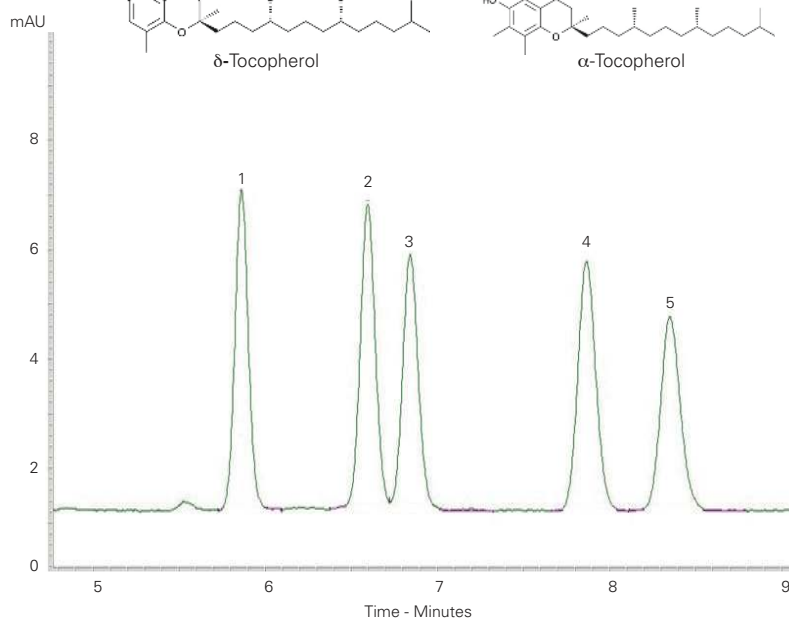
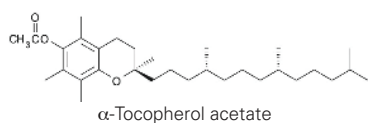
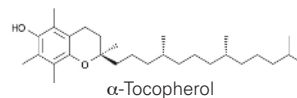
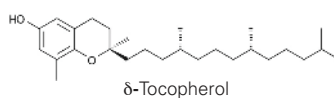
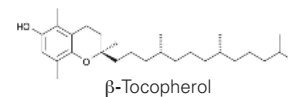
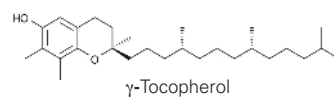
Column: ACE Excel 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: EXL-1110-1546U
Mobile Phase: A: 0.1% H₃PO₄/MeCN (1:3 v/v)
 B: MeCN
Gradient:

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

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

Analytes

1. γ-Tocopherol
2. β-Tocopherol
3. δ-Tocopherol
4. α-Tocopherol
5. α-Tocopherol acetate



Reproduced with permission of WIREC-WESSLING International Research and Educational Centre, Budapest, Hungary



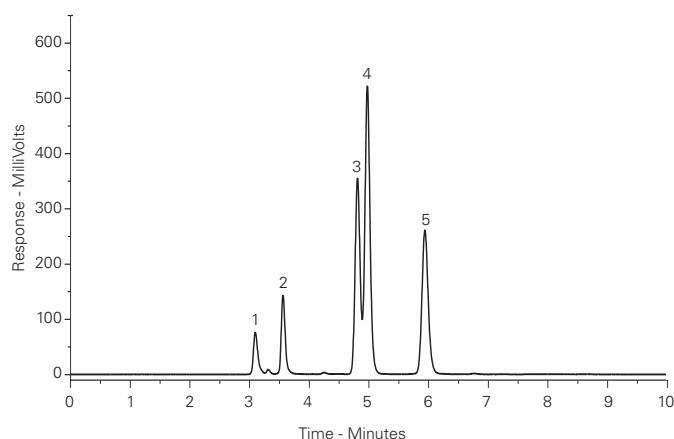
Tocopherols Application #AN2790

Conditions

Column: ACE 5 SIL
Dimensions: 250 x 4.6 mm
Part Number: ACE-127-2546
Mobile Phase: Hexane/IPA (98:2 v/v)
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: Ambient
Detection: UV-Vis, 450 nm

Analytes

1. γ-Tocopherol
2. α-Tocopherol
3. β-Tocopherol
4. β-Tocopherol
5. δ-Tocopherol



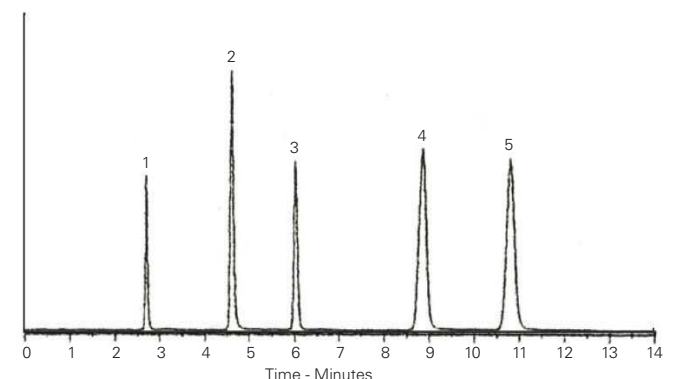
Tricyclic Antidepressants Application #AN3920

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeOH/25 mM KH₂PO₄ pH 6.0 in H₂O (80:20 v/v)
Flow Rate: 1 mL/min
Temperature: 22 °C
Detection: UV, 215 nm

Analytes

1. Norephedrine
2. Nortriptyline
3. Toluene
4. Imipramine
5. Amitriptyline



Toxins from Amanita Phalloides Mushrooms by LC-HRMS Application #AN4060

Conditions

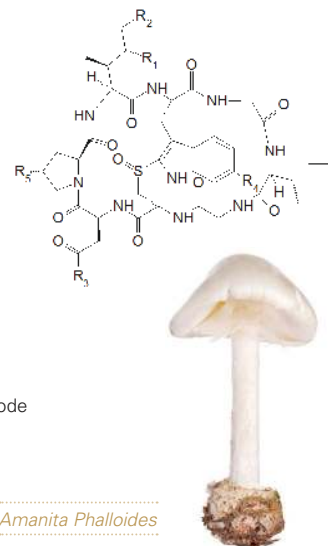
Column: ACE 3 AQ
Dimensions: 150 x 3.0 mm
Part Number: ACE-116-1503
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0 | 15 |
| 17 | 100 |
| 22 | 100 |
| 22 | 15 |
| 30 | 15 |

Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 50 °C
Detection: Thermo Exactive MS
 ESI in positive ion mode

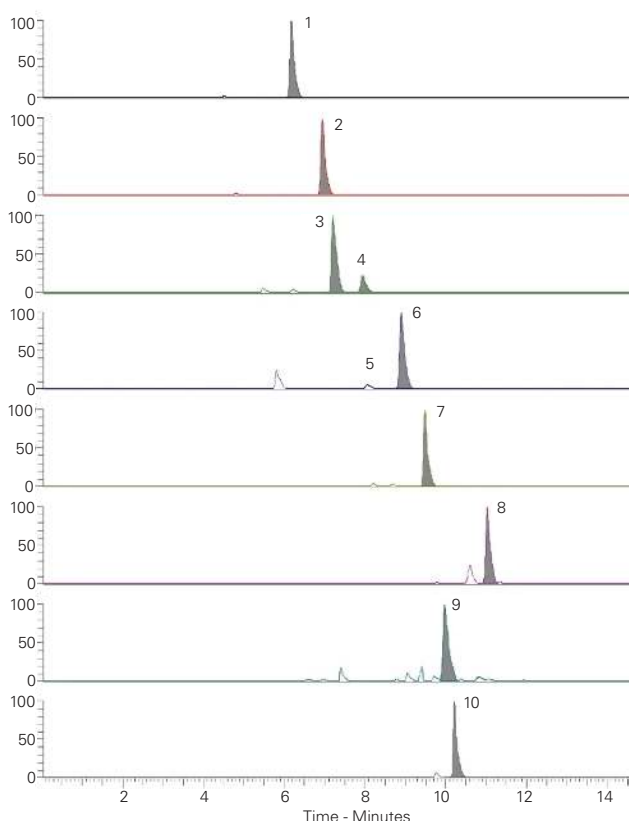
Analyte

1. Amatoxins



Amanita Phalloides

| Peak | Analyte | R1 | R2 | R3 | R4 | R5 | Exact Mass |
|------|------------------|----|----|-----------------|----|----|------------|
| 1 | α - Amanitin | OH | OH | NH ₂ | OH | OH | 918.35417 |
| 2 | β - Amanitin | OH | OH | OH | OH | OH | 919.338182 |
| 3 | γ - Amanitin | H | OH | NH ₂ | OH | OH | 902.359252 |
| 4 | Amaninamide | OH | OH | NH ₂ | H | OH | 902.359252 |
| 5 | Amanin | OH | OH | OH | H | OH | 903.343267 |
| 6 | ε - Amanitin | H | OH | OH | OH | OH | 903.343267 |
| 7 | Amanullin | H | H | NH ₂ | OH | OH | 886.364337 |
| 8 | Proamanullin | H | H | NH ₂ | OH | H | 870.369423 |
| 9 | Amanullinic Acid | H | H | OH | OH | OH | 887.348353 |
| 10 | Bacitracin (IS) | - | - | - | - | - | 1421.7489 |



Reproduced with permission of Fera Science Ltd, York, UK

Tricyclic Antidepressants (Gradient)

Application #AN1690

Conditions

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

Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 50 |
| 6.0 | 70 |
| 7.0 | 70 |
| 7.5 | 50 |

Flow Rate: 1.2 mL/min

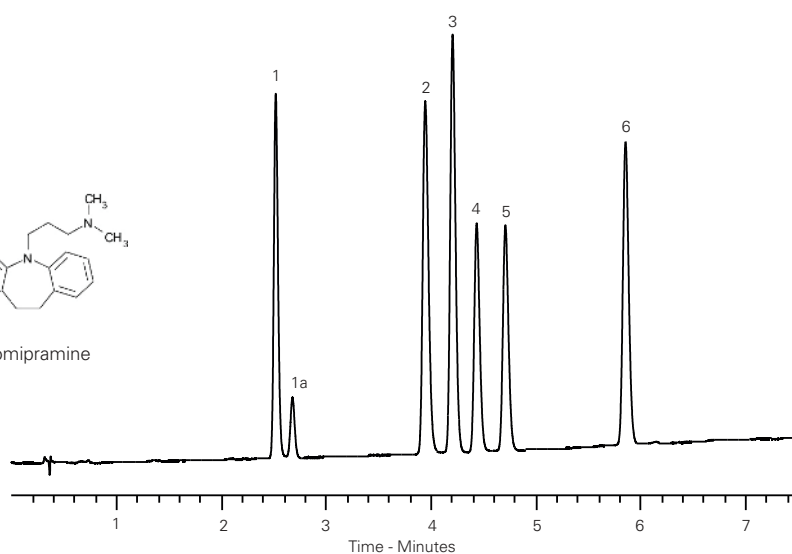
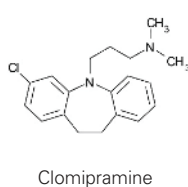
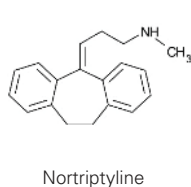
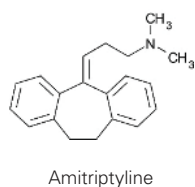
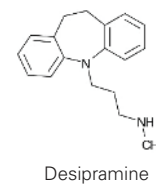
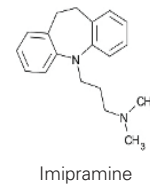
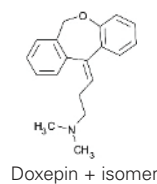
Injection: 2 µL

Temperature: 40 °C

Detection: UV, 260 nm

Analytes

1. Doxepin + isomer
2. Imipramine
3. Desipramine
4. Amitriptyline
5. Nortriptyline
6. Clomipramine



Tricyclic Antidepressants (Isocratic)

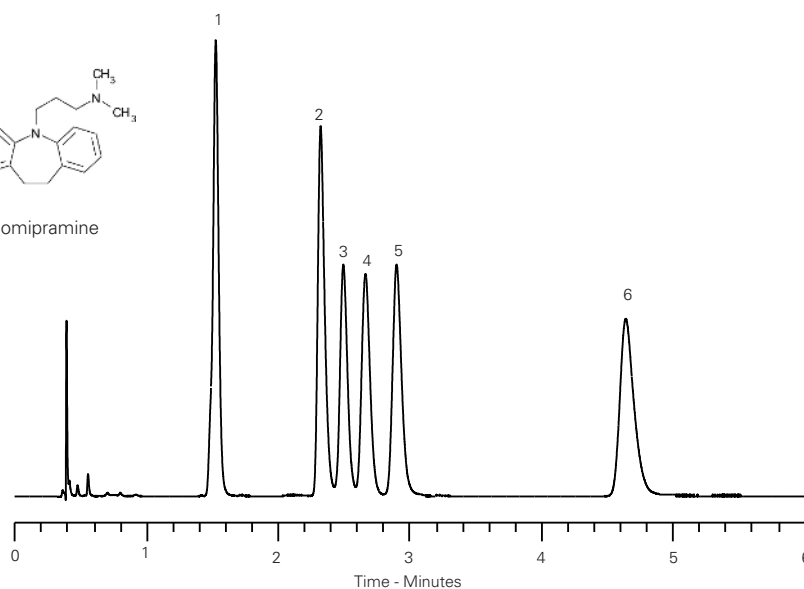
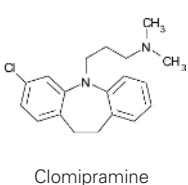
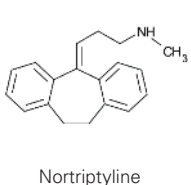
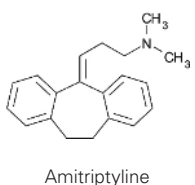
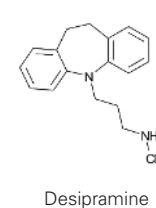
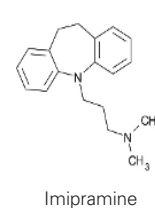
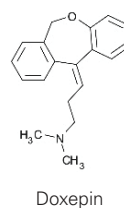
Application #AN1680

Conditions

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

Analytes

1. Doxepin
2. Imipramine
3. Desipramine
4. Amitriptyline
5. Nortriptyline
6. Clomipramine





Tricyclic Antidepressants (Isocratic Rapid Analysis)

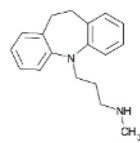
Application #AN1700

Conditions

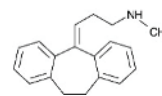
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 20 mM ammonium acetate pH 6.3
 MeCN/H₂O (65:35 v/v)
Flow Rate: 1.5 mL/min
Injection: 10 µL
Temperature: 60 °C
Detection: UV, 215 nm

Analytes

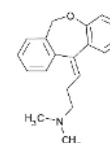
1. Desipramine
2. Nortriptyline
3. Doxepin
4. Imipramine
5. Amitriptyline



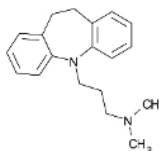
Desipramine



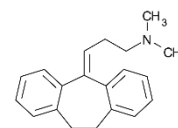
Nortriptyline



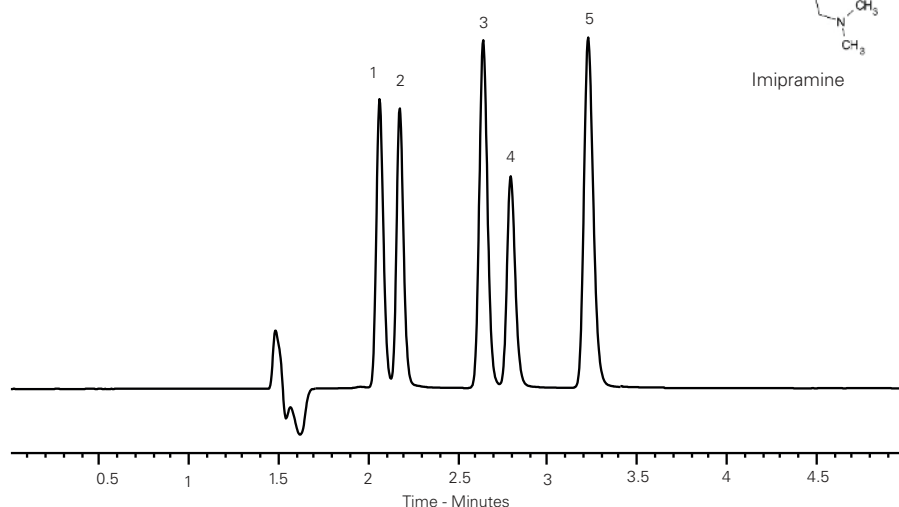
Doxepin



Imipramine



Amitriptyline



ACE Method Development Kits

Intelligent Solutions for Method Development



- **Highly cost effective** - 2 and 3 column kits available for the same price as a single column
- **4 different Method Development Kits** available in dimensions from microbore (0.5 mm id) through to analytical (4.6 mm id) for rapid, systematic method development.
- Carefully selected ACE phases enabling the power of selectivity to be fully exploited
- Each ACE phase provides different selectivity due to differing interactions

FREE Application Support and FREE Method Development Service

Learn more: www.ace-hplc.com or email: info@ace-hplc.com

Triple API Pharmaceutical and Related Substances using Ultra Resolution

Application #AN3560

Conditions

Column: ACE Excel 1.7 SuperC18
Dimensions: 100 x 3.0 mm; 2 x 100 x 3.0 mm (coupled); 3 x 100 x 3.0 mm (coupled)
Part Number: EXL-1711-1003U
Mobile Phase: A: H₂O
 B: MeCN
 C: 200 mM ammonium formate pH 3.0

Analytes

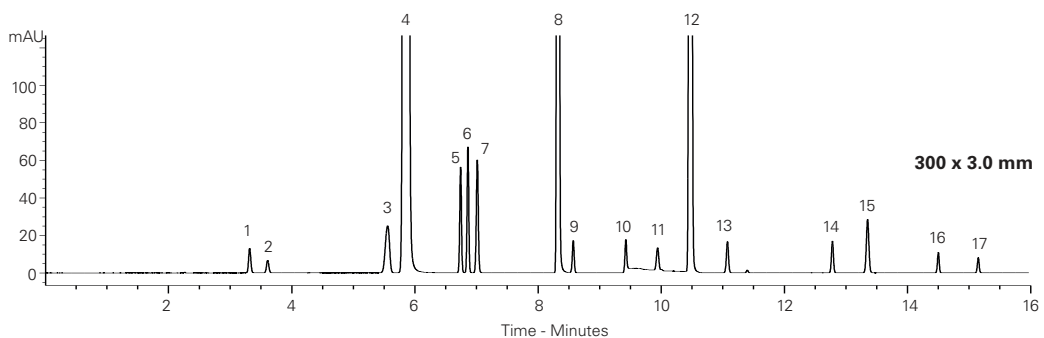
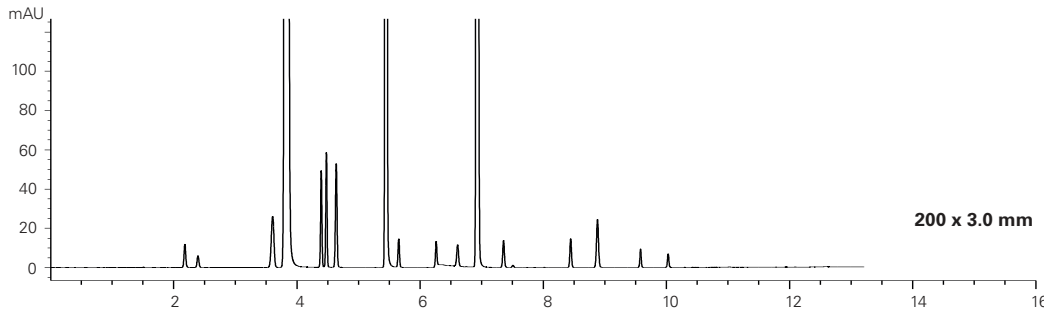
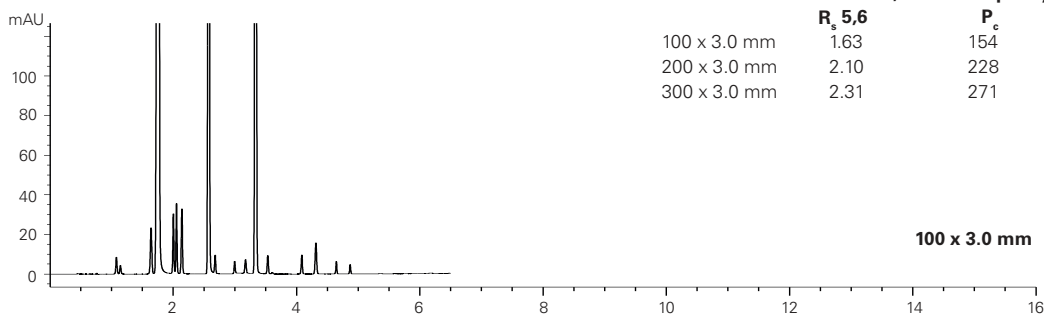
- | | | |
|------------------|---------------------------|---------------------------------|
| 1. 2-Aminophenol | 7. 4-Hydroxybenzoic acid | 13. 4-Nitrophenol |
| 2. Hydroquinone | 8. Caffeine | 14. 4-Chloroacetanilide |
| 3. Theobromine | 9. 2-Acetamidophenol | 15. 2-Nitrophenol |
| 4. Paracetamol | 10. 2-Hydroxybenzoic acid | 16. Acetylsalicylsalicylic acid |
| 5. Paraxanthine | 11. Phenol | 17. Salsalate |
| 6. Theophylline | 12. Aspirin | |

Gradient:

| Time (mins) | Time (mins) | | | %A | %B | %C |
|-------------|--------------|--------------|--------------|----|----|----|
| | 100 x 3.0 mm | 200 x 3.0 mm | 300 x 3.0 mm | | | |
| - | 0.00 | 0.00 | 0.00 | 90 | 5 | 5 |
| 0.00 | 1.21 | 2.41 | 2.41 | 90 | 5 | 5 |
| 5.00 | 11.21 | 17.41 | 17.41 | 20 | 75 | 5 |
| 6.00 | 12.21 | 18.41 | 18.41 | 20 | 75 | 5 |
| 6.50 | 13.21 | 19.41 | 19.41 | 90 | 5 | 5 |

Flow Rate: 0.8 mL/min
Temperature: 80 °C
Detection: UV, 270 nm

| Dimensions | Resolution, R _s 5,6 | Peak Capacity, P _c |
|--------------|--------------------------------|-------------------------------|
| 100 x 3.0 mm | 1.63 | 154 |
| 200 x 3.0 mm | 2.10 | 228 |
| 300 x 3.0 mm | 2.31 | 271 |





Tyrosine, Tryptophan and Tramadol by HPLC with Fluorescence Detection

Application #AN4180

Conditions

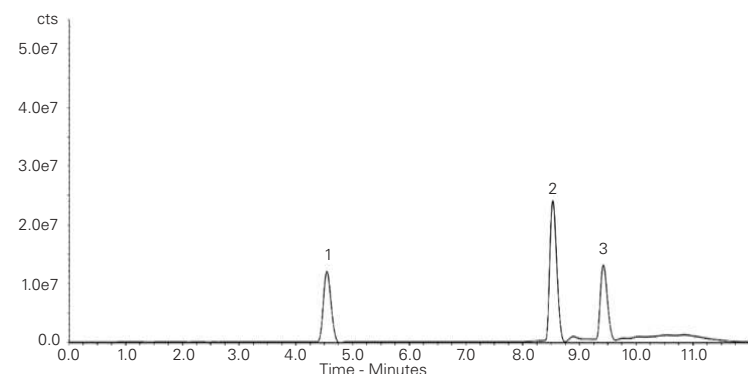
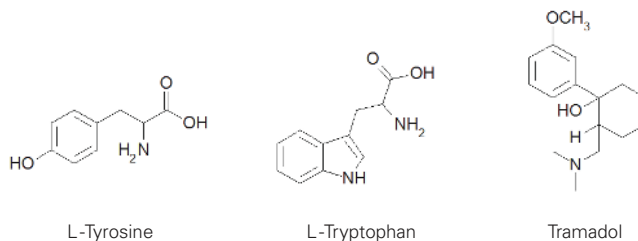
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: A: 50 mM NaH₂PO₄ in H₂O
 B: MeCN/H₂O (60:40 v/v)
Gradient:

| Time (mins) | %B |
|-------------|-----|
| 0.0 | 0 |
| 5.0 | 10 |
| 8.0 | 100 |
| 9.0 | 100 |
| 9.5 | 0 |
| 14.0 | 0 |

Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: Fluorescence, λ_{Ex} 280 nm, λ_{Em} 340 nm

Analytes

1. L-Tyrosine
2. L-Tryptophan
3. Tramadol



Reproduced with permission of Centre for the Research and Technology in Agro-Environmental and Biological Sciences, University of Trás-os-Montes and Alto Douro (UTAD-CITAB), Portugal

USP Monograph – 17α-Ethinylestradiol

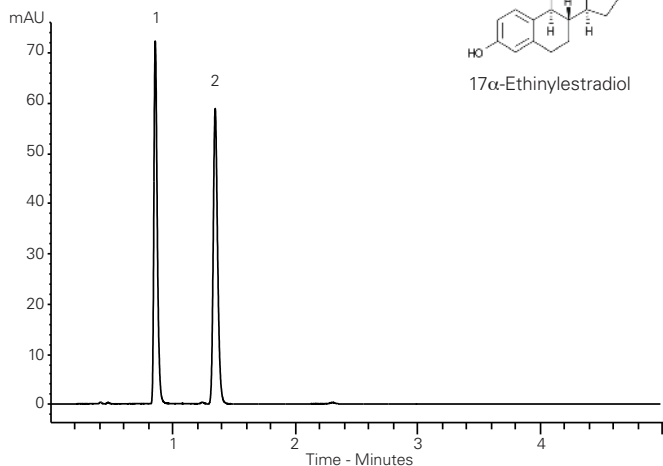
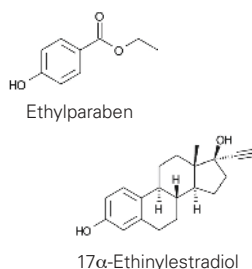
Application #AN1710

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: H₂O/MeCN (50:50 v/v)
Flow Rate: 0.43 mL/min
Injection: 3.1 µL
Temperature: Ambient (22 °C)
Detection: UV, 280 nm

Analytes

1. Ethylparaben
2. 17α-Ethinylestradiol



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Amlodipine Besylate

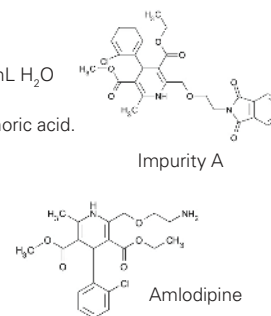
Application #AN2550

Conditions

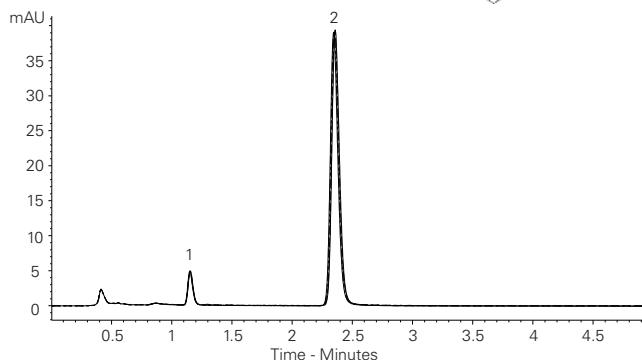
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 75 x 3.0 mm
Part Number: CORE-25A-7503U
Mobile Phase: MeOH/MeCN/buffer pH 3.0 (35:15:50 v/v/v)
Buffer: 7.0 mL triethylamine in 900 mL H₂O to 1000 mL volumetric flask. Adjust to pH 3.0 with phosphoric acid. Dilute to volume with H₂O
Flow Rate: 0.8 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 237 nm

Analytes

1. Impurity A
2. Amlodipine



Chromatogram shows 6 injections overlaid



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Budesonide

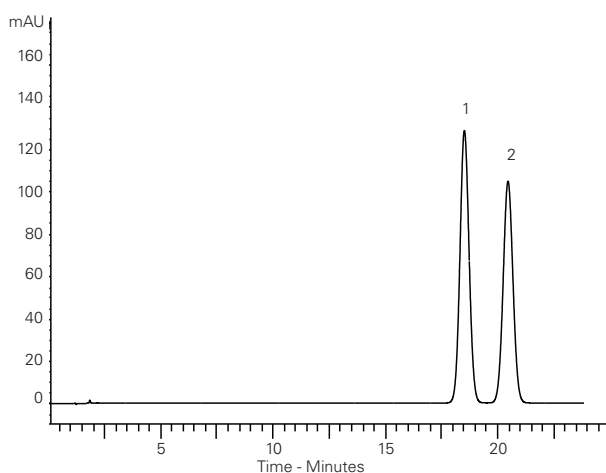
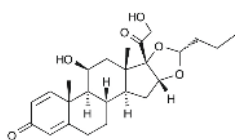
Application #AN1720

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 18 mM monobasic sodium phosphate pH 3.2 in H₂O/MeCN (68:32 v/v)
Flow Rate: 1.5 mL/min
Injection: 20 µL
Temperature: Ambient (22 °C)
Detection: UV, 254 nm

Analytes

1. Budesonide B
2. Budesonide A



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Doxepin

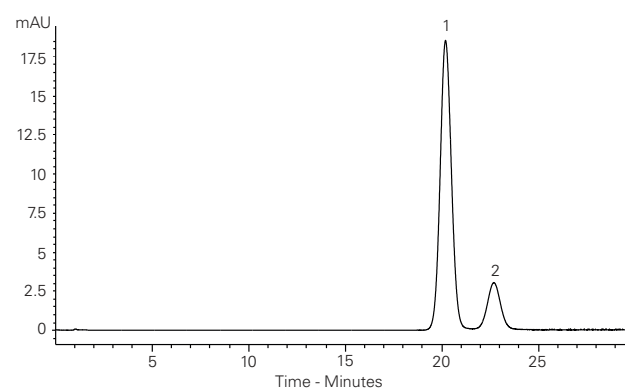
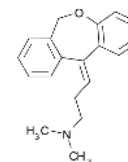
Application #AN1730

Conditions

Column: ACE 3 C8
Dimensions: 50 x 4.6 mm
Part Number: ACE-112-0546
Mobile Phase: 0.2 M monobasic NaH₂PO₄ pH 2.5 in H₂O/MeOH (30:70 v/v)
Flow Rate: 0.56 mL/min
Injection: 4.5 µL
Temperature: 50 °C
Detection: UV, 254 nm

Analytes

1. Doxepin isomer
2. Doxepin isomer



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Estradiol

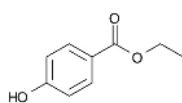
Application #AN1740

Conditions

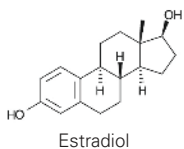
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 4.6 mm
Part Number: CORE-25A-1046U
Mobile Phase: H₂O/MeCN (45:55 v/v)
Flow Rate: 1.39 mL/min
Injection: 10.1 µL
Temperature: Ambient (22 °C)
Detection: UV, 205 nm

Analytes

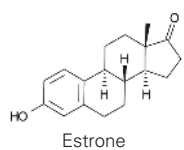
1. Ethylparaben
2. Estradiol
3. Estrone



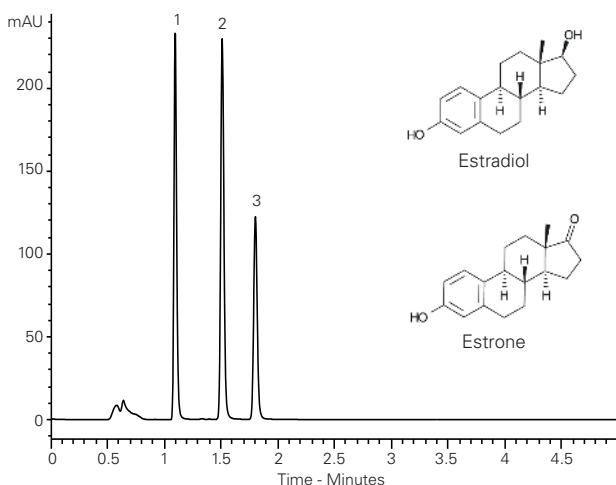
Ethylparaben



Estradiol



Estrone



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Glimepiride

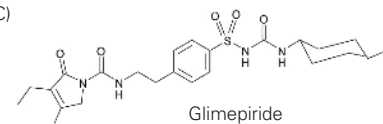
Application #AN1760

Conditions

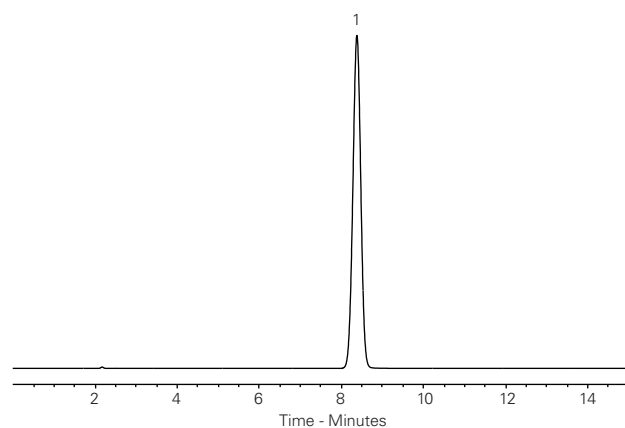
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 8 mM monobasic sodium phosphate pH 2.4/MeCN (1:1 v/v)
Flow Rate: 1.32 mL/min
Injection: 16 µL
Temperature: Ambient (22 °C)
Detection: UV, 228 nm

Analyte

1. Glimepiride



Glimepiride



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.



USP Monograph – Guaifenesin

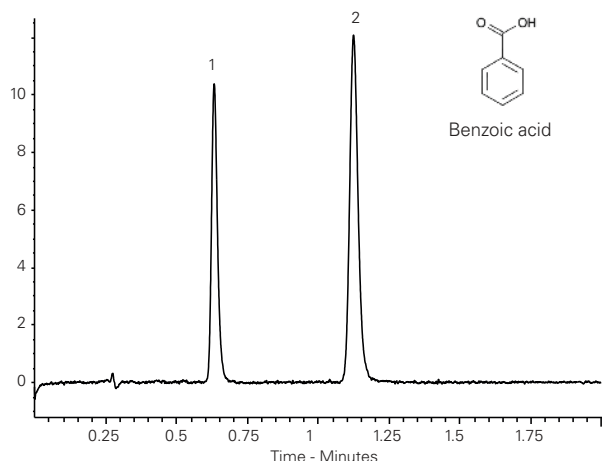
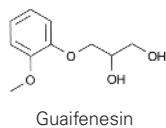
Application #AN1750

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: H₂O/MeOH/Glacial acetic acid (60:40:1.5 v/v/v)
Flow Rate: 0.85 mL/min
Injection: 1.5 µL
Temperature: Ambient (22 °C)
Detection: UV, 276 nm

Analytes

1. Guaifenesin
2. Benzoic acid



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Hydrocortisone

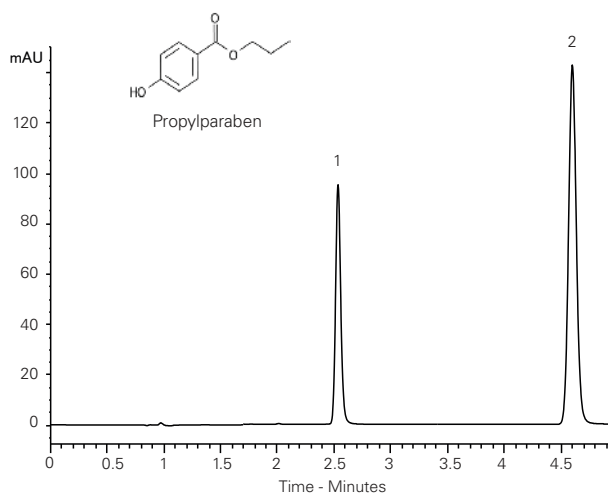
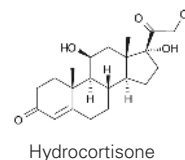
Application #AN1770

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 4.6 mm
Part Number: CORE-25A-1046U
Mobile Phase: H₂O/MeCN/MeOH (50:25:25 v/v/v)
Flow Rate: 1 mL/min
Injection: 5.8 µL
Temperature: Ambient (22 °C)
Detection: UV, 254 nm

Analytes

1. Hydrocortisone
2. Propylparaben



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Hydroquinone

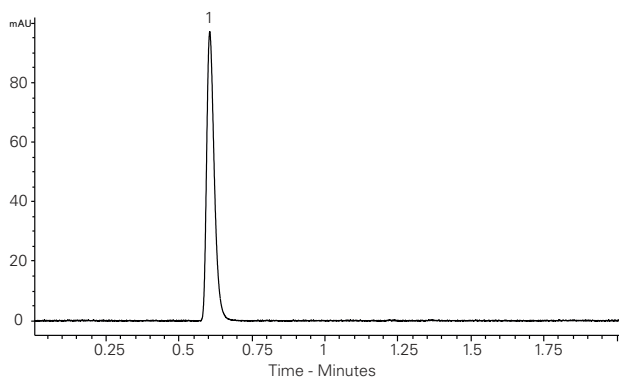
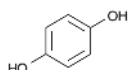
Application #AN1780

Conditions

Column: ACE Excel 2 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-101-0503U
Mobile Phase: H₂O/MeOH (45:55 v/v)
Flow Rate: 0.45 mL/min
Injection: 0.9 µL
Temperature: Ambient (22 °C)
Detection: UV, 280 nm

Analyte

1. Hydroquinone



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Indomethacin

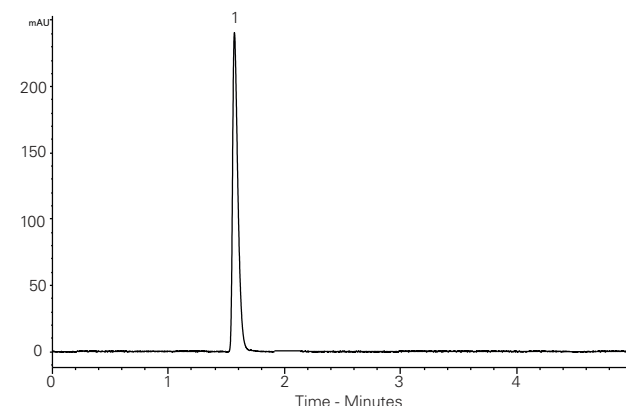
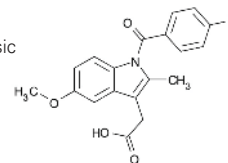
Application #AN1790

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 0.01 M monobasic sodium phosphate and 0.01 M dibasic sodium phosphate in MeCN/H₂O (1:1 v/v)
Flow Rate: 1.32 mL/min
Injection: 13 µL
Temperature: Ambient (22 °C)
Detection: UV, 254 nm

Analyte

1. Indomethacin



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Metronidazole

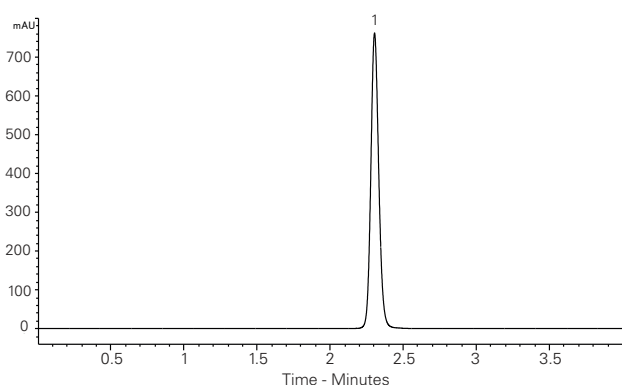
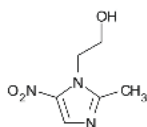
Application #AN1800

Conditions

Column: ACE 3 C8
Dimensions: 75 x 4.6 mm
Part Number: ACE-112-7546
Mobile Phase: H₂O/MeOH (4:1 v/v)
Flow Rate: 1 mL/min
Injection: 15 µL
Temperature: 30 °C
Detection: UV, 319 nm

Analyte

1. Metronidazole



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Naproxen

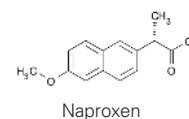
Application #AN1810

Conditions

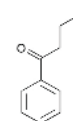
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: H₂O with glacial acetic acid (49:1)/MeCN (50:50 v/v)
Flow Rate: 0.51 mL/min
Injection: 2.8 µL
Temperature: Ambient (22 °C)
Detection: UV, 254 nm

Analytes

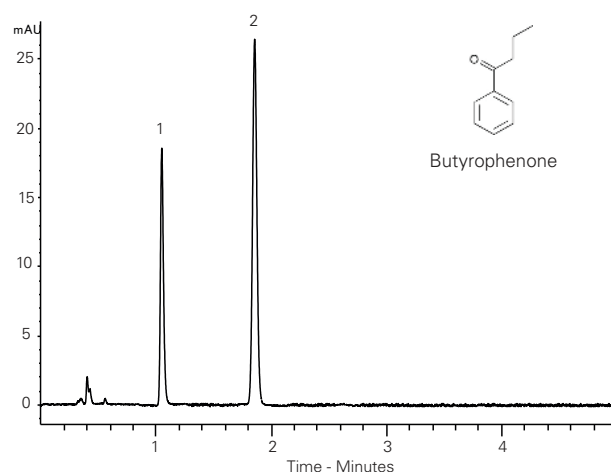
1. Naproxen
 2. Butyrophenone



Naproxen



Butyrophenone



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

USP Monograph – Paracetamol/Aspirin/Caffeine

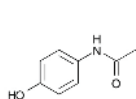
Application #AN1820

Conditions

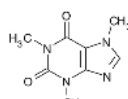
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 4.6 mm
Part Number: CORE-25A-0546
Mobile Phase: H₂O with glacial acetic acid (69:3)/MeOH (72:28 v/v)
Flow Rate: 2 mL/min
Injection: 2.5 µL
Temperature: 45 °C
Detection: UV, 275 nm

Analytes

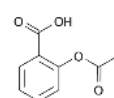
1. Paracetamol
 2. Caffeine
 3. Aspirin
 4. Benzoic acid
 5. Salicylic acid



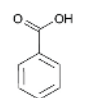
Paracetamol



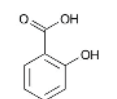
Caffeine



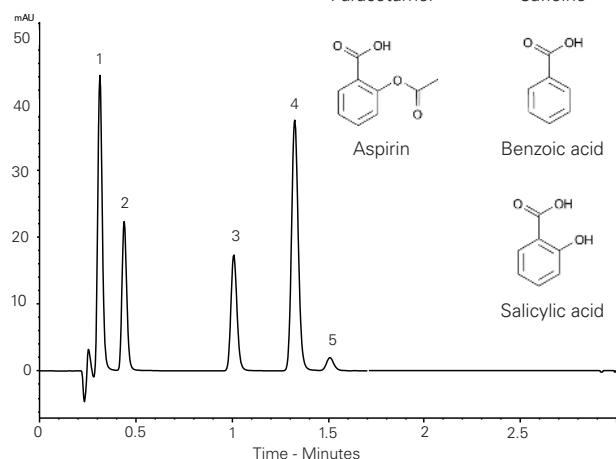
Aspirin



Benzoic acid



Salicylic acid



Translated method according to USP <621> guidance. Always check the latest and official method information from the relevant pharmacopoeia prior to analysis.

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

email: info@ace-hplc.com



Vanilla Flavourings – Natural and Artificial

Application #AN4390

Conditions

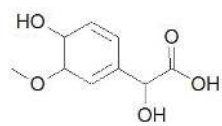
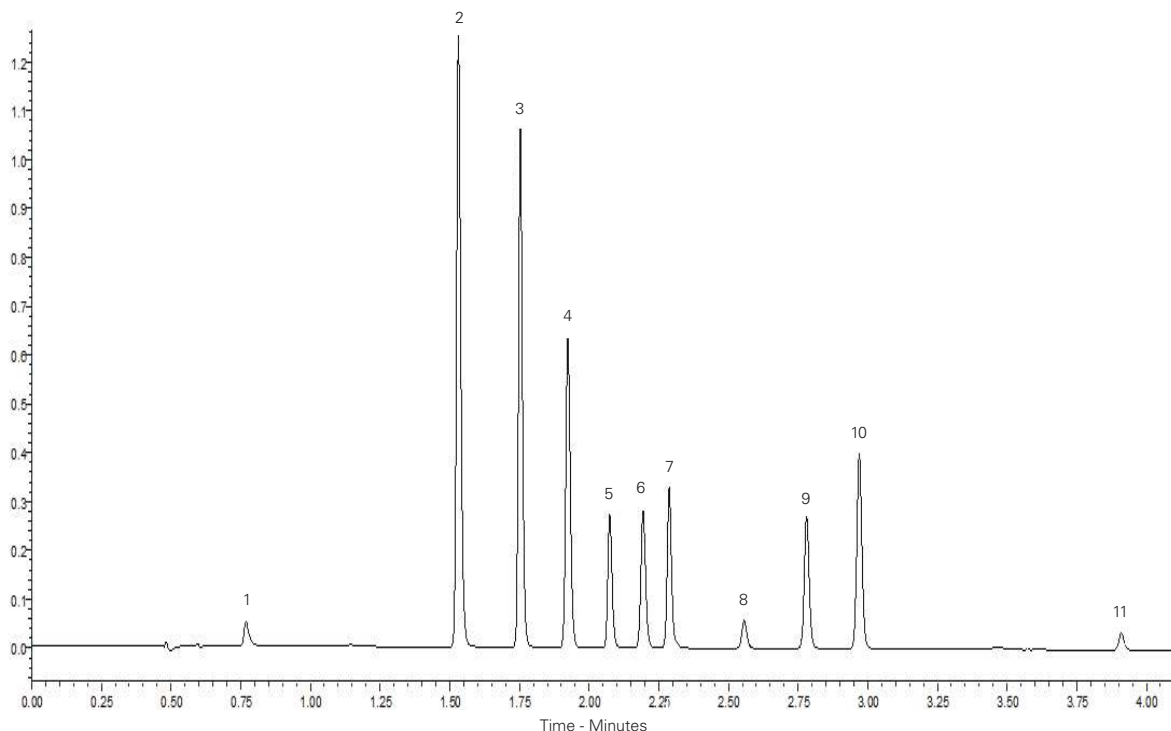
Column: ACE UltraCore 2.5 SuperPhenylHexyl
Dimensions: 100 x 2.1 mm
Part Number: CORE-25B-1002U
Mobile Phase: A: 10 mM ammonium formate in H₂O
 B: MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 5 |
| 5.5 | 70 |

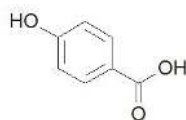
Flow Rate: 0.5 mL/min
Injection: 3 µL
Temperature: 50 °C
Detection: UV, 254 nm

Analytes

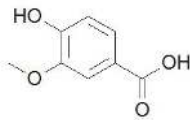
1. Vanillylmandelic acid
2. 4-Hydroxybenzoic acid
3. Vanillic acid
4. 4-Hydroxybenzaldehyde
5. p-Coumaric acid
6. Vanillin
7. Ferulic acid
8. Guaiacol
9. Ethyl vanillin
10. Coumarin
11. Eugenol



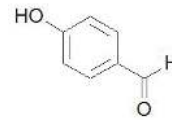
Vanillylmandelic acid



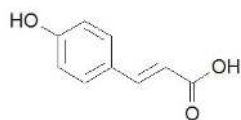
4-Hydroxybenzoic acid



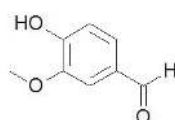
Vanillic acid



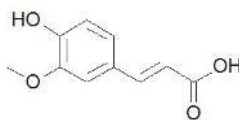
4-Hydroxybenzaldehyde



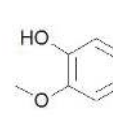
p-Coumaric acid



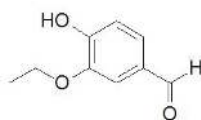
Vanillin



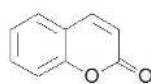
Ferulic acid



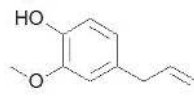
Guaiacol



Ethyl vanillin



Coumarin



Eugenol

Vanillins

Application #AN1620

Conditions

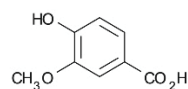
Column: ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: EXL-1112-1546U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 30 |
| 10.0 | 55 |
| 10.5 | 55 |
| 15.0 | 30 |
| 20.0 | 30 |

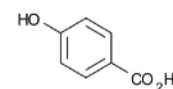
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 40 °C
Detection: UV, 260 nm

Analytes

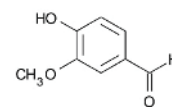
1. Vanillic acid
2. 4-Hydroxybenzoic acid
3. Vanillin
4. 4-Hydroxybenzaldehyde
5. Guaiacol
6. Ethyl Vanillin
7. Eugenol



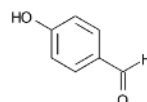
Vanillic acid



4-Hydroxybenzoic acid



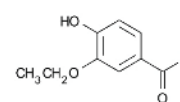
Vanillin



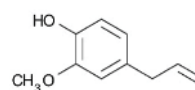
4-Hydroxybenzaldehyde



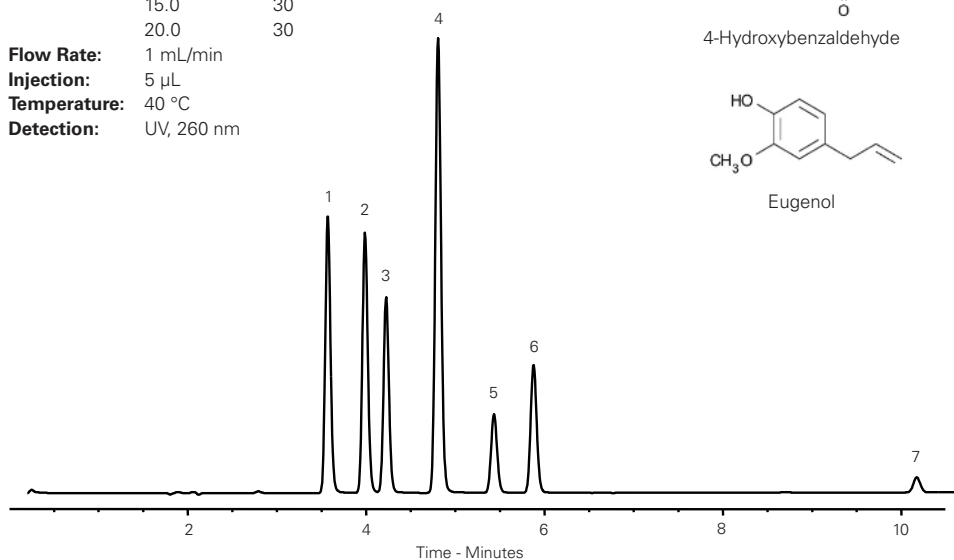
Guaiacol



Ethyl Vanillin



Eugenol



Vanillins – Fast Analysis

Application #AN2240

Conditions

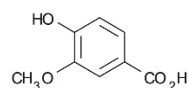
Column: ACE Excel 1.7 C18-Amide
Dimensions: 50 x 3.0 mm
Part Number: EXL-1712-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 25 |
| 1.32 | 75 |
| 1.49 | 75 |
| 1.60 | 25 |

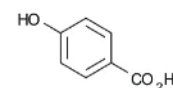
Flow Rate: 1.3 mL/min
Injection: 1 µL
Temperature: 45 °C
Detection: UV, 260 nm

Analytes

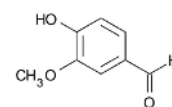
1. Vanillic acid
2. 4-Hydroxybenzoic acid
3. Vanillin
4. 4-Hydroxybenzaldehyde
5. Guaiacol
6. o-Vanillin
7. Ethyl Vanillin
8. Eugenol



Vanillic acid



4-Hydroxybenzoic acid



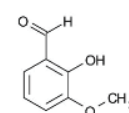
Vanillin



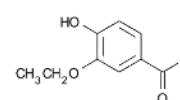
4-Hydroxybenzaldehyde



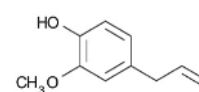
Guaiacol



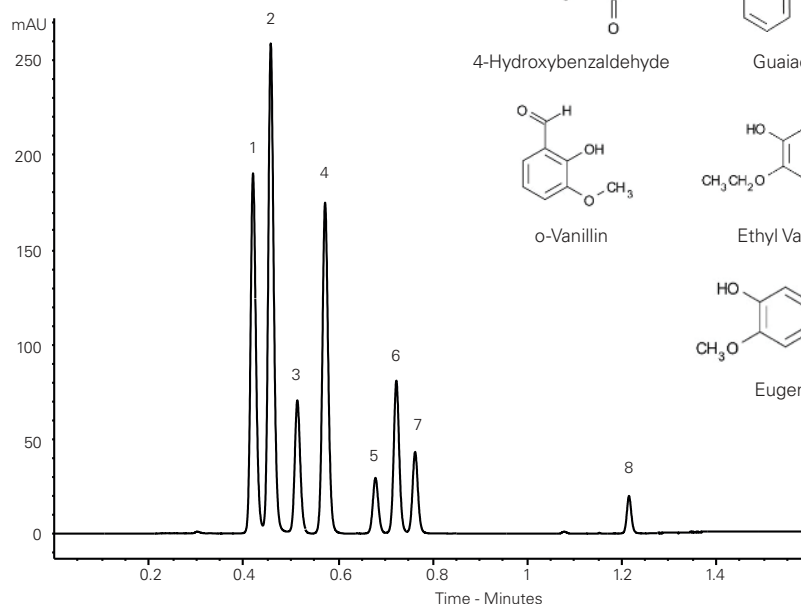
o-Vanillin



Ethyl Vanillin



Eugenol





Vitamin D2/D3

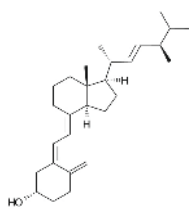
Application #AN1840

Conditions

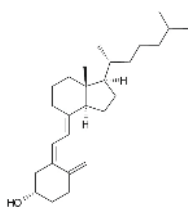
Column: ACE Excel 2 C18-Amide
Dimensions: 50 x 3.0 mm
Part Number: EXL-1012-0503U
Mobile Phase: 100% MeCN
Flow Rate: 0.43 mL/min
Injection: 2 µL
Temperature: 20 °C
Detection: UV, 265 nm

Analytes

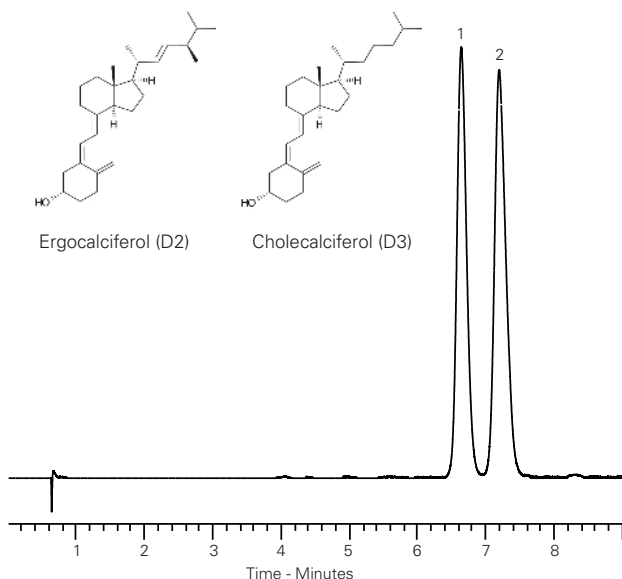
1. Ergocalciferol (D2)
2. Cholecalciferol (D3)



Ergocalciferol (D2)



Cholecalciferol (D3)



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

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

25-Hydroxy Vitamin D in Serum by LC-MS/MS

Application #AN2390

Conditions

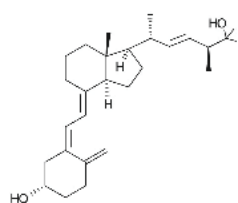
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

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

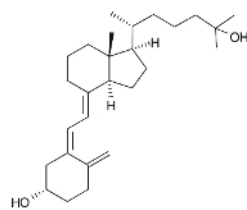
Flow Rate: 0.4 mL/min
Injection: 15 µL
Temperature: 40 °C
Detection: Quattro Premier XE triple quad MS
 MRM positive ESI mode
 Desolvation temperature: 450 °C
 Ion source temperature: 150 °C

Analytes

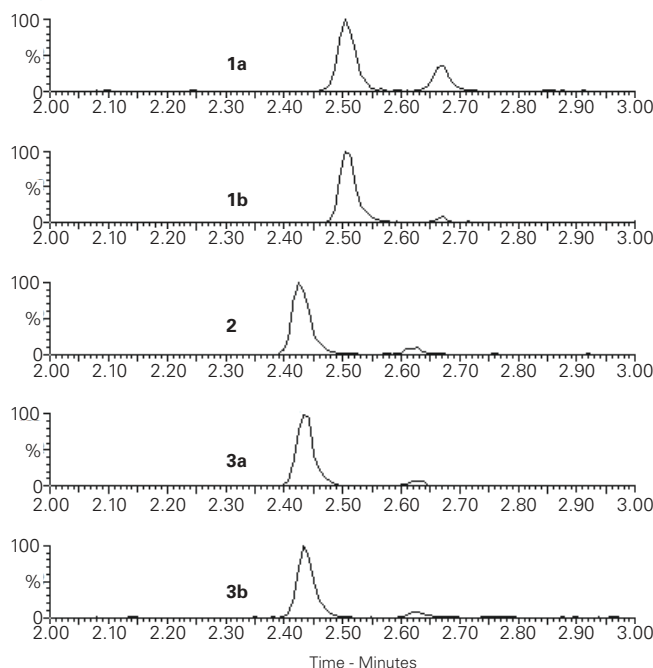
- 1a. 25-OH Vitamin D2
(*m/z* 395.5 → 269.5)
- 1b. 25-OH Vitamin D2
(*m/z* 395.5 → 119.2)
2. d6-25-OH Vitamin D3 (IS)
(*m/z* 389.6 → 263.5)
- 3a. 25-OH Vitamin D3
(*m/z* 383.5 → 257.5)
- 3b. 25-OH Vitamin D3
(*m/z* 383.5 → 107.2)



25-OH Vitamin D2



25-OH Vitamin D3



1,25-Dihydroxyvitamins D2 and D3 in Serum by LC-MS/MS

Application #AN4070

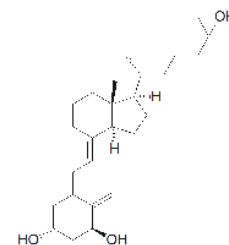
Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: MeCN/H₂O (50:50 v/v) containing 30 μ L methylamine per 500 mL
Flow Rate: 0.5 mL/min
Injection: 20 μ L
Temperature: 40 °C
Detection: AB Sciex 5500 triple quad MS
 ESI in positive ion mode
 IonSpray Voltage: 5500 V
 Temperature: 550 °C

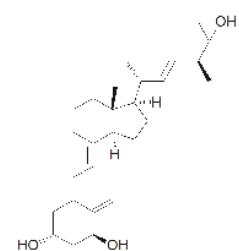
Sample: 1,25 diOH vitamin D2 and 1,25 diOH vitamin D3 metabolites are extracted from serum using supported liquid extraction. Sensitivity of LC-MS/MS analysis is maximised through use of PTAD (9-phenyl-1,2,4-triazole-3,5-dione) derivatisation and complexation with methylamine.

Analytes

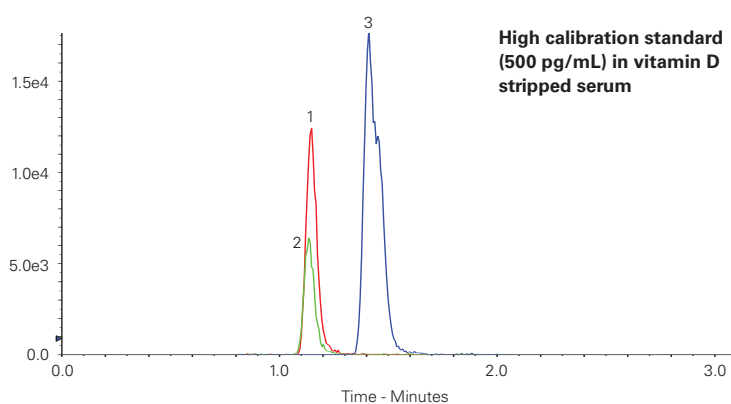
- 1,25-diOH vitamin D3-PTAD-methylamine complex
(m/z 623.4 \rightarrow 314.1)
- d3-1,25-diOH vitamin D3-PTAD-methylamine complex (I.S.)
(m/z 626.4 \rightarrow 317.1)
- 1,25-diOH vitamin D2-PTAD-methylamine complex
(m/z 635.4 \rightarrow 314.1)



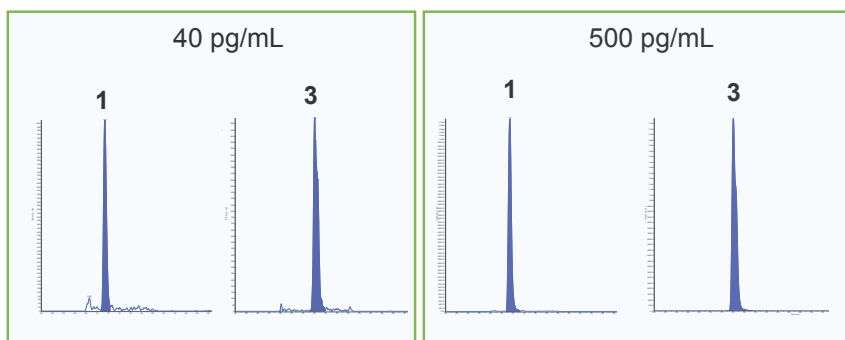
1,25-dihydroxy vitamin D3



1,25-dihydroxy vitamin D2



Low and high calibration standards in charcoal stripped (vitamin D free) serum, analysed as PTAD-methylamine complexes



Reproduced with permission of Biotage GB Ltd, UK. For further details of sample preparation see Biotage App Note AN857



Vitamins – Fat Soluble

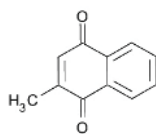
Application #AN2420

Conditions

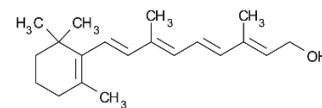
Column: ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: EXL-1112-1546U
Mobile Phase: MeOH/MeCN (90:10 v/v)
Flow Rate: 1 mL/min
Temperature: 20 °C
Detection: UV, 280 nm

Analytes

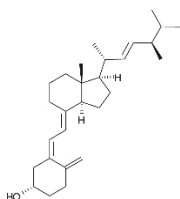
1. Menadione (Vitamin K3)
2. Retinol (Vitamin A)
3. Vitamin A acetate
4. Ergocalciferol (Vitamin D2)
5. Cholecalciferol (Vitamin D3)
6. Vitamin E acetate
7. α-Tocopherol (Vitamin E)
8. Vitamin K1



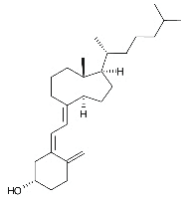
Menadione (Vitamin K3)



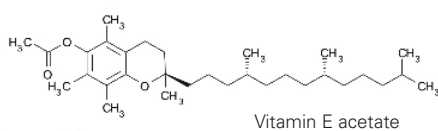
Retinol (Vitamin A)



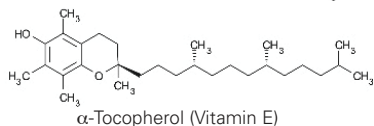
Ergocalciferol (Vitamin D2)



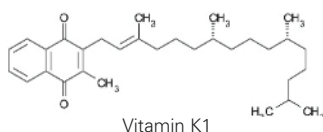
Cholecalciferol (Vitamin D3)



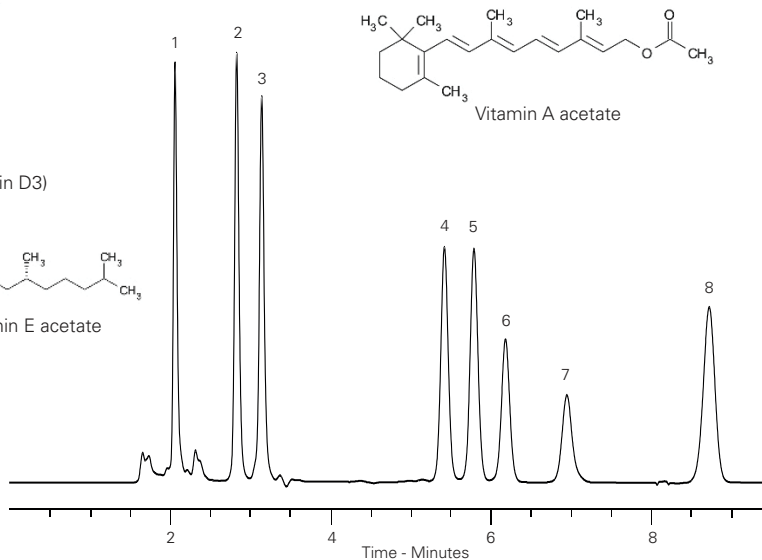
Vitamin E acetate



α-Tocopherol (Vitamin E)



Vitamin K1



Vitamins – Water Soluble (Gradient I)

Application #AN2940

Conditions

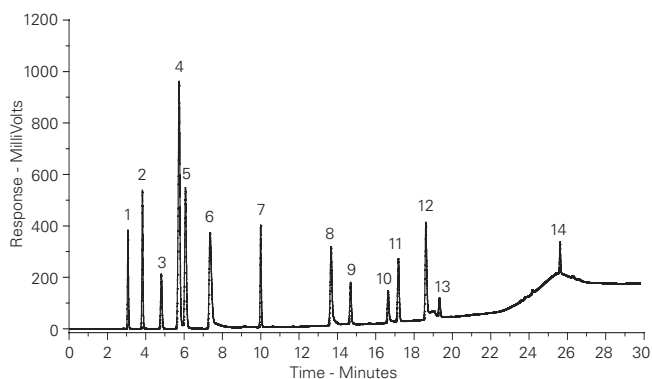
Column: ACE 5 C8
Dimensions: 250 x 4.6 mm
Part Number: ACE-122-2546
Mobile Phase: A: 50 mM KH₂PO₄ pH 2.5 in H₂O
 B: MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.0 | 0 |
| 3.0 | 0 |
| 16.5 | 45 |
| 19.5 | 80 |

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 205 nm

Analytes

1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Niacinamide (Vitamin B3)
5. Nicotinic acid
6. Pyridoxal
7. Pyridoxine
8. p-Aminobenzoic acid
9. Pantothenic acid (Vitamin B5)
10. Folic acid (Vitamin B9)
11. Cyanocobalamin (Vitamin B12)
12. Riboflavin (Vitamin B2)
13. d-Biotin (Vitamin B7)
14. Thiocotic acid



Vitamins – Water Soluble (Gradient II)

Application #AN2930

Conditions

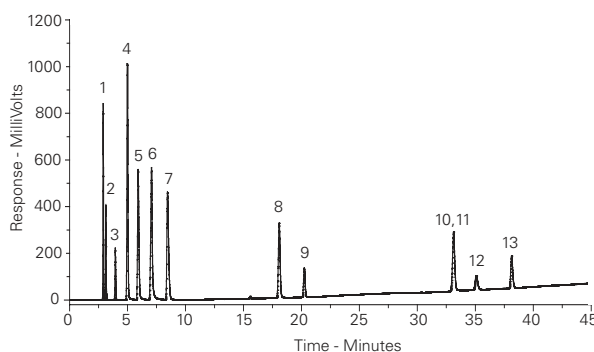
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 50 mM KH₂PO₄ pH 3.0 in H₂O
 B: MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 3 |
| 5 | 3 |
| 45 | 45 |
| 50 | 80 |

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 205 nm

Analytes

1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Nicotinic acid
5. Pyridoxal
6. Impurity
7. Pyridoxine
8. p-Aminobenzoic acid
9. Pantothenic acid (Vitamin B5)
10. Folic acid (Vitamin B9)
11. Cyanocobalamin (Vitamin B12)
12. d-Biotin (Vitamin B7)
13. Riboflavin (Vitamin B2)



Vitamins – Water Soluble (Gradient III) Application #AN1870

Conditions

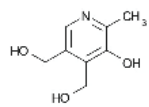
Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: A: 20 mM potassium phosphate pH 2.83 in H₂O
 B: 20 mM potassium phosphate pH 2.83 in MeOH
 H₂O (50:50 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 20 |
| 15 | 70 |

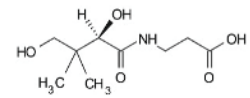
Flow Rate: 1.5 mL/min
Injection: 1 µL
Temperature: 40 °C
Detection: UV, 205 nm

Analytes

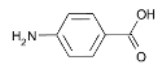
1. Pyridoxine (Vitamin B6)
2. Pantothenic acid (Vitamin B5)
3. p-Aminobenzoic acid
4. Folic acid (Vitamin B9/ Vitamin M)
5. D-Biotin (Vitamin B7/ Vitamin H)
6. Cyanocobalamin (Vitamin B12)
7. Riboflavin (Vitamin B2)



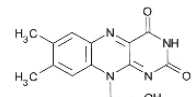
Pyridoxine (Vitamin B6)



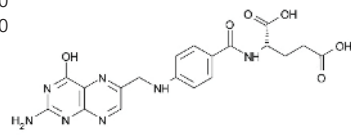
Pantothenic acid (Vitamin B5)



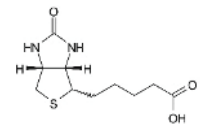
p-Aminobenzoic acid



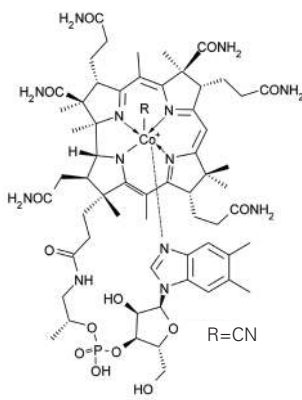
Riboflavin (Vitamin B2)



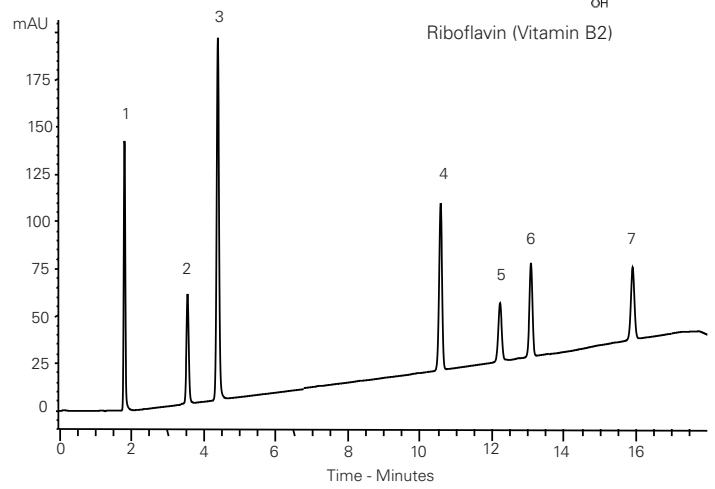
Folic acid (Vitamin B9/Vitamin M)



D-Biotin (Vitamin B7/Vitamin H)



Cyanocobalamin (Vitamin B12)



Vitamins – Water Soluble (Gradient IV) Application #AN1880

Conditions

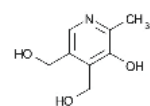
Column: ACE Ultracore 2.5 SuperPhenylHexyl
Dimensions: 50 x 2.1 mm
Part Number: CORE-25B-0502U
Mobile Phase: A: 20 mM KH₂PO₄, pH 2.7
 B: 20 mM KH₂PO₄, pH 2.7 in MeOH/H₂O (50:50 v/v)
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0.00 | 20 |
| 1.50 | 60 |
| 3.00 | 70 |
| 3.75 | 70 |
| 4.50 | 20 |
| 9.00 | 20 |

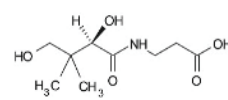
Flow Rate: 0.4 mL/min
Injection: 1 µL
Temperature: 40 °C
Detection: UV, 205 and 254 nm

Analytes

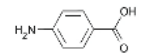
1. Pyridoxine
2. Pantothenic acid
3. p-Aminobenzoic acid
4. Folic acid
5. D-Biotin
6. Cyanocobalamin
7. Riboflavin



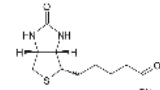
Pyridoxine



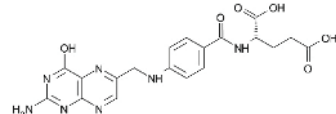
Pantothenic acid



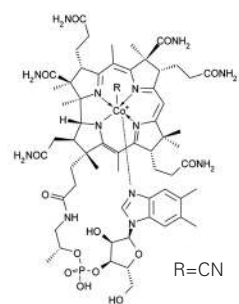
p-Aminobenzoic acid



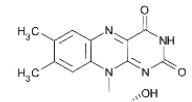
D-Biotin



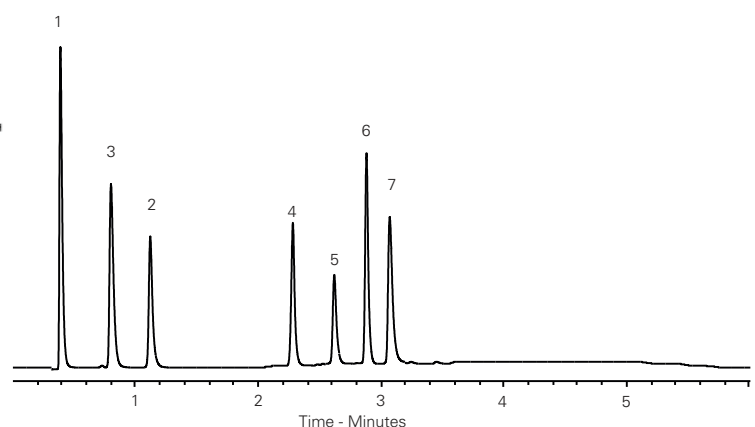
Folic acid



Cyanocobalamin



Riboflavin





Vitamins – Water Soluble (Isocratic I)

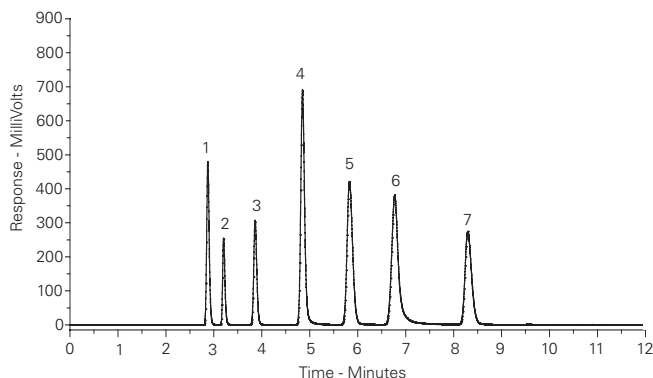
Application #AN2990

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM KH₂PO₄ pH 3.0 in H₂O/MeOH (97:3 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 205 nm

Analytes

1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Nicotinic acid
5. Pyridoxal
6. Impurity
7. Pyridoxine



Vitamins – Water Soluble (Isocratic II)

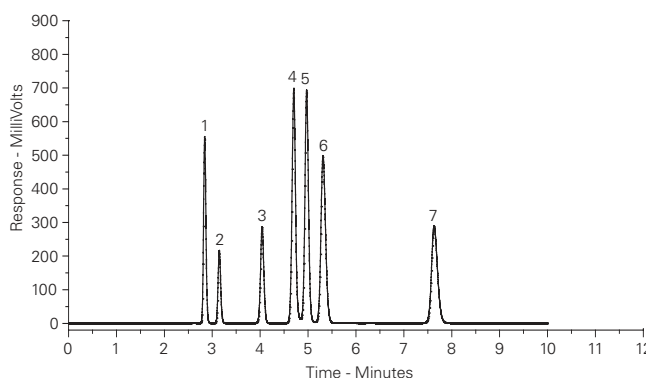
Application #AN2980

Conditions

Column: ACE 5 C8
Dimensions: 250 x 4.6 mm
Part Number: ACE-122-2546
Mobile Phase: 50 mM KH₂PO₄ pH 2.5 in H₂O/MeOH (97:3 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 205 nm

Analytes

1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Nicotinamide (Vitamin B3)
5. Pyridoxal
6. Nicotinic acid
7. Pyridoxine



Vitamins in Fruit Juice by Fast LC-MS

Application #AN2610

Conditions

Column: ACE Excel 3 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1110-1002U
Mobile Phase: A: 15 mM formic acid, adjusted to pH 3.8 with ammonia solution
 B: MeOH

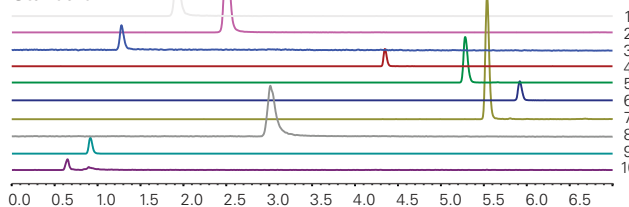
| Gradient: | Time (mins) | %B |
|-----------|-------------|----|
| | 0.00 | 1 |
| | 1.00 | 1 |
| | 3.00 | 8 |
| | 3.10 | 25 |
| | 6.00 | 50 |
| | 6.50 | 50 |
| | 6.51 | 1 |
| | 9.00 | 1 |

Flow Rate: 0.4 mL/min
Temperature: 30 °C
Detection: LCMS-8040 triple quad MS
 ESI positive mode (ESI negative for ascorbic and citric acid)
 DL temperature: 250 °C
 Heat block temperature: 400 °C

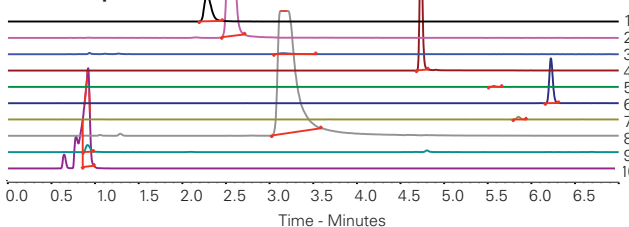
Analytes

1. Thiamine (Vitamin B1) (*m/z* 266.10 → 122.15)
2. Pyridoxine (Vitamin B6) (*m/z* 170.20 → 152.15)
3. Nicotinic acid (Vitamin B3) (*m/z* 124.00 → 78.00)
4. Pantothenic acid (Vitamin B5) (*m/z* 220.30 → 90.05)
5. Cyanocobalamin (Vitamin B12) (*m/z* 678.50 → 147.05)
6. Riboflavin (Vitamin B2) (*m/z* 377.20 → 243.10)
7. Biotin (Vitamin B7) (*m/z* 245.10 → 227.05)
8. Nicotinamide (Vitamin B3) (*m/z* 123.20 → 80.05)
9. Ascorbic acid (Vitamin C) (*m/z* 175.10 → 114.80)
10. Citric acid (*m/z* 191.10 → 87.15)

Standard



Juice sample



Vitamins in Green Vegetables by LC-MS/MS - Water Soluble

Application #AN1860

Conditions

Column: ACE 3 C4-300
Dimensions: 150 x 2.1 mm
Part Number: ACE-213-1502
Mobile Phase: A: 10 mM ammonium acetate
 pH 4.5 in H₂O
 B: 0.1% acetic acid in MeOH
 C: 0.3% acetic acid in MeOH

| Gradient: | Time (mins) | %A | %B | %C |
|-----------|-------------|----|-----|----|
| | 0 | 90 | 10 | 0 |
| | 3 | 90 | 10 | 0 |
| | 4 | 50 | 0 | 50 |
| | 7 | 50 | 0 | 50 |
| | 10 | 0 | 100 | 0 |

Flow Rate: 0.2 mL/min

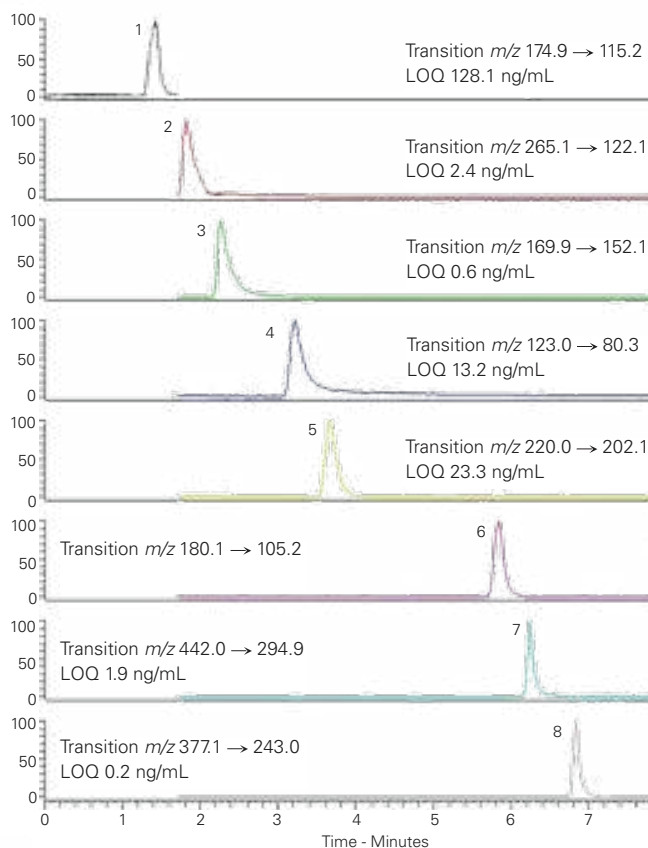
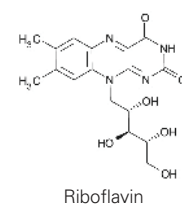
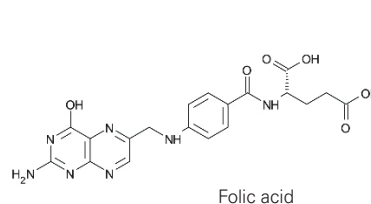
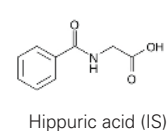
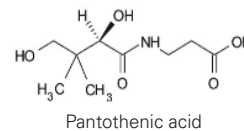
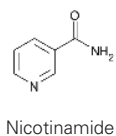
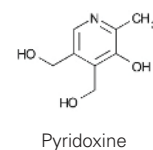
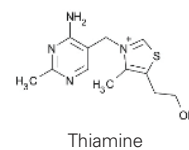
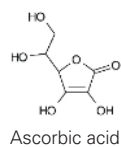
Injection: 10 µL

Temperature: 20 °C

Detection: TSQ triple quad MS; SRM mode
 -ESI for vitamin C
 +ESI for vitamin B

Analytes

1. Ascorbic acid
2. Thiamine
3. Pyridoxine
4. Nicotinamide
5. Pantothenic acid
6. Hippuric acid (IS)
7. Folic acid
8. Riboflavin



Reproduced with permission of Foodomics Laboratory, CIAL-CSIC, Madrid, Spain



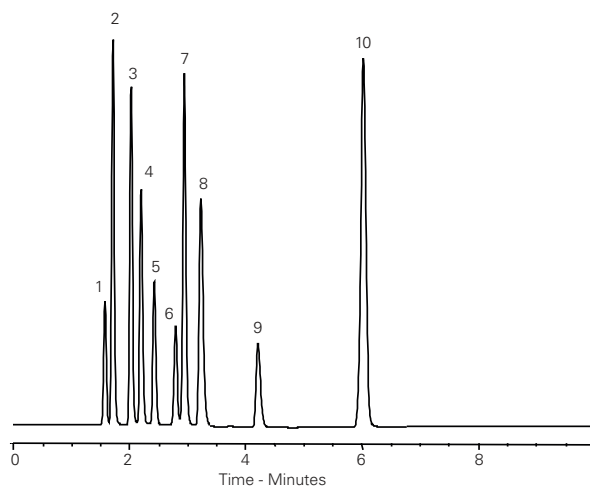
Vitamins and Polar Molecules - Water Soluble
Application #AN1850

Conditions

Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: 0.1 % phosphoric acid in H₂O/MeOH (96.5:3.5 v/v)
Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: 22 °C
Detection: UV, 260 nm

Analytes

1. Pyridoxamine (Vitamin B6)
2. Thiamine (Vitamin B1)
3. Isonicotinamide
4. Nicotinamide
5. L-Ascorbic acid (Vitamin C)
6. Orotic Acid
7. Hypoxanthine
8. Pyridoxal (Vitamin B6)
9. Pyridoxine (Vitamin B6)
10. p-Aminobenzoic acid



Water Soluble Artificial Colours
Application #AN3010

Conditions

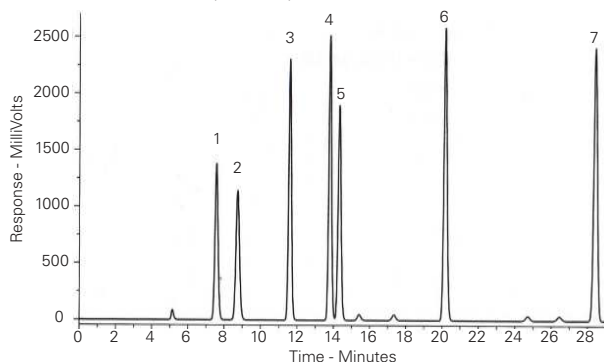
Column: ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-111-1046
Mobile Phase: A: 3 mM tetrabutylammonium bromide and 5 mM KH₂PO₄ in H₂O
 B: 5 mM tetrabutylammonium bromide in MeOH
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 45 |
| 20 | 70 |
| 30 | 45 |
| 40 | 45 |

Flow Rate: 0.8 mL/min
Injection: 10 µL
Temperature: Ambient
Detection: UV-Vis, 420 nm, 520 nm and 600 nm

Analytes

1. Amaranth
2. Sunset Yellow
3. Allura Red
4. Red 2G
5. Ponceau 4R
6. Carmoisine
7. Erythrosine



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

Whey Proteins from Whole Milk
Application #AN3000

Conditions

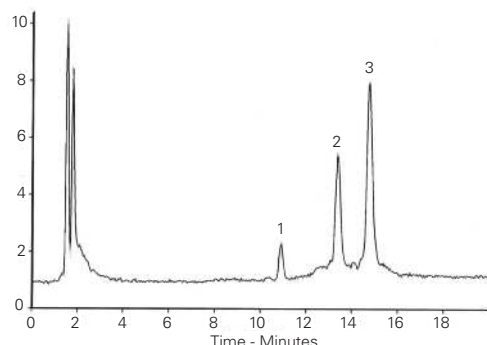
Column: ACE 3 C4-300
Dimensions: 150 x 2.1 mm
Part Number: ACE-213-1502
Mobile Phase: A: 0.5% formic acid in H₂O
 B: 0.5% formic acid in MeCN
Gradient:

| Time (mins) | %B |
|-------------|----|
| 0 | 35 |
| 16 | 43 |
| 17 | 80 |
| 20 | 80 |
| 21 | 35 |
| 31 | 35 |

Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: ESI-MS (+ve)

Analytes

1. α-Lactalbumin
2. β-Lactoglobulin B
3. β-Lactoglobulin A



Reproduced with permission of University of Vienna, Austria

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

Wine Acid Analysis

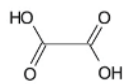
Application #AN1890

Conditions

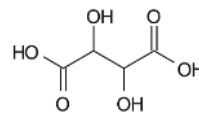
Column: ACE Excel 3 C18-Amide
Dimensions: 250 x 2.1 mm
Part Number: EXL-1112-2502U
Mobile Phase: 40 mM ammonium phosphate pH 2.5 in H₂O
Flow Rate: 0.21 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 214 nm

Analytes

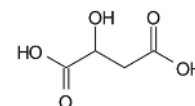
1. Oxalic acid
2. Tartaric acid
3. Malic acid
4. Lactic acid
5. Ascorbic acid
6. Citric acid



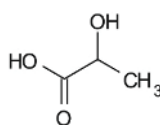
Oxalic acid



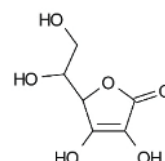
Tartaric acid



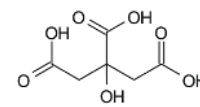
Malic acid



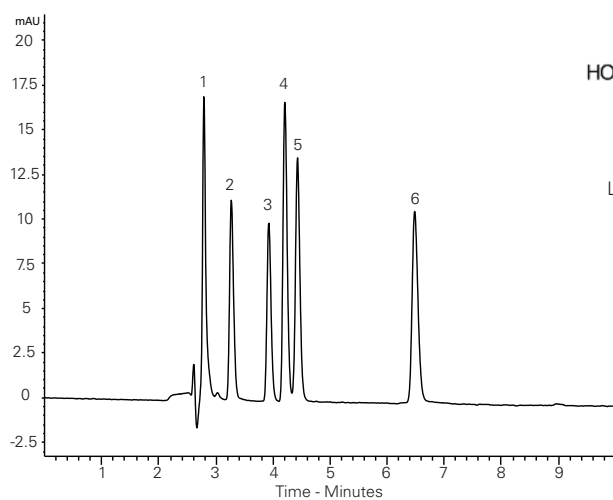
Lactic acid



Ascorbic acid



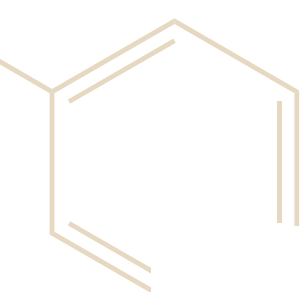
Citric acid





Analyte Index

| A | |
|---|---|
| Abamectin | 124 |
| AB-CHMINACA | 51 |
| Abscisic acid | 139 |
| ¹¹ C-ABP688 | 101 |
| Acebutalol | 44 |
| Acephate | 124, 128, 132 |
| Acesulfame K | 22, 41, 58 |
| 2-Acetamidophenol | 33, 42, 43, 116, 117 |
| 4-Acetamidophenol | 33 |
| Acetaminophen (paracetamol) | 32, 33, 61, 71, 108, 116, 117, 133, 140, 171, 175 |
| Acetamiprid | 104, 124, 128, 132 |
| Acetanilide | 33, 42, 43 |
| Acetophenone | 82 |
| Acetylcarnitine | 21 |
| 6-Acetylcodeine | 69 |
| Acetylclaidzin | 89 |
| 4-Acetyl-2-fluorobiphenyl | 76 |
| Acetylgénistin | 89 |
| Acetylglycitin | 89 |
| 6-Acetylmorphine | 111 |
| N-Acetyl pomalidomide | 141 |
| N-Acetylprocainamide | 74, 135 |
| Acetylsalicylic acid (aspirin) | 32, 33, 42, 43, 61, 107, 108, 112, 133, 171, 175 |
| Acetylsalicylsalicylic acid | 43, 171 |
| Aclonifen | 128 |
| Acrivastine | 36 |
| Adenine | 109 |
| Adenine arabinoside | 109 |
| Adenosine | 47, 109 |
| Adipic acid | 97, 99 |
| Adrenaline (epinephrine) | 53, 54, 55, 105 |
| Aflatoxin B1 | 103 |
| Aflatoxin B2 | 103 |
| Aflatoxin G1 | 103 |
| Aflatoxin G2 | 103 |
| Agmatine | 25 |
| Ajoene | 77 |
| AKB48F | 51 |
| AKB48 N-5-OH-pentyl | 51 |
| AKB48 N-pentanoic | 51 |
| Alachlor | 128, 132 |
| Alanine (Ala) | 24, 25, 26, 28 |
| Aldicarb | 124, 128, 132 |
| Aldicarb sulfone | 124, 128, 132 |
| Aldicarb sulfoxide | 124, 128, 132 |
| Aldosterone | 155 |
| Alfentanil | 69 |
| Alitame | 41 |
| Alkylated diphenylamine (ADPA) | 95 |
| Allethrin | 124 |
| Alliin | 77 |
| Allura Red | 184 |
| Alprazolam | 46, 68, 69 |
| Alprenolol | 45 |
| AM2201 N-4-OH-pentyl | 51 |
| AM2201 5/6-OH-indole | 51 |
| Amanin | 168 |
| Amaninamide | 168 |
| α -Amanitin | 168 |
| β -Amanitin | 168 |
| γ -Amanitin | 168 |
| ϵ -Amanitin | 168 |
| Amanullin | 168 |
| Amanullinic acid | 168 |
| Amaranth | 41, 184 |
| Ametoctradin | 124 |
| Ametryn | 128 |
| Amiloride | 43, 66, 74, 134 |
| L-2-Amino adipic acid | 25 |
| p-Aminobenzoic acid | 33, 146, 180, 181, 184 |
| 7-Aminoclonazepam | 46, 68, 69 |
| 6-Amino-m-cresol | 82 |
| Aminodesmethylflunitrazepam | 69 |
| 4-Aminodiphenylamine | 82 |
| 7-Aminoflunitrazepam | 46, 68, 69 |
| 4-Amino-2-hydroxytoluene | 82 |
| 2-Aminoindane | 148 |
| Aminomethylphosphonic acid (AMPA) | 80 |
| Aminonitrazepam | 69 |
| 4-Amino-3-nitrophenol | 82 |
| m-Aminophenol | 82 |
| o-Aminophenol | 82, 116, 117 |
| p-Aminophenol | 82, 116 |
| 3-Aminophthalic acid | 141 |
| Aminopyralid | 128 |
| Aminorex | 69 |
| Amiodarone | 69 |
| Amisulpride | 69 |
| Amitriptyline | 69, 134, 168, 169, 170 |
| Amitrole | 128 |
| Amlodipine | 69, 86, 172 |
| Ammonium ion | 25, 27 |
| Amoxicillin | 30 |
| AMPA (aminomethylphosphonic acid) | 80 |
| Amphetamine | 31, 68, 69 |
| α -Amyrin | 48 |
| β -Amyrin | 48 |
| Andrographolide | 34 |
| Androstenedione | 155 |
| Androsterone | 155 |
| Angiotensin I | 35 |
| Angiotensin II | 35, 119, 120 |
| Angiotensin III | 35 |
| Anhydroecgonine methyl ester | 69 |
| Antimycin A1a | 38 |
| Antimycin A1b | 38 |
| Antimycin A2a | 38 |
| Antimycin A2b | 38 |
| Antimycin A3a | 38 |
| Antimycin A3b | 38 |
| Antimycin A4a | 38 |
| Antimycin A4b | 38 |
| Antimycin A5 | 38 |
| Antimycin A6 | 38 |
| Apomyoglobin | 147 |
| Ara-C | 63 |
| Arginine (Arg) | 23, 24, 25, 26, 27, 28 |
| Aripiprazole | 69 |
| Artemisinin | 41 |
| Ascorbic acid (vitamin C) | 61, 109, 112, 140, 180, 182-5 |
| Asparagine (Asn) | 24, 25, 28 |
| Aspart (insulin) | 88 |
| Aspartame | 22, 41 |
| Aspartic acid (Asp) | 24, 25, 26, 28 |
| Aspirin (acetylsalicylic acid) | 32, 33, 42, 43, 61, 107, 108, 112, 133, 171, 175 |
| Atazanavir | 39 |
| Atenolol | 43, 44, 45, 69, 134 |
| Atomoxetine | 69 |
| Atorvastatin | 154 |
| Atrazine | 124, 128, 132 |
| Atrazine-desethyl | 128 |
| Atrazine-desisopropyl | 128 |
| Avenacin A-1 | 43 |
| Avenacin A-2 | 43 |
| Avenacin B-1 | 43 |
| Avenacin B-2 | 43 |
| Avermectin B1a | 128 |
| Avermectin B1b | 128 |
| Avobenzene | 163 |
| Azamethiphos | 128 |
| Azinphos-ethyl | 124, 128 |
| Azinphos-methyl | 124, 128 |
| Azinphos-methyl OA | 124 |
| Aziprotryne | 128 |
| Azoxystrobin | 124, 128 |
| B | |
| Bacitracin | 168 |
| Benalaxyl | 128 |
| Bendiocarb | 124 |
| Bendroflumethiazide | 32, 43, 65, 66, 107 |
| Benfluralin | 83 |
| Benfuracarb | 128 |
| Benomyl | 132 |
| Benoxacor | 124 |
| Benthiavalicarb-isopropyl | 128 |
| Benzalkonium chloride | 115 |
| Benzamide | 135 |
| Benzedrone | 69 |
| Benzoic acid | 33, 112, 115, 140, 144, 174, 175 |
| Benzophenone | 87 |
| Benzophenone-3 | 163 |
| Benzoyllecgonine (BZE) | 68, 69 |
| Benzyl alcohol | 23 |
| 3',4'-di-O-Benzyl-7O-(2-hydroxyethyl)-3-O-methylquercetin | 48 |
| Benzylparaben | 116 |
| Benzylpiperazine | 69 |
| Betamethasone | 61 |
| Bifenazate | 124, 128 |
| Bifenox | 128 |
| Bifenthrin | 128 |
| Biochanin A | 89 |
| d-Biotin (vitamin B7/vitamin H) | 180, 181, 182 |
| Bis(1,3-dichloro-2-propyl) phosphate (BDPCP) | 113 |
| Bis(2-ethylhexyl) phosphate (BEHP) | 113 |
| Bisoprolol | 69 |
| Bitertanol | 124, 128 |
| Bixafen | 128 |
| 9'-cis-Bixin | 35 |
| 9'-trans-Bixin | 35 |
| α -Boldenone | 157 |



| | | | | | | |
|--|--|---|------------------------|--|---------------------------------|----|
| β-Boldenone | 157 | 7-Carboxyporphyrin I | 142 | Clomethiazole | 69 | |
| Boscalid | 124, 128 | Carfentrazone-ethyl | 124, 128 | Clomipramine | 69, 135, 169 | |
| Bovine insulin | 88, 89 | Carglumic acid | 52 | Clonazepam | 46, 68, 69 | |
| BPO-dG#1 | 45 | Carmoisine | 184 | Clonidine | 59, 69 | |
| BPO-dG#2 | 45 | Carnitine | 21 | Clopidogrel | 59 | |
| BPO-dG#3 | 45 | Carvedilol | 43, 44, 134, 135 | Cloquintocet-mexyl | 128 | |
| BPO-dG#4 | 45 | α-Casein | 102 | Cloransulam methyl | 124 | |
| Brassinolide | 139 | β-Casein | 102 | Clothianidin | 104, 124, 128, 132 | |
| Bromazepam | 46, 68, 69 | Catechin | 58, 137, 145 | Clozapine | 69 | |
| Bromfenvinfos-ethyl | 128 | Catechin hydrate | 115 | CMPP (2-(4-chloro-2-methylphenoxy) propionic acid) | 136 | |
| Brompheniramine | 48 | Catechol | 56, 133 | Cobicistat | 152 | |
| 2-Bromophenol | 62 | Cathine | 69 | Cocaethylene | 69 | |
| Bromuconazole A | 128 | Cathinone | 69 | Cocaine | 68, 69, 94 | |
| Bromuconazole B | 128 | 2C-B-FLY | 69 | Codeine | 68, 70, 111 | |
| Budesonide A | 173 | Cefquinome | 57 | Coproporphyrin I | 142 | |
| Budesonide B | 173 | Cetirizine | 36 | Coproporphyrin III | 142 | |
| Bufalin | 118 | Chloramphenicol | 57 | Cordycepin | 109 | |
| Bufotenidine | 49 | Chlorantranilprole | 124, 128 | Corticosterone | 156, 157 | |
| Bufotenine (N, N-dimethylserotonin) | 49, 118 | Chlorbromuron | 128 | Cortisol | 62, 144 | |
| Buphedrone | 69 | Chlordiazepoxide | 39, 69 | Cortisone | 144, 156 | |
| Buphedrone ephedrine | 69 | Chlorfenvinphos | 124, 128 | Cortisone-21-acetate | 156 | |
| Bupirimate | 124, 128 | Chloridazon | 128 | Cotinine | 70 | |
| Bupivacaine | 69, 134 | Chlorimuron ethyl | 124 | Coumaphos | 124, 128 | |
| Buprenorphine | 68 | 4-Chloroacetanilide | 116, 117, 171 | Coumaric acid | 146 | |
| Buprenorphine glucuronide | 69 | m-Chloroacetophenone | 82 | p-Coumaric acid | 136, 176 | |
| Buprofezin | 124, 128 | o-Chloroacetophenone | 82 | Coumarin | 176 | |
| Bupropion | 69 | p-Chloroacetophenone | 82 | 6-CP | 136 | |
| Butter Yellow | 88 | 2-Chlorodeoxyadenosine | 47 | mCPP (m-chlorophenylpiperazine) | 70 | |
| n-Butylbenzene | 104 | Chlorogenic acid (3-Caffeoylquinic acid) | 50, 58, 137 | Creatinine | 70 | |
| Butylone | 69 | 4-Chloro-2-methylphenol (PCOC) | 136 | m-Cresol | 136 | |
| i-Butylparaben | 116 | 4-Chloro-2-methylphenoxyacetic acid (MCPA) | 136 | o-Cresol | 136 | |
| n-Butylparaben | 116 | 4-(4-Chloro-2-methylphenoxy)butanoic acid (MCPB) | 136 | p-Cresol | 74, 133 | |
| 2-(4-Butylphenyl)propanoic acid | 87 | 2-(4-Chloro-2-methylphenoxy)propionic acid (CMPP) | 136 | Crotamine | 151 | |
| gamma-Butyrolactone (GBL) | 77 | 2-Chlorophenol | 136 | Crotapotin | 151 | |
| Butyrophenone | 175 | 4-Chlorophenol | 116, 117, 136 | Crotoxyphos | 124 | |
| Butyrylcarnitine | 21, 97 | 2-Chloro-p-phenylenediamine | 82 | Crufomate | 124 | |
| Butyrylglycine | 98 | Chloroquine | 69 | Cryptochlorogenic acid (4-caffeoylquinic acid) | 50 | |
| BZE (Benzoylecgonine) | 68, 69 | 4-Chlororesorcinol | 82 | Cyanazine | 128, 132 | |
| C | | | Chlorpheniramine | 36, 37, 69 | Cyanidin-3, 5-diglucoside | 36 |
| C1,2 (N-sulfocarbamoylgonyautoxins) | 118 | Chlorpromazine | 69 | Cyanidin-3-glucoside | 36 | |
| Cadaverine | 25, 140 | Chlorpyrifos | 124, 128 | Cyanidin-3-sambubioside | 36 | |
| Cadusafos | 124, 128 | Chlorpyrifos-methyl | 128 | Cyanidin-3-sambubioside-5-glucoside | 36 | |
| Caffeic acid | 48, 60, 136, 146 | Chlorpyrifos OA | 124 | Cyanocobalamin (vitamin B12) | 180, 181, 182 | |
| Caffeine | 22, 33, 39, 50, 56, 58, 61, 69, 134, 135, 171, 175 | Chlortetracycline | 166 | Cyantranilprole | 124 | |
| 3-Caffeoylquinic acid (chlorogenic acid) | 50, 58, 137 | Chlortoluron | 128 | Cyazofamid | 124, 128 | |
| 4-Caffeoylquinic acid (cryptochlorogenic acid) | 50 | Cholecalciferol (vitamin D3) | 178, 180 | Cyclamate | 22, 41 | |
| 5-Caffeoylquinic acid (neochlorogenic acid) | 50 | Cichoric acid | 137 | Cyclizine | 70 | |
| Caftaric acid | 137 | Cimetidine | 114 | Cycloate | 128 | |
| Calycosin | 48 | Cinidon-ethyl | 128 | Cycloartenol | 48 | |
| Camfetamine | 69 | Cinnamic acid | 112, 145 | Cyclosporin A | 62 | |
| Cannabidiol | 52 | trans-Cinnamoylglycine | 98 | Cyclosporin B | 62 | |
| Carbamazepine | 69 | Ciprofibrate | 57 | Cyclosporin C | 62 | |
| Carbamazepine 10,11-epoxide | 69 | Citalopram | 69 | Cyclosporin D | 62 | |
| Carbaryl | 124, 128, 132 | Citric acid | 98, 182, 185 | Cyclosporin E | 62 | |
| Carbendazim | 124, 128, 132 | Clenbuterol | 58 | Cyclosporin G | 62 | |
| Carbofuran | 124, 128, 132 | Clethodim | 124, 128 | Cyclosporin L | 62 | |
| Carbosulfan | 128 | Clindamycin | 92 | Cyclosporin U | 62 | |
| Carboxin | 124, 128 | Clobazam | 69 | Cycloxydim A | 128 | |
| 5-Carboxyporphyrin I | 142 | Clofarabine | 47 | Cycloxydim B | 128 | |
| 6-Carboxyporphyrin I | 142 | Clofentazine | 124, 128, 132 | Cyflufenamid | 124 | |
| | | Clomazone | 128 | Cyfluthrin | 132 | |
| | | | | Cymoxanil | 124, 128 | |

| | | | | | |
|---|----------------|---|---------------|--|------------------|
| Cyphenothrin | 124 | N-Desmethyltramadol | 70 | Dimethenamid | 124, 128 |
| Cyproconazole | 128, 132 | O-Desmethyltramadol | 70 | Dimethoate | 124, 128, 132 |
| Cyprodinil A | 128 | Desmethylvenlafaxine | 70 | Dimethocaine | 70 |
| Cyprosulfamide | 124 | N-Desmethyl zopiclone | 70 | Dimethomorph | 124, 128, 132 |
| Cyromazine | 124 | Desomorphine | 70 | 1,2-Dimethoxybenzene | 159 |
| Cysteine (Cys) | 24, 25, 26, 28 | Desoxypropadrol | 70 | 1,3-Dimethoxybenzene | 159 |
| Cytarabine | 63 | Detemir (insulin) | 88 | 1,4-Dimethoxybenzene | 159 |
| Cytidine | 63, 109 | Dexamethasone | 61 | 3,4-Dimethoxycinnamic acid | 112 |
| Cytochrome C | 147 | Dextromethorphan | 36, 37, 70 | 1,4-Dimethylnaphthalene | 104 |
| Cytosine | 109 | DHEA (Didehydroepiandrosterone) | 155 | 2,4-Dimethylphenol | 136 |
| D | | | | | |
| dADP | 109 | Diaphenhiuron | 128 | 3,4-Dimethylphenol | 136 |
| dAMP | 109 | Dialifos | 124 | 3,5-Dimethylphenol | 136 |
| dATP | 109 | Diamorphine | 70 | N,N-Dimethyl-1,4-phenylenediamine HCl | 82 |
| 2,4-D (2,4-Dichlorophenoxyacetic acid) | 136 | Diazepam | 46, 68, 70 | N,N-Dimethylserotonin (bufotenine) | 49, 118 |
| Daidzein | 89 | Diazinon | 124, 128 | Dimoxystrobin | 128 |
| Daidzin | 89 | Diazinon OA | 124 | Dinactin | 101 |
| Darunavir | 39 | Dibucaine | 76 | Diniconazole | 128 |
| 2,4-DB (4-(2,4-dichlorophenoxy)butanoic acid) | 136 | Dibutyltin | 114 | 1,2-Dinitrobenzene | 23, 133 |
| dcGTx (decarbamoylegonautoxin) | 118 | 3,4-Dicaffeoylquinic acid (isochlorogenic acid B) | 50 | 1,3-Dinitrobenzene | 39, 75, 133, 134 |
| dcNEO (decarbamoyleneosaxitoxin) | 118 | 3,5-Dicaffeoylquinic acid (isochlorogenic acid A) | 50 | Dinitrophenol | 70 |
| 2,4-DCP (2,4-dichlorophenol) | 136 | 4,5-Dicaffeoylquinic acid (isochlorogenic acid C) | 50 | 2,4-Dinitrotoluene | 75 |
| dcSTX (decarbamoyle saxitoxin) | 118 | Dichlorfluandil | 128 | Dinotefuran | 124, 132 |
| DDT (4,4-dichlorodiphenyltrichloroethane) | 52 | Dichloromid | 124 | Dioxacarb | 124 |
| Decarbamoyleneosaxitoxin (dcNEO) | 118 | 4,4-Dichlorodiphenyltrichloroethane (DDT) | 52, 153 | Dioxathion | 124 |
| Decarbamoyle saxitoxin (dcSTX) | 118 | 2,4-Dichlorophenol (2,4-DCP) | 62, 136 | Diphenhydramine | 36, 70, 87 |
| DEF | 124 | 2,6-Dichlorophenol | 136 | Diphenylprolinol (D2PM) | 70 |
| Dehydroandrographolide | 34 | 2,4-Dichlorophenoxyacetic acid (2,4-D) | 136 | Dipipanon | 70 |
| Dehydroaripiprazole | 70 | 4-(2,4-Dichlorophenoxy)butanoic acid (2,4-DB) | 136 | Disulfoton | 128 |
| Dehydrobufotenine | 118 | 2-(2,4-Dichlorophenoxy)propionic acid (2,4-DP) | 136 | Disulfoton sulfone | 124, 128 |
| Deisopropylatrazine | 132 | Dichlorvos | 124 | Disulfoton sulfoxide | 124, 128 |
| Deltorpin-II | 65 | Diclobutrazol A | 128 | Ditalimfos | 128 |
| Demeclocycline | 166 | Diclofenac | 107, 108 | Diuron | 124, 128 |
| Demeton-S-methyl | 128 | Dicrotophos | 124, 128, 132 | DMA | 132 |
| Demeton-S-methyl sulfone | 128, 132 | Didanosine | 65 | DMPF | 132 |
| Demeton-S-methyl sulfoxide | 132 | 12,18-Didecarboxysirohaem | 64 | DMST | 124, 128 |
| Demeton-S-sulfone | 124 | Didehydroepiandrosterone (DHEA) | 155 | Dodine | 124, 128 |
| Deoxyadenosine | 47, 109 | Didesmethylcitalopram | 70 | Donepezil | 70 |
| Deoxyalliin | 77 | Didesmethylsibutramine | 39 | Dopamine | 53, 54, 55, 105 |
| 14-Deoxyandrographiside | 34 | Dienestrol | 157 | DOTATATE | 66 |
| 14-Deoxyandrographolide | 34 | Diethofencarb | 124, 128 | Dothiepin | 70 |
| 11-Deoxycortisol | 155 | Diethylpropion | 39 | Doxepin | 169, 170, 173 |
| 21-Deoxycortisol | 155 | Diethylstilbestrol | 157 | Doxorubicin | 63 |
| Deoxycytidine | 109 | N,N-Diethyltoluene-2,5-diamine | 82 | Doxycycline | 166 |
| Deoxyguanosine | 47, 109 | Difenconazole | 128 | Doxylamine | 36, 37 |
| Deoxyinosine | 109 | Diflubenzuron | 124, 128 | 2,4-DP ((2-(2,4-dichlorophenoxy)propionic acid) | 136 |
| Deoxythymidine | 47 | Diflufenican | 128 | Dulcin | 41 |
| Deoxyuridine | 47, 109 | Diflunisal | 133 | Dulcoside A | 42 |
| Dermorphin | 65 | Digoxin | 70 | E | |
| Desacetyl cinobufagin | 118 | Dihydrocodeine | 68, 70, 111 | EAM2201 | 51 |
| Desacetyl rifabutin | 150 | Dihydrocyclosporin A | 62 | Ecgonine ethyl ester | 70 |
| Desacetyl rifampicin | 150 | Dihydrostreptomycin | 29 | Ecgonine methyl ester | 70 |
| Desacetyl rifapentine | 150 | 1,3-Dihydroxybenzene | 133 | EDDP (2-ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine) | 68, 70, 111 |
| Desethyl atrazine | 132 | 3 β ,25-Dihydroxy-5-cholesten-7-one | 114 | Efavirenz | 39 |
| Desethyl hydroxychloroquine | 86 | 3 β ,27-Dihydroxy-5-cholesten-7-one | 114 | Elvitegravir | 152 |
| Desfluoro paroxetine | 119 | 7 α ,25-Dihydroxycholesterol | 114 | Emamectin | 124 |
| Desipramine | 70, 169, 170 | 7 β ,25-Dihydroxycholesterol | 114 | Emtricitabine | 152 |
| Desmedipham | 128 | 7 α ,27-Dihydroxycholesterol | 114 | Entacapone | 73 |
| Desmethylcitalopram | 70 | 7 β ,27-Dihydroxycholesterol | 114 | Epanolol | 73 |
| N-Desmethylclozapine | 70 | 2',6'-Dihydroxy-4'-methoxydihydrochalcone | 48 | Ephedrine | 31, 39 |
| Desmethylflunitrazepam | 70 | 7,3'-Dihydroxy-4'-methoxy-8-methylflavone | 48 | Epicatechin | 53, 58, 137, 145 |
| Desmethylfluoxetine | 70 | 1,5-Dihydroxynaphthalene | 82 | Epigallocatechin | 53, 137 |
| N-Desmethylmirtazapine | 70 | 2,7-Dihydroxynaphthalene | 82 | Epigallocatechin gallate | 53 |
| Desmethyl-olanzapine | 70 | 3,4-Dihydroxynorephedrine | 55 | Epinastine | 73 |
| Desmethyl-pirimitcarb | 128 | 3,4-Dihydroxyphenylacetic acid | 85 | Epinephrine (adrenaline) | 53, 54, 55, 105 |
| N-Desmethylsibutramine | 39 | 1,25-Dihydroxy vitamin D2 | 179 | Epoxiconazole | 128 |
| | | 1,25-Dihydroxy vitamin D3 | 179 | | |
| | | Diltiazem | 70 | | |
| | | Dimethachlor | 128 | | |

| H | |
|---|---|
| Haloiperidol | 70 |
| Hellebrigenin | 118 |
| Hellebrigenol-3-O-sulfate | 118 |
| Hepcidin-25 | 83 |
| Heptafluorobutyric acid | 121 |
| Heptenofos | 129 |
| Hexaconazole | 125, 129, 132 |
| Hexaflumuron | 129, 132 |
| Hexanoylcarnitine | 21 |
| Hexanoylglycine | 98 |
| Hexazinone | 129 |
| Hexestrol | 157 |
| Hexobarbital | 134 |
| Hexythiazox | 125, 129 |
| hGMCFSF | 149 |
| Higromycin-B | 29 |
| Hippuric acid | 70, 84, 183 |
| Histamine | 25 |
| Histidine (His) | 24, 25, 26, 28 |
| HNP-1 (Human neutrophil peptide 1) | 64 |
| HNP-2 (Human neutrophil peptide 2) | 64 |
| HNP-3 (Human neutrophil peptide 3) | 64 |
| Holo-transferrin | 147 |
| Homosalate | 163 |
| Homovanillic acid | 85 |
| HT-2-toxin | 103 |
| Human insulin | 89 |
| Hydrochlorothiazide | 23, 32, 43, 66, 86, 133, 134 |
| Hydrocodone | 68, 70, 111 |
| Hydrocortisone | 156, 174 |
| Hydromorphone | 68, 70, 111 |
| Hydroquinidine | 148 |
| Hydroquinine | 148 |
| Hydroquinone | 116, 117, 171, 174 |
| 2-Hydroxyadipic acid | 98 |
| α -Hydroxyalprazolam | 46, 68, 70 |
| 4-Hydroxyamphetamine | 70 |
| 4-Hydroxybenzaldehyde | 176, 177 |
| 2-Hydroxybenzoic acid (salicylic acid) | 33, 42, 43, 61, 108, 112, 133, 139, 140, 171, 175 |
| 3-Hydroxybenzoic acid | 33 |
| 4-Hydroxybenzoic acid | 33, 58, 144, 171, 176, 177 |
| Hydroxybupropion | 70 |
| gamma-Hydroxybutyric acid (GHB) | 77, 99 |
| 2-Hydroxybutyric acid | 99 |
| 3-Hydroxybutyric acid | 99 |
| 4-Hydroxybutyric acid | 77, 99 |
| 3-Hydroxycarbofuran | 124, 128 |
| Hydroxychloroquine | 86 |
| 7 α -Hydroxycholesterol | 114 |
| 7 β -Hydroxycholesterol | 114 |
| 22(R)-Hydroxycholesterol | 114 |
| 22(S)-Hydroxycholesterol | 114 |
| 24(S)-Hydroxycholesterol | 114 |
| 25-Hydroxycholesterol | 114 |
| 27-Hydroxycholesterol | 114 |
| 2-Hydroxyethylflurazepam | 46, 68 |
| 2-Hydroxyglutaric acid | 98 |
| 3-Hydroxyglutaric acid | 98 |
| 5-Hydroxyhexanoic acid | 99 |
| 6-Hydroxyindole | 82 |
| 5-Hydroxyindoleacetic acid | 105 |
| 3-Hydroxyisobutyric acid | 99 |
| 2-Hydroxyisocaproic acid | 99 |
| 4-Hydroxyisophthalic acid | 43 |
| 3-Hydroxyisovaleric acid | 98 |
| Hydroxyitraconazole | 90 |
| 15-Hydroxy lubiprostone | 94 |
| 15-Hydroxy lubiprostone-d4 | 94 |
| 4-Hydroxymethamphetamine | 70 |
| DL-4-Hydroxy-3-methoxymandelic acid | 85 |
| 3-Hydroxy-2-methylbutyric acid | 98 |
| 3-Hydroxy-3-methylglutaric acid | 98 |
| 2-Hydroxy-3-methylvaleric acid | 99 |
| 8-Hydroxymirtazapine | 70 |
| 7-Hydroxymirtazapine | 70 |
| 3-Hydroxyphenazepam | 70 |
| 2-Hydroxyphenylacetic acid | 99 |
| 4-Hydroxyphenylacetic acid | 99 |
| 5-Hydroxy pomalidomide | 141 |
| 7-Hydroxy pomalidomide | 141 |
| 11 α -Hydroxyprogesterone | 156, 157 |
| 17 α -Hydroxyprogesterone | 155 |
| 21-Hydroxyprogesterone | 156, 157 |
| Hydroxyproline | 23, 25 |
| 7-Hydroxyquetiapine | 70 |
| 9-Hydroxyrisperidone | 70 |
| Hydroxystanozolol | 157 |
| 5-Hydroxythiabendazole | 124 |
| α -Hydroxytriazolam | 46, 68 |
| 25-Hydroxy vitamin D2 | 178 |
| 25-Hydroxy vitamin D3 | 178 |
| Hydroxyzine | 135 |
| Hyperoside | 75 |
| I | |
| Ibuprofen | 32, 87, 107, 133, 134 |
| Imazalil | 125, 129 |
| Imazosulfuron | 125 |
| Imidacloprid | 104, 125, 129, 132 |
| Imipramine | 70, 168, 169, 170 |
| Imiprothrin | 125 |
| Indapamide | 43, 65, 66 |
| Indaziflam | 125 |
| Indomethacin | 107, 108, 133, 134, 174 |
| Indoxacarb | 125, 129, 132 |
| Insulin aspart | 88 |
| Insulin detemir | 88 |
| Insulin glargine | 88 |
| Insulin lispro | 88 |
| Insulin R | 88 |
| 5-Iodo-2-aminoindane | 70 |
| Ipcnazole | 125, 129 |
| Iprodione | 129 |
| Iprovalicarb | 125, 129 |
| Irbesartan | 34 |
| Isoamylamine | 25 |
| 2-(4-Isobutylphenyl)ethanone | 87 |
| 2-(4-Isobutylphenyl)propanamide | 87 |
| 2-(3-Isobutylphenyl)propanoic acid | 87 |
| Isobutyrylcarnitine | 21, 97 |
| Isobutyrylglycine | 98 |
| Isochlorogenic acid A (3,5-dicaffeoylquinic acid) | 50 |
| Isochlorogenic acid B (3,4-dicaffeoylquinic acid) | 50 |
| Isochlorogenic acid C (4,5-dicaffeoylquinic acid) | 50 |
| Isocitric acid | 98 |
| Isocyclosporin A | 62 |
| Isofenfos | 125, 129 |
| Isofenfos-methyl | 129 |
| Isoformonetin | 48 |
| Isoleucine (Ile) | 23, 24, 25, 26, 27, 28 |
| Isoliquritigenin | 48 |
| J | |
| Jasmonic acid | 139 |
| JWH-018 | 51, 164 |
| JWH-018 N-4-OH-pentyl | 164 |
| JWH-018 5-OH-indole | 51 |
| JWH-018 N-5-OH-pentyl | 51 |
| JWH-018 N-pentanoic | 51, 164 |
| JWH-019 N-6-OH-hexyl | 51 |
| JWH-073 | 51, 164 |
| JWH-073 N-3-OH-butyl | 164 |
| JWH-073 N-4-OH-butyl | 51 |
| JWH-081 | 51 |
| JWH-081 N-5-OH-pentyl | 51 |
| JWH-122 | 51 |
| JWH-122 N-5-OH-pentyl | 51 |
| JWH-122 N-4-pentyl | 51 |
| JWH-200 | 164 |
| JWH-210 | 51 |
| JWH-210 5-OH-indole | 51 |
| JWH-250 | 164 |
| JWH-250 N-5-OH-pentyl | 51, 164 |
| K | |
| Kaempferol | 75, 76 |
| Kanamycin | 29 |
| Ketamine | 68, 70 |
| Ketoprofen | 32, 107, 108, 134 |
| 11-Ketoprogesterone | 156, 157 |
| Kresoxim-methyl | 125, 129 |
| L | |
| Labetalol | 45 |
| α -Lactalbumin | 184 |
| Lactic acid | 185 |
| Lactofen | 125 |
| β -Lactoglobulin A | 102, 184 |
| β -Lactoglobulin B | 102, 184 |
| Lactose | 159, 161 |
| Lactulose | 159 |
| Lamotrigine | 70 |
| Lansoprazole | 37, 91, 147 |
| Lapatinib | 91 |
| Lenacil | 125, 129 |
| Leptophos OA | 125 |
| Leucine (Leu) | 23, 24, 25, 26, 27, 28 |
| Leucine enkephalin | 119, 120 |
| Leucomalachite green | 96 |
| Levamisole | 70 |
| Levetiracetam | 70 |
| Levodopa | 53 |
| Lidocaine (lignocaine) | 70, 92, 94 |
| Isopilocarpine | 139 |
| Isoprenaline | 105 |
| Isoprocarb | 125, 129 |
| 2-Isopropylphenol | 62 |
| Isoprothiolane | 129 |
| Isoproturon | 125, 129 |
| Isorhamnetin | 75 |
| Isovalerylcarnitine | 21, 97 |
| Isovalerylglycine | 98 |
| Isoxadifen-ethyl | 129 |
| Isoxaflutole | 129 |
| Isoxanthohumol | 138 |
| Itraconazole | 90 |



Lignocaine (lidocaine) 70, 92, 94
 Lincomycin 92
 Linuron 125, 129
 Liqueiritigenin 48
 Lispro (insulin) 88
 Lopinavir 39
 Loratadine 36
 Lorazepam 46, 68, 70
 Lorcaserin 39
 Lormetazepam 70
 Losartan 34
 Lovastatin hydroxy acid 143
 Lovastatin lactone 143
 LSD 70
 Lufenuron 129
 Lurbinctedin 95
 Lysine (Lys) 23, 24, 25, 26, 27, 28
 Lysophosphatidylcholine 93
 Lysophosphoethanolamine 93
 Lyso-SM-509 47

M

Malachite green 96
 Malaaxon 129
 Malathion 125
 Malathion OA 125
 Maleic acid 36, 37, 48, 96, 98, 112
 Malic acid 185
 Malonic acid 99
 Maltose 159
 MAM2201 N-4-OH-pentyl 51
 6-MAM (6-monoacetylmorphine) 68, 111
 Mandipropamid 125, 129, 132
 Marinobufagin 118
 MCAT 70
 MCPA (4-chloro-2-methylphenoxyacetic acid) 136
 MCPB (4-(4-chloro-2-methylphenoxy)butanoic acid) 136
 MDA (3,4-methylenedioxy-amphetamine) 31, 68, 70
 MDAI (5,6-methylenedioxy-2-aminoindane) 70
 MDEA (3,4-methylenedioxy-N-ethylamphetamine) 31, 68, 70
 MDMA (3, 4-methylenedioxy-methamphetamine) 31, 68, 70, 96
 MDPV (methylenedioxypropylvalerone) 70
 Mecarbam 129
 Meclofenamic acid 107, 108
 Mefenamic acid 107, 108, 133
 Mefenpyr-diethyl 125
 MEGX (monoethylglycinexylidide) 70
 Melamine 96
 Menadione (vitamin K3) 180
 MeOPP (p-methoxyphenylpiperazine) 70
 Mepaniprym 125, 129
 Mephedrone (4-methylmethcathinone, 4-MMC) 56, 70
 Mepronil 129
 Mescaline 70
 Mesoporphyrin IX 142
 Mesotrione 125, 129
 Metaflumizone 125, 129
 Metalaxyl 125, 129
 Metaldehyde 125
 Metamitron 129
 Metanephrine 54, 55
 Metanil Yellow 88
 Metazachlor 129

Metconazole 125, 129
 Metformin 70
 Methacrifos 129
 Methadone 63, 68, 70, 111
 Methamidophos 125, 129, 132
 Methamphetamine 31, 68, 71
 Methaqualone 71
 Methdilazine 134
 Methedrone 71
 Methidathion 125
 Methiocarb 125, 129
 Methiocarb sulfone 125, 129
 Methiocarb sulfoxide 125, 129
 Methionine (Met) 23, 24, 25, 26, 27, 28
 Methionine enkephalin 119, 120
 Methiopropamine 71, 148
 Methocarbamol 71
 Methomyl 125, 129, 132
 Methotrexate 100
 Methoxetamine 71
 4-Methoxyamphetamine (PMA) 71, 96
 Methoxybenzene 159
 4-Methoxycinnamic acid 112
 Methoxyfenozide 125, 129
 3-Methoxy-4-hydroxyphenylglycol (MHPG) 105
 3-Methoxytyramine 54, 71
 2-Methoxy-4-vinylphenol 62
 2'-C-Methyladenosine 109
 3-Methyladipic acid 99
 2-Methylbutyrylcarnitine 21, 97
 2-Methylbutyrylglycine 98
 3-Methylcatechol 56
 4-Methylcatechol 56
 3-Methylcrotonylglycine 98
 S-Methyl-L-cysteine 24
 3,4-Methylenedioxy-amphetamine (MDA) 31, 68, 70
 3,4-Methylenedioxy-N-ethylamphetamine (MDEA) 31, 68, 70
 3,4-Methylenedioxy-methamphetamine (MDMA) 31, 68, 70, 96
 4-Methylethcathinone (4-MEC) 56, 71
 Methyl gallate 115
 3-Methylglutaric acid 99
 Methylhexanamine 71
 2-Methylhippuric acid 84
 Methylmalonic acid 98
 4-Methylmethcathinone (mephedrone, 4-MMC) 56, 70
 2-Methylnaphthalene 104
 Methylone 71
 Methylparaben 23, 58, 59, 74, 116, 144
 Methylphenidate 71
 2-Methylphenol 62
 5-Methyl-2-phenyl-1,2-dihydropyrazol-3-one 82
 2-(4-Methylphenyl)propanoic acid 87
 Methylphenylsulfone 133, 162
 Methylphenylsulfoxide 133, 134, 162
 Methylprednisolone 61
 2-Methylresorcinol 56, 82
 N-Methylserotonin 118
 Methylsuccinic acid 97, 98
 Methyltestosterone 157
 17 α -Methyltestosterone 100
 Methylthioadenosine 47
 4-Methylthioamphetamine 31
 5-Methyltryptamine 71
 (3S)-7-O-Methylvestitol 48

Metobromuron 129
 Metoclopramide 71
 Metolachlor 129
 Metolcarb 125
 Metoprolol 43, 44, 45, 134
 Metoxuron 129
 Metrafenone 129
 Metribuzin 125, 129
 Metronidazole 23, 134, 175
 Mevinfos A 125, 130
 Mevinfos B 125, 130
 MHPG (3-methoxy-4-hydroxyphenylglycol) 105
 Microcystin LR 102
 Microcystin RR 102
 Microcystin YR 102
 Midazolam 46, 68, 71
 Mirtazapine 71
 Mitragynine 71
 Modafinil 71
 Molinate 130
 6-Monoacetylmorphine (6-MAM) 71, 111
 Monocrotophos 125, 130, 132
 Monodecarboxysirohaem 64
 Mono-N-desethylamiodarone 71
 Monolinuron 125, 130
 Morphine 68, 71, 111
 Morphine 3- β -D-glucuronide 111
 Morphine 6- β -D-glucuronide 111
 Myclobutanil 125, 130
 Myricetin 133

N

Nadolol 45
 Naloxone 71
 1-Naphthol 82, 133, 136
 2-Naphthol 136
 Naphyrone 71
 Napropamide 130
 Naproxen 107, 108, 175
 Naringenin 48
 Nefopam 71
 NEO (neosaxitoxin) 118
 Neoandrographolide 34
 Neochlorogenic acid (5-caffeoylquinic acid) 50
 Neohesperidin dihydrochalcone 22, 41
 Neosaxitoxin (NEO) 118
 Neotame 41
 Neurotensin 119
 Niacinamide (vitamin B3) 180, 182
 Nicotinamide 109, 182, 183, 184
 Nicosulfuron 125
 Nicotine 132
 Nicotinic acid 180, 182
 Nifoxipam 71
 Nimesulide 107, 108, 133
 Nimetazepam 71
 Nitenpyram 130
 Nitrazepam 46, 68, 71
 m-Nitroaniline 106
 o-Nitroaniline 106
 p-Nitroaniline 106
 Nitrobenzene 39, 75, 134
 4-Nitrocatechol 56
 Nitrofurazone 106
 2-Nitrophenol 116, 117, 171
 4-Nitrophenol 116, 117, 171
 2-Nitro-p-phenylenediamine 82

| | | | | | |
|---------------------------------------|-------------------------|---|---|--|---------------|
| Procyanidin pentamer..... | 137 | Quinoxifen..... | 126, 130 | Sorbic acid..... | 33, 58, 144 |
| Procyanidin tetramer..... | 137 | Quizalofop-ethyl..... | 126 | Sotalol..... | 43, 45, 151 |
| Procyclidine..... | 71 | | | Spectinomycin..... | 29 |
| Profenofos..... | 130 | R | | Spermidine..... | 25 |
| Proxoydim..... | 126 | Ranitidine..... | 114, 149 | Sphingomyelin phosphoethanolamine..... | 93 |
| Progesterone..... | 155 | Rebaudioside A..... | 42 | Spinetoram..... | 126 |
| Proline (Pro)..... | 23, 25, 26, 27, 28 | Rebaudioside B..... | 42 | Spinosyn A..... | 126, 130 |
| Promecarb..... | 126 | Rebaudioside C..... | 42 | Spinosyn D..... | 126, 130 |
| Promethazine..... | 36, 71, 162 | Rebaudioside D..... | 42 | Spirodiclofen..... | 126, 130 |
| Prometryn..... | 130, 132 | Rebaudioside F..... | 42 | Spiromesifen..... | 126, 130 |
| Propachlor..... | 130 | Red 2G..... | 184 | Spiromesifen alcohol..... | 126 |
| Propamocarb..... | 126, 130 | Remacemide..... | 135 | Spironolactone..... | 43, 65, 66 |
| Propaquizafop..... | 126, 130 | Remifentanil..... | 71 | Spirotetramat..... | 126, 130 |
| Propargite..... | 126, 130, 132 | Reserpine..... | 74 | Spiroxamine..... | 126, 130 |
| Propazine..... | 130, 132 | Resmethrin..... | 126 | Stanozolol..... | 32 |
| Propetamfos..... | 126, 130 | Resorcinol..... | 56, 82, 136 | Steviolbioside..... | 42 |
| Propham..... | 130 | Retinol (vitamin A)..... | 180 | Stevioside..... | 42 |
| Propiconazole..... | 130 | Reversed tri-iodothyronine (rT3)..... | 167 | Streptomycin..... | 29 |
| Propionylcarnitine..... | 21 | Rhamnose..... | 160 | STX (saxitoxin)..... | 118 |
| Propionylglycine..... | 98 | Rhodamine B..... | 88 | Suberylglycine..... | 98 |
| Propiophenone..... | 135 | Riboflavin (vitamin B2)..... | 180, 181, 182, 183 | Succinic acid..... | 98 |
| Propisochlor..... | 130 | Ribonuclease A..... | 147 | Sucralose..... | 22, 41 |
| Propofol..... | 71 | Rifabutin..... | 150 | Sucrose..... | 159, 160, 161 |
| Propofol glucuronide..... | 71 | Rifampicin..... | 150 | Sudan I..... | 88 |
| Propoxur..... | 126, 130 | Rifapentine..... | 150 | Sudan II..... | 88 |
| Propoxyphene..... | 71 | Rimonabant..... | 39 | Sudan III..... | 88 |
| Propranolol..... | 43, 44, 45, 71 | Rimsulfuron..... | 126 | Sudan IV..... | 88 |
| Propylbenzene..... | 133 | Risperidone..... | 71 | Sudan Black..... | 88 |
| Propylparaben..... | 58, 59, 116, 144, 174 | Ritalinic acid..... | 71 | Sudan Orange G..... | 88 |
| Propyzamide..... | 130 | Ritonavir..... | 39 | Sudan Red B..... | 88 |
| Proquinazid..... | 130 | Rotenone..... | 126, 130 | Sudan Red 7B..... | 88 |
| Prostaglandin F2 α | 147 | Rubusoside..... | 42 | Sudan Red G..... | 88 |
| 8-iso-Prostaglandin F2 α | 147 | Rutin..... | 75, 76, 89 | Sufentanil..... | 71 |
| Prosulfocarb..... | 130 | | | Sulfachloropyridazine..... | 161 |
| Prosulfuron..... | 126, 130 | S | | Sulfadiazine..... | 161 |
| Prothioconazole..... | 130 | Saccharin..... | 22, 41, 58 | Sulfadimethoxine..... | 161 |
| Prothioconazole-desthio..... | 130 | Saflufenacil..... | 126 | Sulfamerazine..... | 161 |
| Protoporphyrin IX..... | 142 | Salbutamol..... | 74 | Sulfamethazine..... | 161 |
| Pseudoephedrine..... | 36, 87 | Salicylaldehyde..... | 33 | Sulfamethoxazole..... | 161 |
| Putrescine..... | 140 | Salicylamide..... | 33, 36, 37, 42, 43 | Sulfamonomethoxine..... | 161 |
| Pymetrozine..... | 126, 130 | Salicylic acid (2-hydroxybenzoic acid)..... | 33, 42, 43, 61, 108, 112, 133, 139, 140, 171, 175 | Sulfapyridine..... | 161 |
| Pyraclostrobin..... | 126, 130 | Salsalate..... | 43, 171 | N-Sulfocarbamoylgonyaurotoxins (C1,2)..... | 118 |
| Pyraflufen-ethyl..... | 126 | Saxitoxin (STX)..... | 118 | Sulfotep..... | 130 |
| Pyrazophos..... | 126, 130 | Scopolamine..... | 36 | Sulfoxaflo..... | 126 |
| Pyridaben..... | 126, 130 | Sebuthylazine..... | 132 | Sulindac..... | 107, 108, 133 |
| Pyridalyl..... | 126 | Secbumeton..... | 130 | Sulphanilamide..... | 134 |
| Pyridapenthion..... | 130 | Sedaxane..... | 126 | Sulprofos..... | 126 |
| Pyridate..... | 130 | Sennoside A..... | 151 | Sumatriptan..... | 162 |
| Pyridoxal..... | 180, 182, 184 | Sennoside B..... | 151 | Sunset Yellow..... | 41, 184 |
| Pyridoxamine..... | 109, 180, 182, 184 | Serine (Ser)..... | 24, 25, 26, 28 | | |
| Pyridoxine (vitamin B6)..... | 180, 181, 182, 183, 184 | Serotonin..... | 105, 118 | T | |
| Pyrifenox..... | 130 | Sertraline..... | 39, 71 | T-2-toxin..... | 103 |
| Pyrimethanil..... | 126, 130 | Sesamol..... | 119 | rT3 (reversed tri-iodothyronine)..... | 167 |
| Pyriproxyfen..... | 126, 130 | Sethoxydim..... | 126 | T3 (tri-iodothyronine)..... | 167 |
| Pyrocatechol..... | 136 | Sibutramine..... | 39 | T4 (thyroxine)..... | 167 |
| Pyroxulam..... | 130 | Sildenafil..... | 71 | Taleranol..... | 157 |
| | | Sildenafil N-oxide..... | 71 | Tartaric acid..... | 185 |
| | | Silthiofam..... | 130 | Tartrazine..... | 41 |
| | | Simazine..... | 126, 130, 132 | Tau-fluvalinate..... | 130 |
| | | Simetryn..... | 130 | Taxol (paclitaxel)..... | 115, 165 |
| | | Simvastatin..... | 155 | TCMTB..... | 126 |
| | | Simvastatin hydroxy acid..... | 153 | Tebuconazole..... | 130 |
| | | Simvastatin lactone..... | 153 | Tebufenozide..... | 126, 130 |
| | | Sinapic acid..... | 112 | Tebufenpyrad..... | 126, 130 |
| | | Sirohaem..... | 64 | Tebuthiuron..... | 126 |
| | | | | Teflubenzuron..... | 130 |
| Q | | | | | |
| Quercetin..... | 58, 76 | | | | |
| Quercitrin..... | 76 | | | | |
| Quetiapine..... | 71, 110 | | | | |
| Quinalfos..... | 126, 130 | | | | |
| Quinidine..... | 148 | | | | |
| Quinine..... | 148 | | | | |
| Quinine sulphate..... | 22 | | | | |
| Quinoclamine..... | 130 | | | | |
| Quinoxaline..... | 74 | | | | |



| | | | | | |
|--|---------------------------------|---|-----------------------------|--|-------------------------------|
| Telithromycin..... | 165 | Tramadol | 71, 172 | Valerylcarntine | 97 |
| Telmisartan | 34 | Trazodone..... | 71 | Valerylglycine..... | 98 |
| Telocinobufagin | 118 | α -Trenbolone..... | 157 | Valine (Val) | 23, 24, 25, 26, 27, 28 |
| Temazepam | 46, 68, 71 | β -Trenbolone..... | 157 | Valsartan | 34, 86 |
| Tembotrione (NH4 adduct)..... | 130 | Triadimefon | 126, 131 | Val-Tyr-Val | 119, 120 |
| Tenofovir disoproxil | 152 | Triadimenol | 126, 131 | Vamidothion..... | 131 |
| Tepraloxymid | 126 | Triallate..... | 131 | Vanillic acid | 146, 176, 177 |
| Terbufos | 130 | Triamcinolone..... | 61 | o-Vanillin | 177 |
| Terbufos sulfone | 126, 130 | Triazofos..... | 126, 131 | Vanillin | 23, 58, 146, 176, 177 |
| Terbufos sulfoxide..... | 126, 130 | Triazolam | 46, 68 | Vanillylmandelic acid (VMA)..... | 53, 176 |
| Terbumeton | 131 | Tribenuron-methyl..... | 126 | Varenciline | 71 |
| Terbutylazine | 126, 131, 132 | Tri-n-butyl phosphate (TBP)..... | 113 | Venlafaxine | 71 |
| Terbutryn..... | 131, 132 | Tributyltin | 114 | Verapamil..... | 71 |
| Terfenadine | 166 | Trichlorfon | 126, 131 | Vestitol..... | 48 |
| Testosterone..... | 100, 155, 166 | 1,2,3-Trichlorobenzene | 133 | Vigabatrin..... | 71 |
| Tetracaine | 134 | Tricyclazole..... | 126, 131 | Virginiamycin | 145 |
| Tetrachlorvinfos..... | 126, 131 | Triethyl phosphate (TEP) | 113 | Vitamin A (retinol)..... | 180 |
| Tetraconazole | 131 | Trifloxystrobin..... | 126, 131 | Vitamin A acetate | 180 |
| Tetracycline..... | 166 | Triflumizole..... | 126, 131 | Vitamin B1 (thiamine) | 109, 180, 182, 183, 184 |
| Δ 9-Tetrahydrocannabinol (THC)..... | 52 | Triflumuron..... | 131 | Vitamin B2 (riboflavin)..... | 180, 181, 182, 183 |
| Tetrahydrocannabinol carboxylic acid (THC-COOH)..... | 68 | Trifluoperazine..... | 71 | Vitamin B3 (niacinamide)..... | 180, 182 |
| 1,2,3,4-Tetrahydro-1-naphthol..... | 134 | Trifluralin | 83 | Vitamin B5 (pantothenic acid)..... | 180, 181, 182, 183 |
| Tetramethrin | 126 | Triforine | 126, 131, 132 | Vitamin B6 (pyridoxine)..... | 180, 181, 182, 183, 184 |
| Tetranactin | 101 | Triglycerides..... | 93 | Vitamin B7 (D-biotin, vitamin H) | 180, 181, 182 |
| Tetrazepam | 71 | Trihexyphenidyl | 71 | Vitamin B9 (folic acid) | 180, 181, 183 |
| TFMPP (trifluoromethylphenylpiperazine)..... | 71 | Tri-iodothyronine (T3) | 167 | Vitamin B12 (cyanocobalamin)..... | 180, 181, 182 |
| THC (Δ 9-Tetrahydrocannabinol)..... | 52 | Triisopropyl phosphate (TiPP)..... | 113 | Vitamin C (ascorbic acid)..... | 61, 109, 112, 140, 180, 182-5 |
| THC-COOH (Tetrahydrocannabinol carboxylic acid) | 68 | 1,2,3-Trimethoxybenzene..... | 159 | Vitamin D2 (ergocalciferol)..... | 178, 180 |
| Theanine..... | 81 | 1,2,4-Trimethoxybenzene..... | 133, 159 | Vitamin D3 (cholecalciferol) | 178, 180 |
| Theobromine..... | 22, 50, 58, 171 | 1,3,5-Trimethoxybenzene..... | 159 | Vitamin E (α -tocopherol)..... | 167, 168, 180 |
| Theogallin..... | 81 | 2,3,6-Trimethylphenol | 136 | Vitamin E acetate | 167, 180 |
| Theophylline..... | 22, 50, 58, 71, 171 | 2,4,6-Trimethylphenol | 62, 136 | Vitamin K1 | 180 |
| Thiamine (vitamin B1) | 109, 180, 182, 183, 184 | 3,4,5-Trimethylphenol..... | 136 | Vitamin K3 (menadione) | 180 |
| Thiabendazole | 126, 131, 132 | Trimethyl phosphate (TMP)..... | 113 | VMA (vanillylmandelic acid) | 53, 176 |
| Thiacloprid..... | 104, 126, 131, 132 | Trinactin | 101 | | |
| Thiamethoxam | 104, 126, 132 | 1,3,5-Trinitrobenzene | 39, 75, 133 | W | |
| Thien carbazone-methyl..... | 131 | Triphenyl phosphate (TPP) | 113 | Warfarin | 71 |
| Thifensulfuron-methyl..... | 126 | Tri-n-propyl phosphate (TPrP)..... | 113 | | |
| Thioanisole..... | 162 | Tripolidine | 36, 37 | X | |
| Thiobencarb | 126 | Tri-m-tolyl phosphate (TMTP)..... | 113 | Xanthine | 50 |
| Thioctic acid..... | 180 | Tri-o-tolyl phosphate (TOTP)..... | 113 | Xanthohumol | 138 |
| Thiodicarb | 126, 131, 132 | Tri-p-tolyl phosphate (TPTP) | 113 | XLR-11 | 164 |
| Thionazin..... | 126 | Tris(2-butoxyethyl) phosphate (TBEP)..... | 113 | | |
| Thiophanate-methyl | 131, 132 | Tris(2-chloroethyl) phosphate (TCEP) | 113 | Z | |
| THJ-018..... | 51 | Tris((2R)-1-chloro-2-propyl) phosphate (TCPP) | 113 | Zaleplon | 68, 71 |
| Threonine (Thr)..... | 24, 25, 26, 27, 28 | Tris(1,3-dichloro-2-propyl) phosphate (TDCPP)..... | 113 | α -Zearalenol | 157 |
| Thymidine | 109 | Triticonazole A..... | 131 | β -Zearalenol | 157 |
| Thymine | 109 | Triticonazole B..... | 131 | Zearalenone | 157 |
| Thyroxine (T4) | 167 | Tryptamine..... | 25 | Zeatin..... | 139 |
| Tiglylglycine | 98 | Tryptophan (Trp) | 25, 27, 28, 172 | Zeranol..... | 157 |
| Tinosorb® M..... | 163 | Tyramine | 25 | Zolpidem..... | 68, 71 |
| Tinosorb® S | 163 | Tyrosine (Tyr) | 23, 24, 25, 26, 28, 53, 172 | Zolpidem phenyl-carboxylic acid | 71 |
| Tobramycin..... | 29 | | | Zopiclone | 71 |
| α -Tocopherol (vitamin E) | 167, 168, 180 | U | | Zopiclone N-oxide | 71 |
| α -Tocopherol acetate..... | 167, 180 | UR-144 | 164 | Zoxamide | 126, 131 |
| β -Tocopherol..... | 167, 168 | UR-144 5-chloro-pentyl..... | 164 | | |
| γ -Tocopherol..... | 167, 168 | UR-144 5-OH-pentyl | 164 | | |
| δ -Tocopherol..... | 167, 168 | UR-144 N-pentanoic | 51, 164 | | |
| Tolclophos-methyl | 131 | Uracil | 109 | | |
| Tolmetin | 107, 108, 133 | Uracil arabinofuranoside..... | 63 | | |
| Toluene | 39, 74, 133, 135, 159, 162, 168 | Uric acid | 85 | | |
| Toluene-2,5-diamine..... | 82 | Uridine..... | 109 | | |
| Toluene-3,4-diamine..... | 82 | Uroporphyrin I..... | 142 | | |
| Toluidine Red | 88 | | | | |
| Tolyfluanid | 131 | V | | | |
| Topramezone | 126, 131 | Valerophenone..... | 134 | | |

Your decision has lasting effects.



Ultra-Inert Base Deactivated UHPLC/HPLC Columns
For Performance, Selectivity and Guaranteed Reproducibility

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.



**ACE products are available through
our international network of distributors**



www.ace-hplc.com



Advanced Chromatography Technologies Ltd, 1 Berry Street, Aberdeen, AB25 1HF, Scotland
Tel: +44 (0) 1224 704 554 • Fax: +44 (0) 1224 841 301 • www.ace-hplc.com • email: info@ace-hplc.com