Accelerating HPLC / UHPLC Method Development With Selectivity: Influence of Column Chemistries

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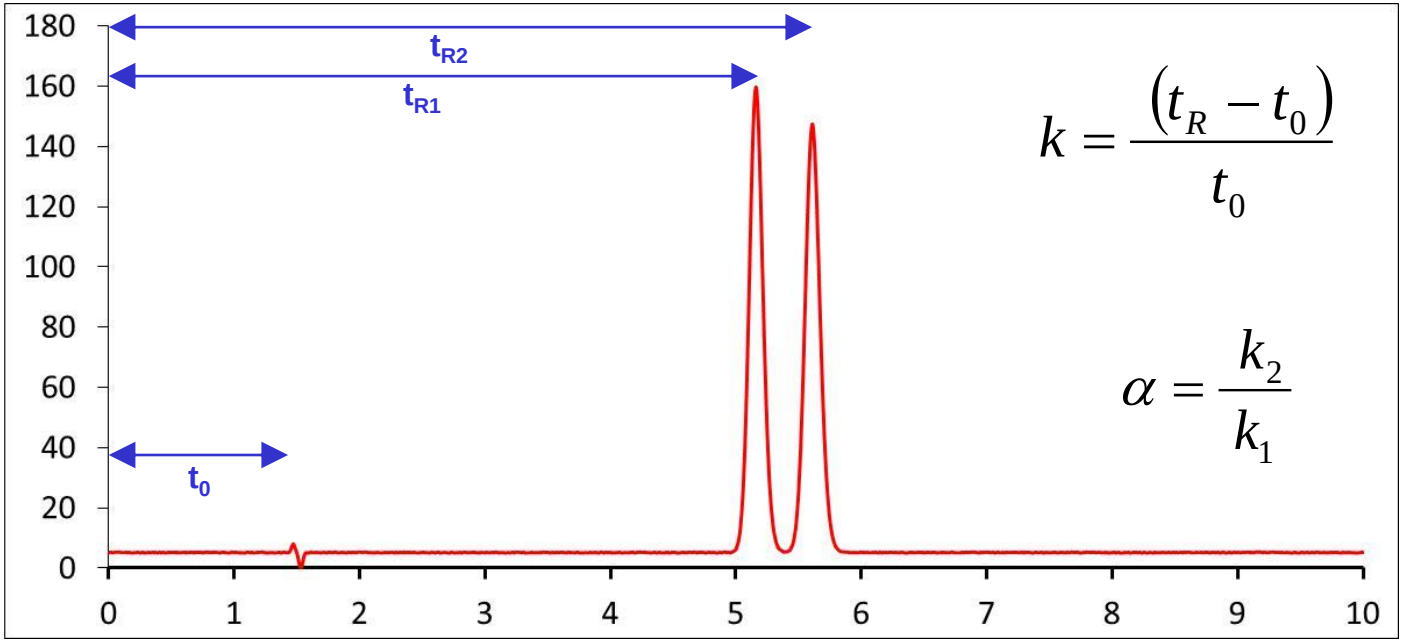
Outline

- What is selectivity?
- Method development workflows
- Maximizing selectivity through rational stationary phase design
- Optimized method development workflows

What is Selectivity?

- Alpha (α) is the symbol used to denote the **separation factor** or **separation selectivity** between 2 adjacent peaks



- **Selectivity** can be thought of as '**peak spacing**'
- Selectivity values should be **> 1.0**

Resolution, Selectivity, Efficiency & Retention

Particle size, column length, dispersion etc

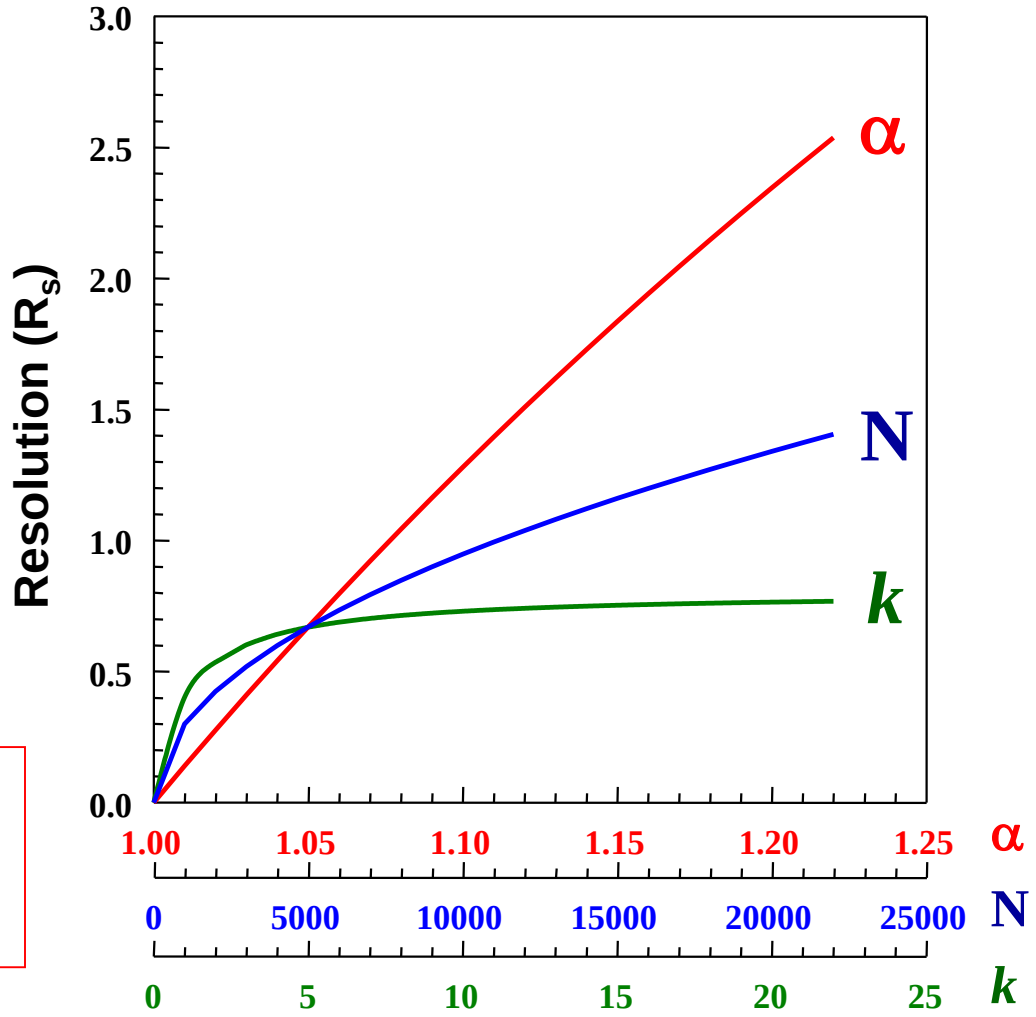
Phase design, eluent etc

Efficiency

Selectivity

Retention

$$R_s = \frac{\sqrt{N}}{4} \cdot \frac{\alpha - 1}{\alpha} \cdot \frac{k}{1+k}$$



Selectivity (α) is the key to resolution and efficiency (N) boosts performance

Zhao, J.H. and P.W. Carr. Analytical Chemistry, (1999) 71, 2623-2632

Which Factors[1] Affect Selectivity?

- **Strongly influenced by physicochemical properties of the analyte, stationary phase, eluent etc**
- **From a practical perspective:**

Isocratic Separations

- Column stationary phase type
- pH (ionisable analytes only)
- Organic modifier type
- % Organic modifier
- Buffer selection
- Column temperature
- Buffer concentration

MOST Influence

LEAST Influence

Gradient Separations

All parameters for isocratic **PLUS**

Gradient steepness,

k^* (t_G, F, V_m, $\Delta\Phi$, M),

$$k^* = \frac{t_G F}{\Delta\Phi V_m M}$$

Dwell volume,

Column dimensions.

1 Adapted from 'Introduction to Modern Liquid Chromatography", 3rd Edition, Snyder, Kirkland, Dolan, 2010, p.29, Wiley & sons

Method Development / Screening Workflow: Overview

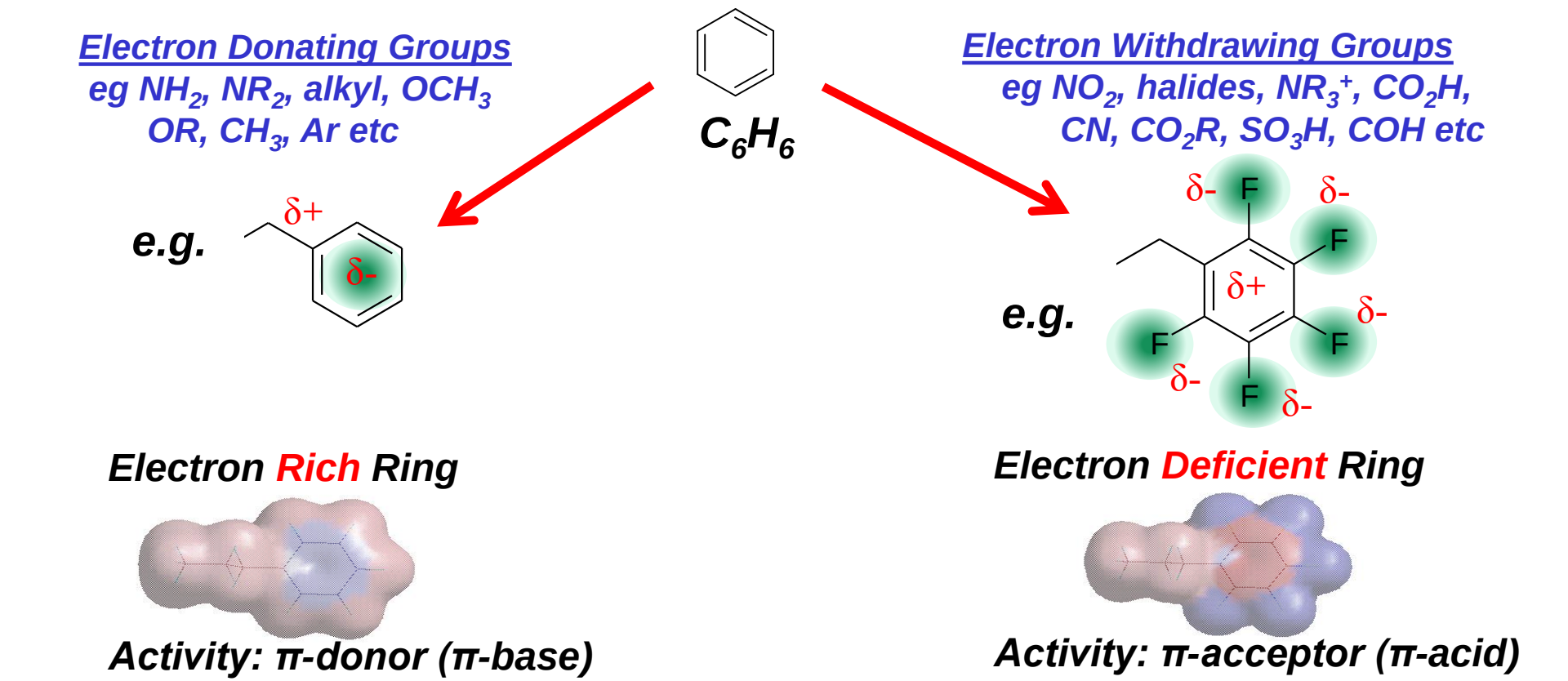
- **Typically multivariate**

- 1 column - 1 temperature - 1 pH - 1 organic modifier - 1 t_G	- 1 column - 2 temperatures - 1 pH - 1 organic modifier - 2 x t_G	- 1 column - 2 temperatures - 1 pH - 2 organic modifier - 2 x t_G	- ≥ 2 columns - 2 temperatures - 1 pH - 2 organic modifier - 2 x t_G	- ≥ 2 column - 2 temperatures - 2 or 3 pH - 2 organic modifier - 2 x t_G
2 x t_G	20C & 60C	MeOH & MeCN	Alkyl chains eg C18, C8 Aromatic eg Phenyl, C18-AR or C18-PFP Polar eg C18-PFP, C18-Amide	pH 2.5 pH 7 pH 10.7

INCREASING COMPLEXITY...BUT KNOWLEDGE RICH

- **Many potential runs to fully explore variables and their effects on retention and selectivity**
- **Would be helpful to reduce parameter options...**

Scientific Led Stationary Phase Design: Aromatic Phases



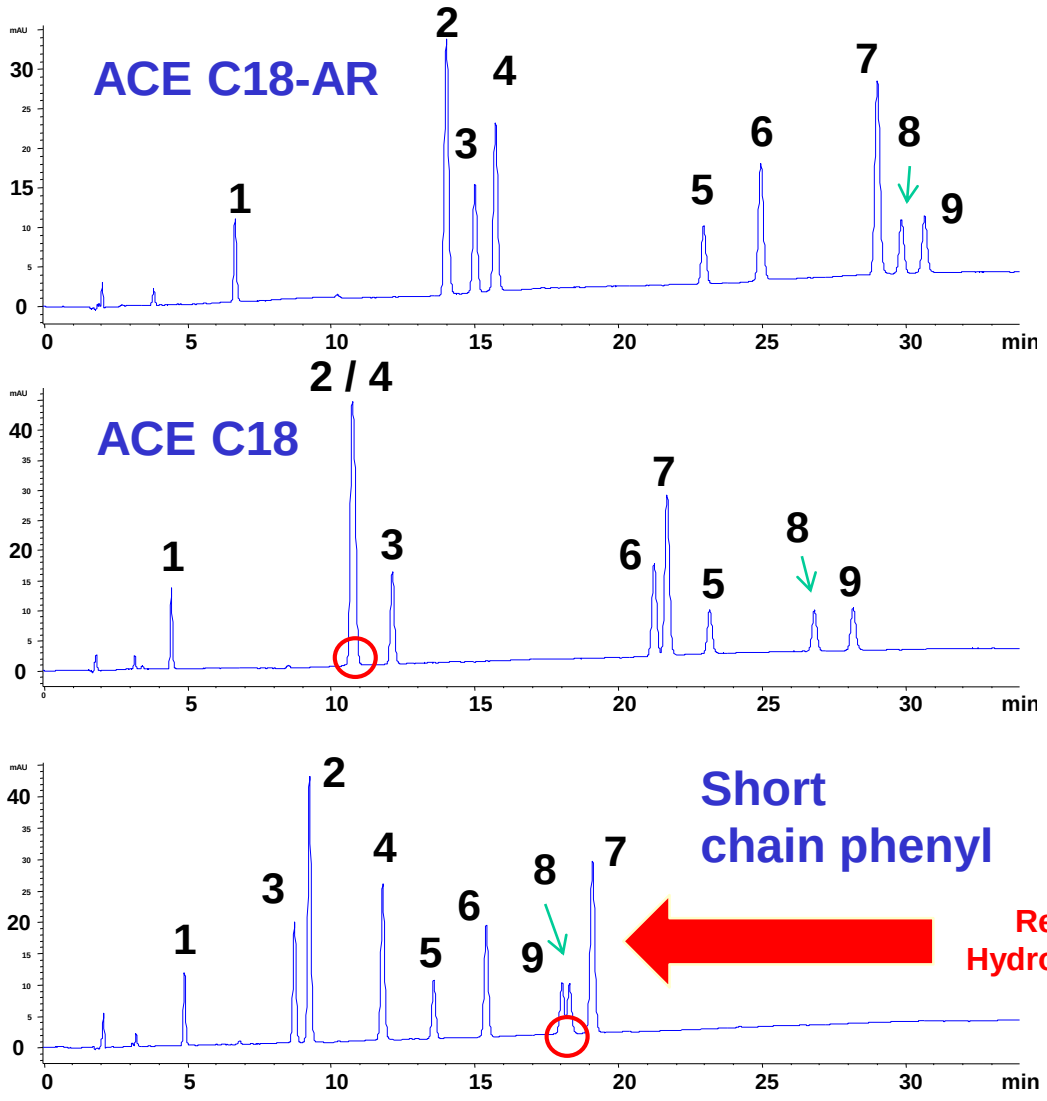
How do we exploit these properties for new stationary phases?

C18+Phenyl = ACE® C18-AR

C18+PFP = ACE® C18-PFP

Both phases have multiple mechanisms of interaction, low bleed and are 100% wettable: i.e. maximize selectivity

ACE® C18-AR Separation Comparisons



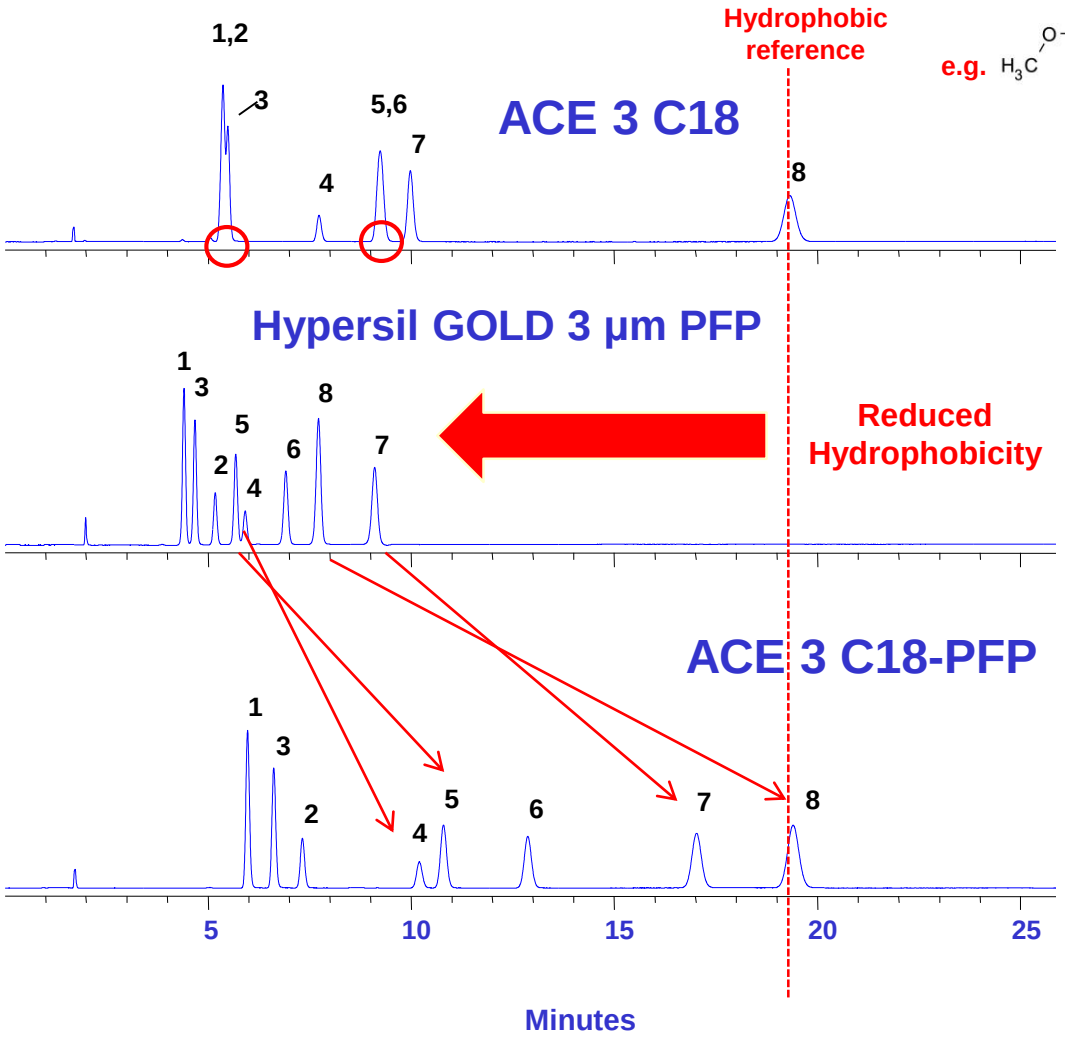
- ACE C18-AR combines hydrophobicity, dipole-dipole and π-π analyte interactions to successfully effect separation
- Mechanisms of C18 and phenyl alone not enough to resolve the NSAID complex mixture
- Elution order, retention and selectivity all seen to differ

1=Bendroflumethazide; 2=Ketoprofen; 3=Naproxen; 4=Sulindac; 5=Ibubrofen; 6=Diclofenac; 7=Indomethacin; 8=Meclofenamic acid; 9=Mefenamic acid;

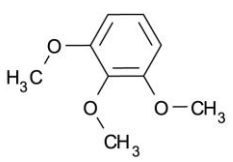
150x4.6 mm id, 1 mL/min, 40C, 254 nm, A = 0.1% v/v formic acid in H_2O B = 0.1% v/v formic acid in MeOH; Gradient:

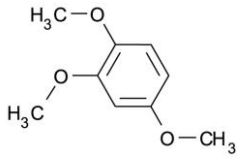
Time	%B
0	52
28	74
33	74

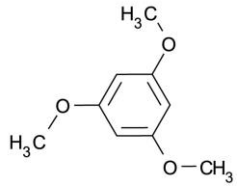
ACE® C18-PFP Example: Methoxybenzene Isomers



e.g.





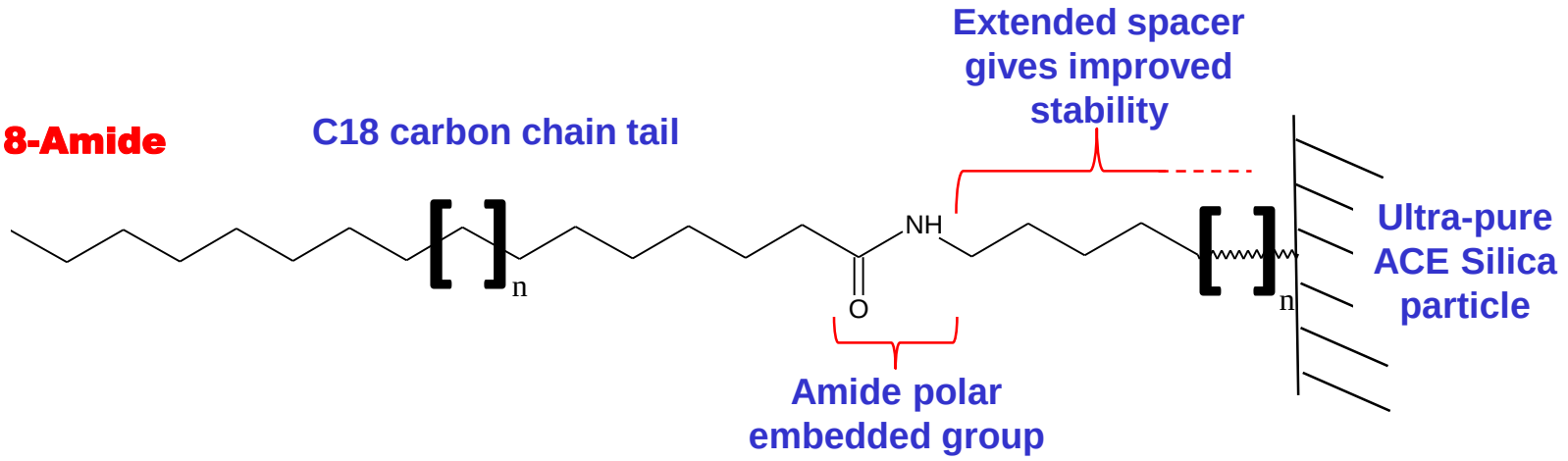


- **C18** or **PFP** mechanisms alone **not enough** to fully resolve the methoxybenzene **isomers**
- **ACE C18-PFP** mechanism **combines hydrophobicity, shape selectivity, dipole-dipole** and **π-π** interactions
- **Elution order**, **retention** and **selectivity** all seen to differ
- Powerful **positional isomer** and **shape** selectivity

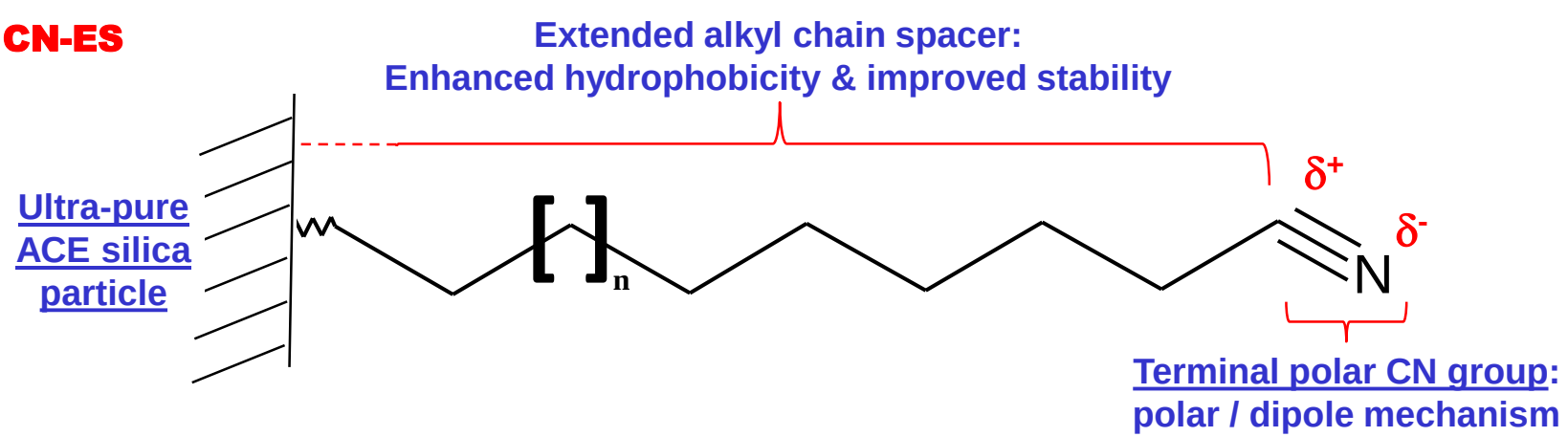
1) 1,2,3-trimethoxybenzene, 2) 1,2,4-trimethoxybenzene, 3) 1,2-dimethoxybenzene, 4) 1,4-dimethoxybenzene 5) methoxybenzene, 6) 1,3-dimethoxybenzene, 7) 1,3,5-trimethoxybenzene, 8) toluene (ref) Mobile phase 50:50 v/v MeOH / H_2O; Column= 150 x 4.6 mm id; 1.00 ml/min; 40C; 254 nm

Scientific Led Stationary Phase Design: Other Phases

ACE C18-Amide



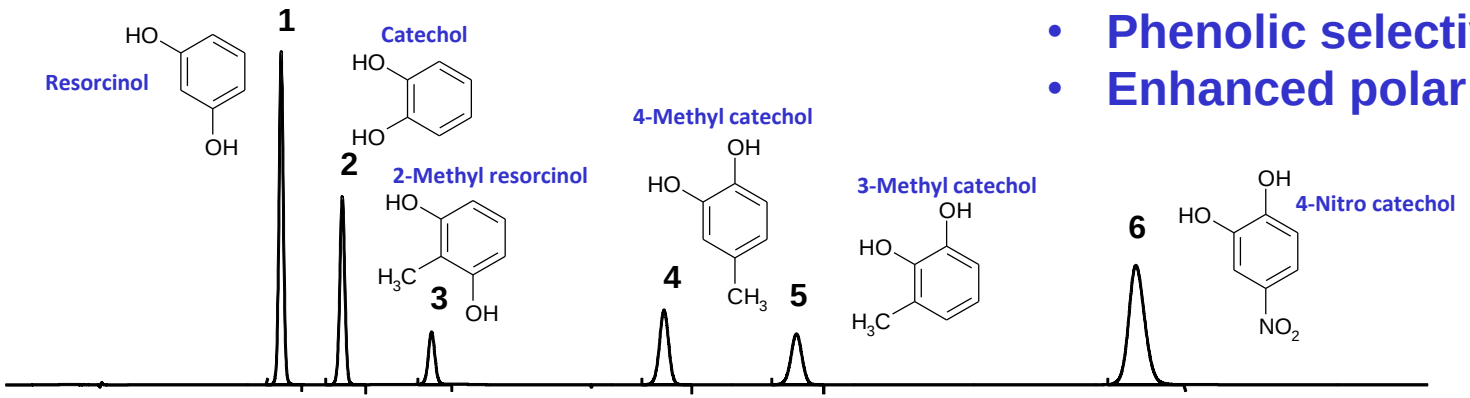
ACE CN-ES



Multiple mechanisms of interaction, low bleed and are 100% wettable: i.e. maximize selectivity

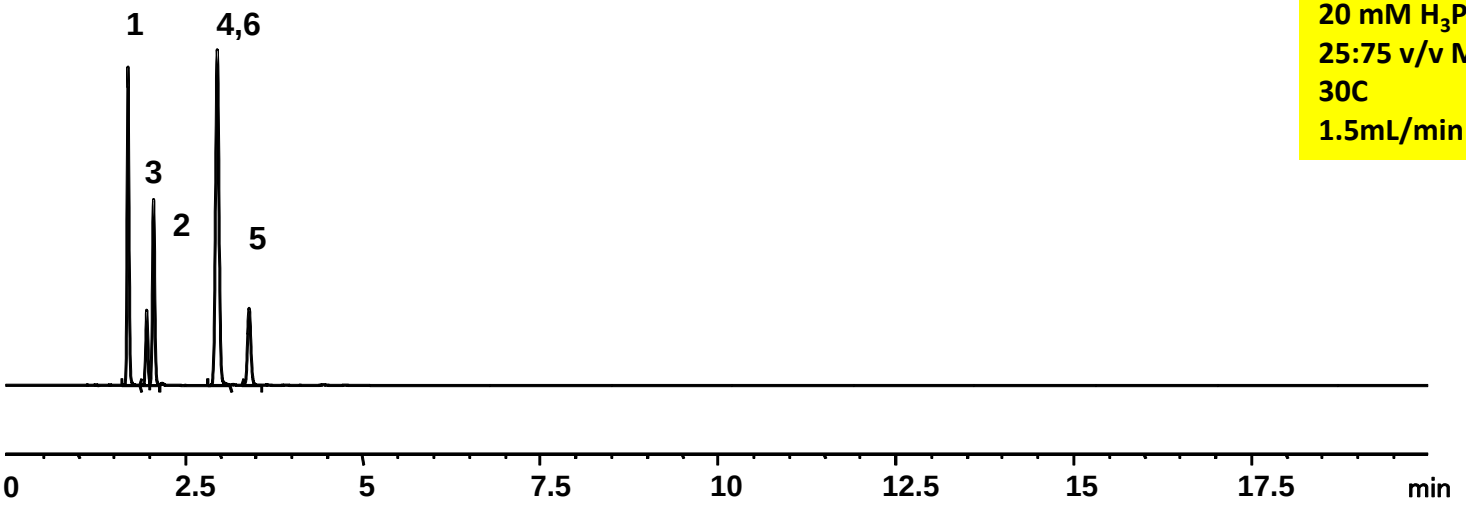
Catechols and Resorcinols Separations

ACE C18-Amide



- **Phenolic selectivity**
- **Enhanced polar retention**

ACE C18

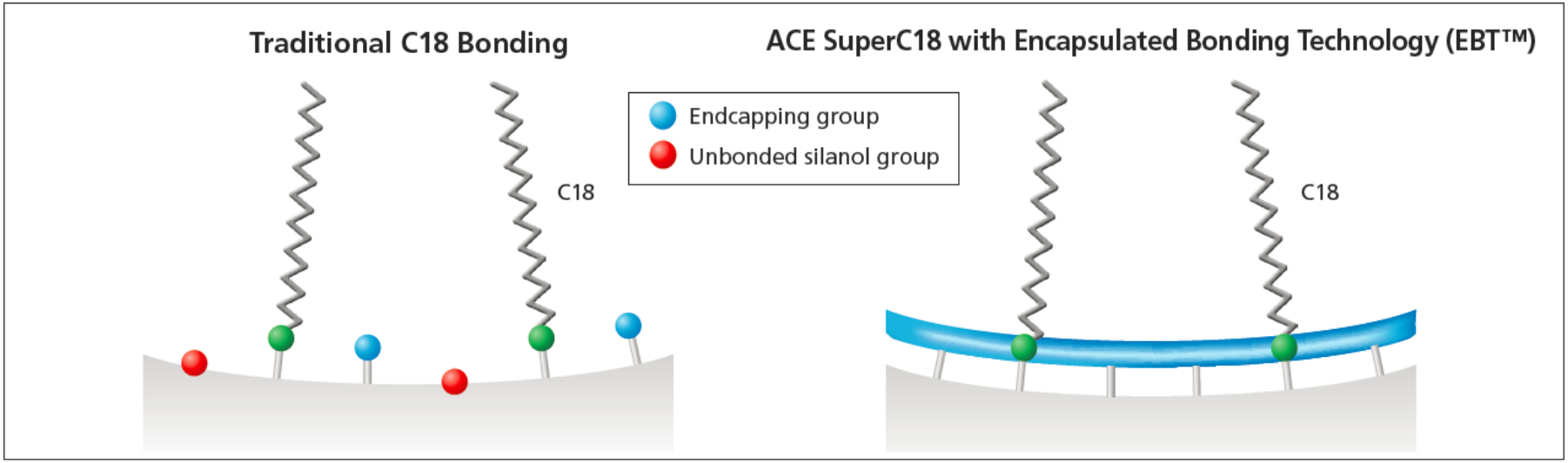


150 x 4.6mm, 3µm
Isocratic analysis

20 mM H_3PO_4 in
25:75 v/v MeCN/H_2O
30C
1.5mL/min

ACE® SuperC18™: Uniquely Designed To Exploit Eluent pH

Encapsulated Bonding Technology (EBT™) for Improved Chromatography and Stability



- **Unique bonding technology** protects the silica surface
- **Extended pH range** compatible silica-based columns
- **Rational** stationary phase design

ACE® SuperC18™: Mid pH Performance

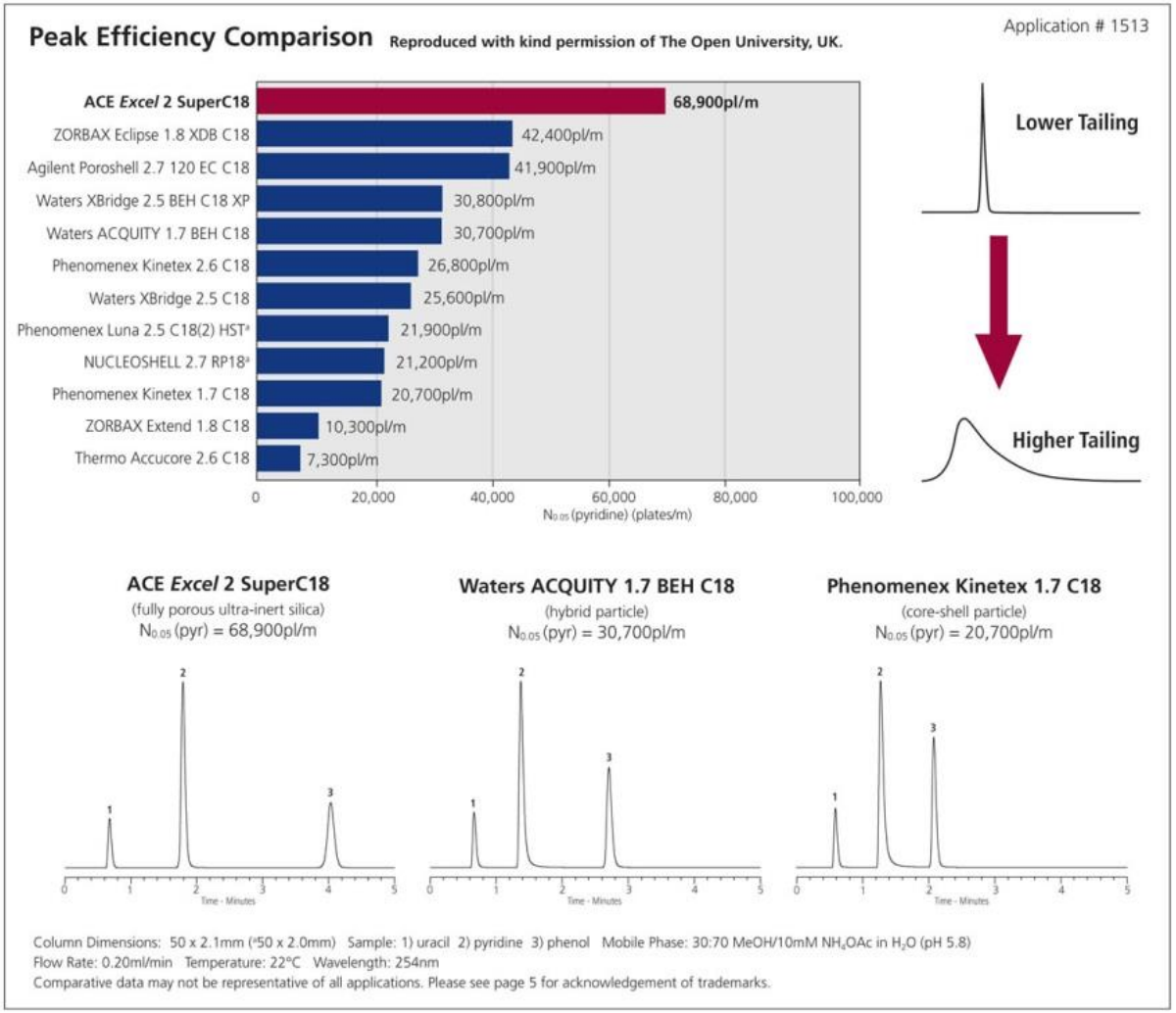
2 µm UHPLC / LC-MS

- Brochure data
- Column inertness
- Pyridine test at mid pH

- Efficiency measured
- Example data shown

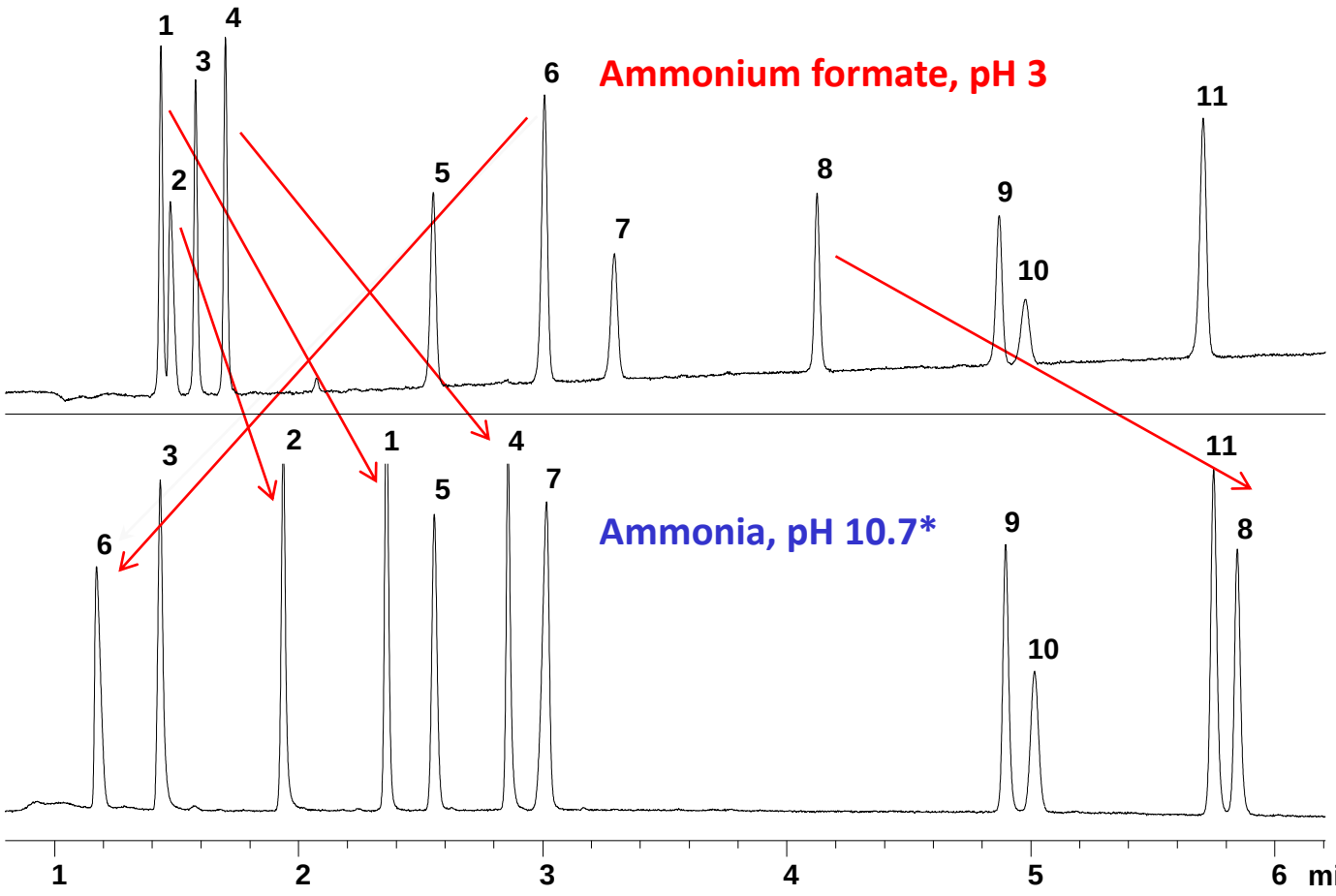
- ACE SuperC18 #1
- Leading competition included

Highest Performing



ACE® SuperC18™: Low / High pH Switching & Selectivity

- **Screening platforms / method development systems**
  - **Significant selectivity changes observed**



A1= 10mM HCOONH4, pH3 (aq)
B1= 10mM HCOONH4, pH 3 in 90% MeCN

A2= 0.1% NH3, pH 10.7 (aq)
B2= 0.1% NH3, pH10.7 in 90% MeCN

ACE Excel 3 SuperC18
50x2.1mm
Gradient: 3 – 100 %B in 7 mins
Flow rate: 0.42 mL/min
Temperature: 40C
Detection: 254 nm
Injection: 2uL

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

*Equivalent to 18mM

ACE® HPLC / UHPLC Columns

ACE® Specifications

PHASE	USP LISTING	FUNCTIONAL GROUP	ENDCAPPED	PARTICLE SIZE (µm)*	PORE SIZE (Å)	SURFACE AREA (m^2/g)	CARBON LOAD (%)	PH RANGE	100% AQ compatible
ACE® Traditional Chemistries									
C18	L1	Octadecyl	Yes	1.7, 2, 3, 5, 10	100	300	15.5	2 – 8	-
C18-HL	L1	Octadecyl	Yes	3, 5, 10, 15	90	400	20.0	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	-
Ph	L11	Phenyl	Yes	2, 3, 5, 10	100	300	9.5	2 – 8	-
CN	L10	Cyano	Yes	2, 3, 5, 10	100	300	5.5	2 – 7	-
AQ	L1	Proprietary	Yes	2, 3, 5, 10	100	300	14.0	2 – 8	YES
SIL	L3	Unbonded	No	2, 3, 5, 10	100	300	N/A	2 – 7	-
ACE NH_2	L8	Proprietary aminopropyl	Proprietary	1.7, 3, 5	100	300	3.5	2 – 7	YES
ACE® Novel Chemistries									
SuperC18	L1	Octadecyl encapsulated	Encapsulated	1.7, 2, 3, 5, 10	90	400	14.8	1.5 – 11.5	-
C18-AR	L1	Octadecyl with integral phenyl	Yes	1.7, 2, 3, 5, 10	100	300	15.5	2 – 8	YES
C18-PFP	L1	Octadecyl with integral PFP	Yes	1.7, 2, 3, 5, 10	100	300	14.3	2 – 8	YES
C18-Amide	L1 / L60	Polar embedded amide	Yes	1.7, 2, 3, 5, 10	100	300	16.4	2 – 8	YES
CN-ES	L10	CN with extended alkyl spacer	Yes	1.7, 2, 3, 5, 10	100	300	12.6	2 – 8	YES
Solid Core Technology ACE® Phases									
UltraCore SuperC18	L1	Octadecyl encapsulated	Encapsulated	2.5 5	95	130 100	7.0 5.4	1.5 – 11.0	-
UltraCore SuperPhenylHexyl	L11	Phenyl Hexyl encapsulated	Encapsulated	2.5 5	95	130 100	4.6 3.6	1.5 – 11.0	-
Large Molecule Wide Pore ACE® Phases									
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® HILIC Phases									
ACE HILIC-A	L3	Proprietary SIL	No	1.7, 3, 5	100	300	N/A	2 – 7	-
ACE HILIC-B	L8	Proprietary aminopropyl	No	1.7, 3, 5	100	300	4.0	2 – 7	-
ACE HILIC-N	pending	Proprietary polyhydroxy	No	1.7, 3, 5	100	300	7.0	2 – 7	-

ACE® Unique Chemistries Key Mechanisms of Interactions

Bonded Phase	Separation Mechanism and Relative Strength[1]				
	Hydrophobic Binding	π-π Interaction	Dipole-Dipole	Hydrogen Bonding	Shape Selectivity
ACE C18	****	-	-	*	**
ACE C18-AR	****	*** (donor)	*	**	***
ACE C18-PFP	****	*** (acceptor)	****	***	****
ACE SuperC18	****	-	-	-	**
ACE C18-Amide	****	-	**	****	**/***
ACE CN-ES	***	*	***	**	*

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

Characterized using the extended Tanaka protocol

ACE® Unique Chemistries Key Mechanisms of Interactions

- **Specifically designed phases to maximize selectivity**

Bonded Phase	Separation Mechanism and Relative Strength[1]				
	Hydrophobic Binding	π-π Interaction	Dipole-Dipole	Hydrogen Bonding	Shape Selectivity
ACE C18	****	-	-	*	**
ACE C18-AR	****	*** (donor)	*	**	***
ACE C18-PFP	****	*** (acceptor)	****	***	****
ACE SuperC18	****	-	-	-	**
ACE C18-Amide	****	-	**	****	**/***
ACE CN-ES	***	*	***	**	*

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

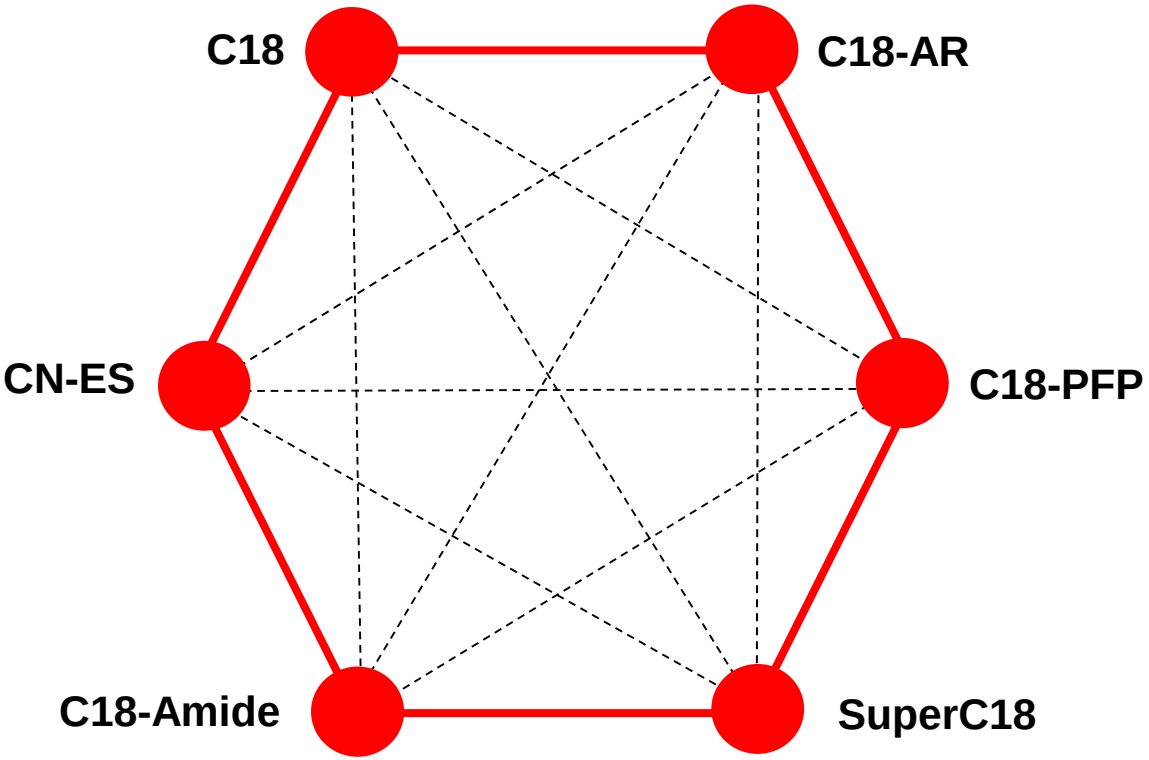
- **Multiple mechanisms of interaction: ideal for method development**

Characterized using the extended Tanaka protocol

Selectivity, Method Development: 6 Column Switcher

- 6 stationary phases, 1 solvent, 1 low pH

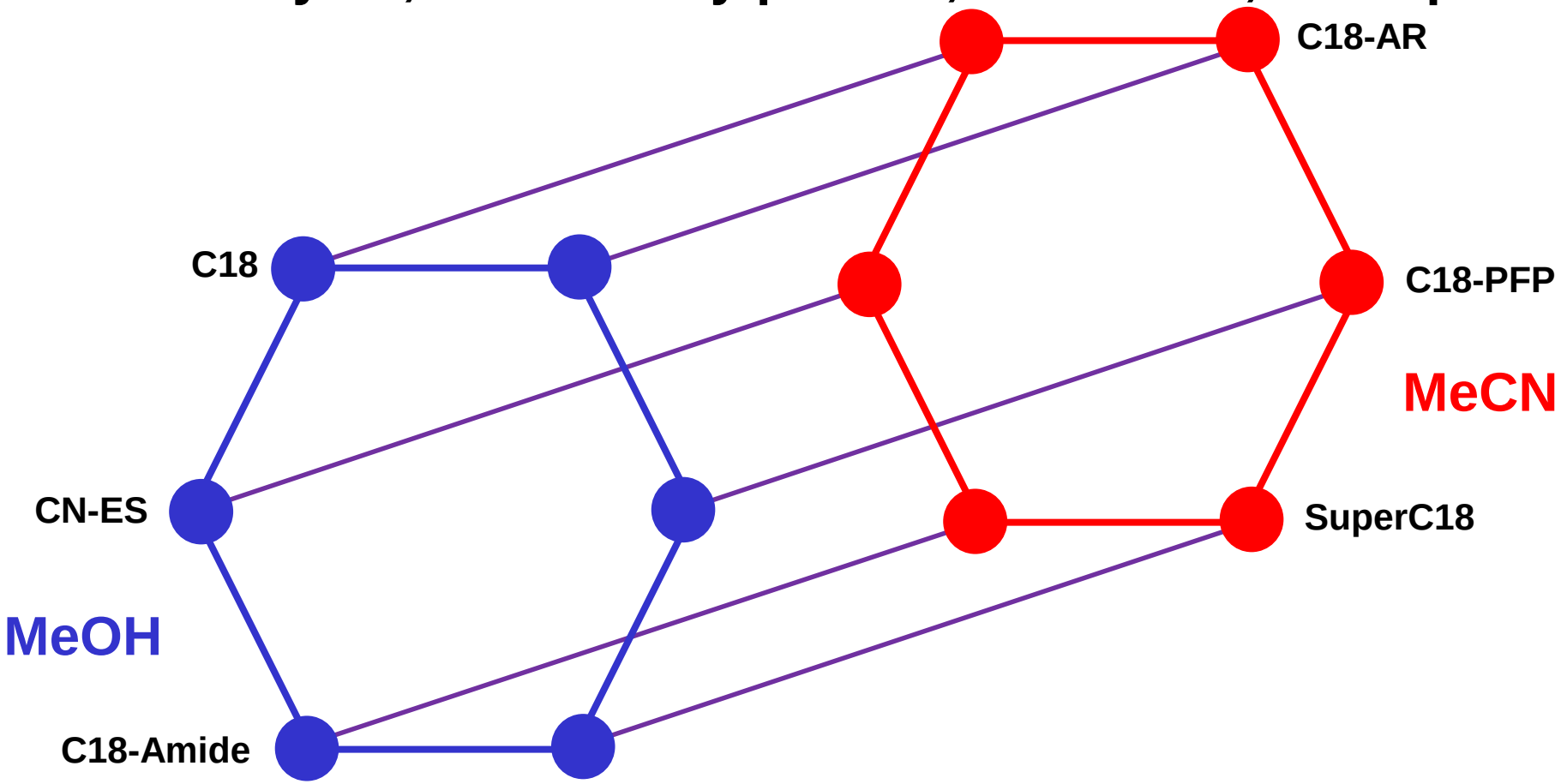
MeCN



6 Column Method Development Platform
Based Upon The Power of Phase Chemistry / Selectivity

Total Selectivity, Method Development: 6 Column Switcher

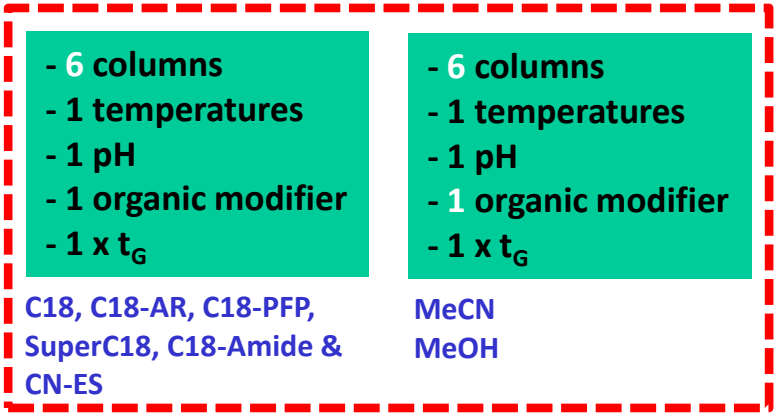
- 45 analytes, 6 stationary phases, 2 solvents, 1 low pH



Total 6 Column Method Development Platform
Based Upon The Power of Selectivity

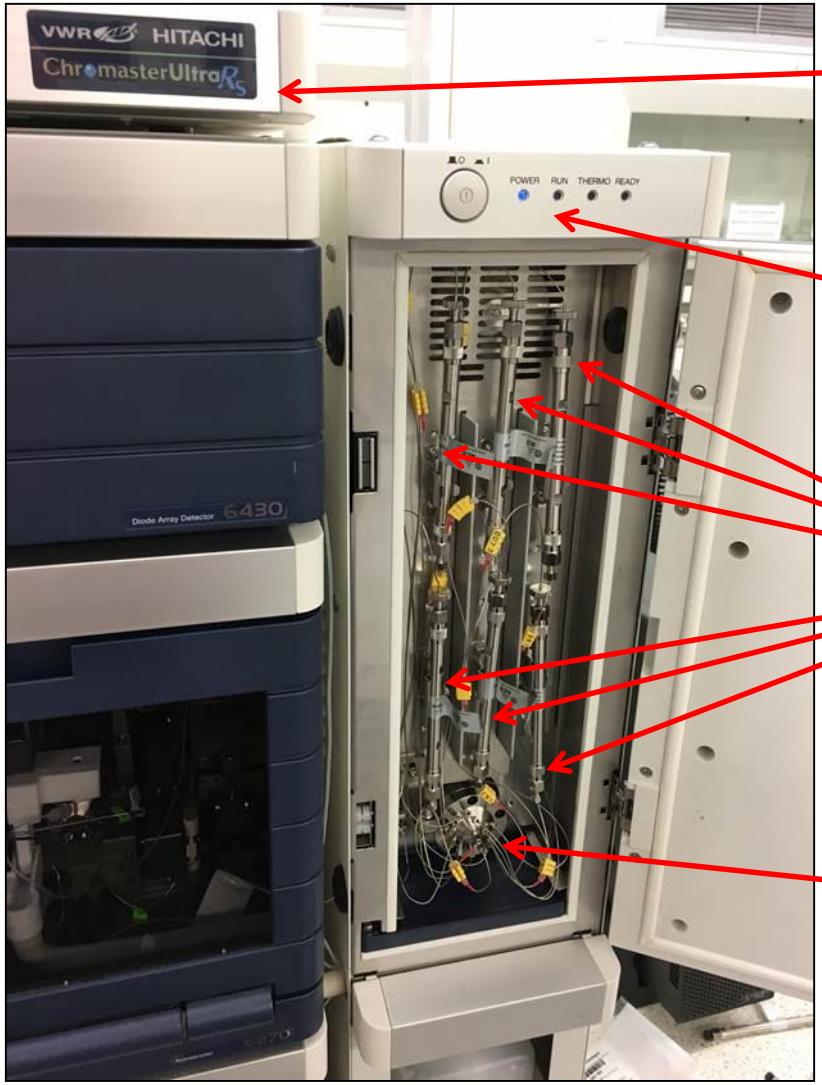
Screening Approach, Method Development Platform #1

Workflow Schematic



6 columns, 2 solvents method development / screening approach based on selectivity data

Total Selectivity, Method Development: Screening Platform



UHPLC Instrument

Thermostatted oven

6 x ACE Column
(100 x 3mm, 2µm)

Switching valve

General LC Method Development Approach

Overview of method development steps

- **Step 1: Scouting runs with general starting conditions**
- Step 2: Optimize for peak shape, run time etc
- Step 3: Validate according to local guidance
- Step 4: Transfer / Implement

General Method Development Initial Conditions

- **Perform a broad scouting gradient run on the samples at acidic eluent pH**

- **How do you calculate your starting conditions?**

For a 100 x 3mm column:

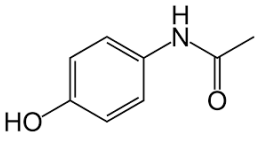
t_G	= 5 minutes
F	= 1.2 mL/min
$\Delta\phi$	= 0.95
V_m	= 0.459 mL
M	= 5

$$k^* = \frac{t_G F}{\Delta\Phi V_m M} = \sim 3$$

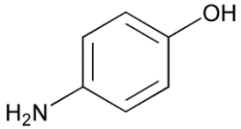
- **Ideally retention (or *k** in gradient elution) should be >2 and <20 for initial method development**

Paracetamol Plus Some Impurities For Method Development

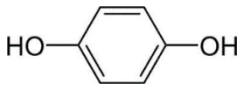
1.	Acetaminophen	API (a.k.a. Paracetamol)
2.	4-aminophenol	synthesis/degradation product
3.	Hydroquinone	deg product of 4-amino phenol
4.	2-aminophenol	Included as would be a synthesis impurity of (8) if not fully removed
5.	2-acetamidophenol	Specified in USP
6.	Phenol	Included as extra compound
7.	4-nitrophenol	Ph. Eur. related substance
8.	2-nitrophenol	Synthesis impurity of 4-amino phenol (39% yield, normally removed by steam distillation)
9.	4-chloroacetanilide	Eu. Ph. Related substance
10.	4-chlorophenol	Potential low level impurity



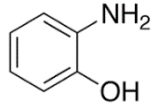
Acetaminophen (Paracetamol)
pKa = 9.86
LogP = 0.34
LogD 5.5 = 0.4
LogD 7.4 = 0.4



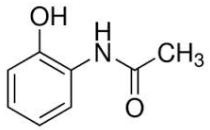
4-aminophenol
pKa = 5.28, 10.17
LogP = -0.29
LogD 5.5 = -0.04
LogD 7.4 = 0.16



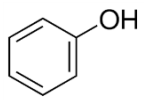
Hydroquinone
pKa = 10.33
LogP = 0.64
LogD 5.5 = 0.53
LogD 7.4 = 0.53



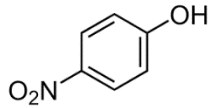
2-aminophenol
pKa = 4.84, 10.01
LogP = 0.44
LogD 5.5 = 0.58
LogD 7.4 = 0.64



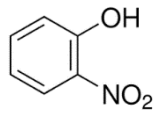
2-acetamidophenol
pKa = 8.79
LogP = 0.72
LogD 5.5 = 0.79
LogD 7.4 = 0.79



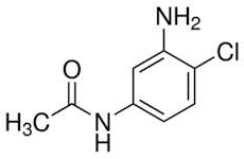
Phenol
pKa = 9.95
LogP = 1.48
LogD 5.5 = 1.63
LogD 7.4 = 1.63



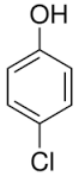
4-nitrophenol
pKa = 7.23
LogP = 1.57
LogD 5.5 = 1.7
LogD 7.4 = 1.31



2-nitrophenol
pKa = 7.23
LogP = 1.71
LogD 5.5 = 1.7
LogD 7.4 = 1.26



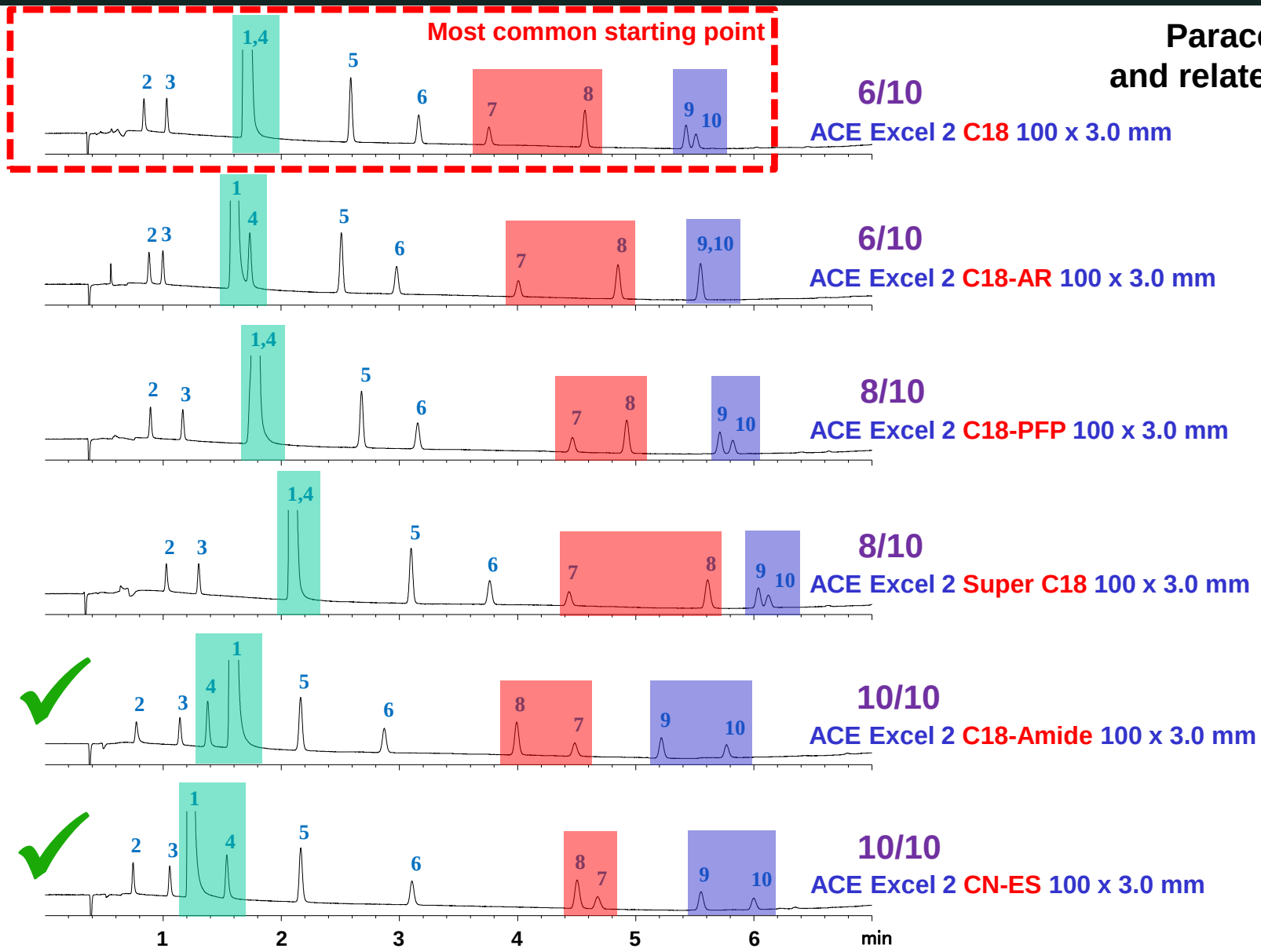
4-chloroacetanilide
pKa = -1.97/14.25
LogP = 2.05
LogD 5.5 = 2.14
LogD 7.4 = 2.14



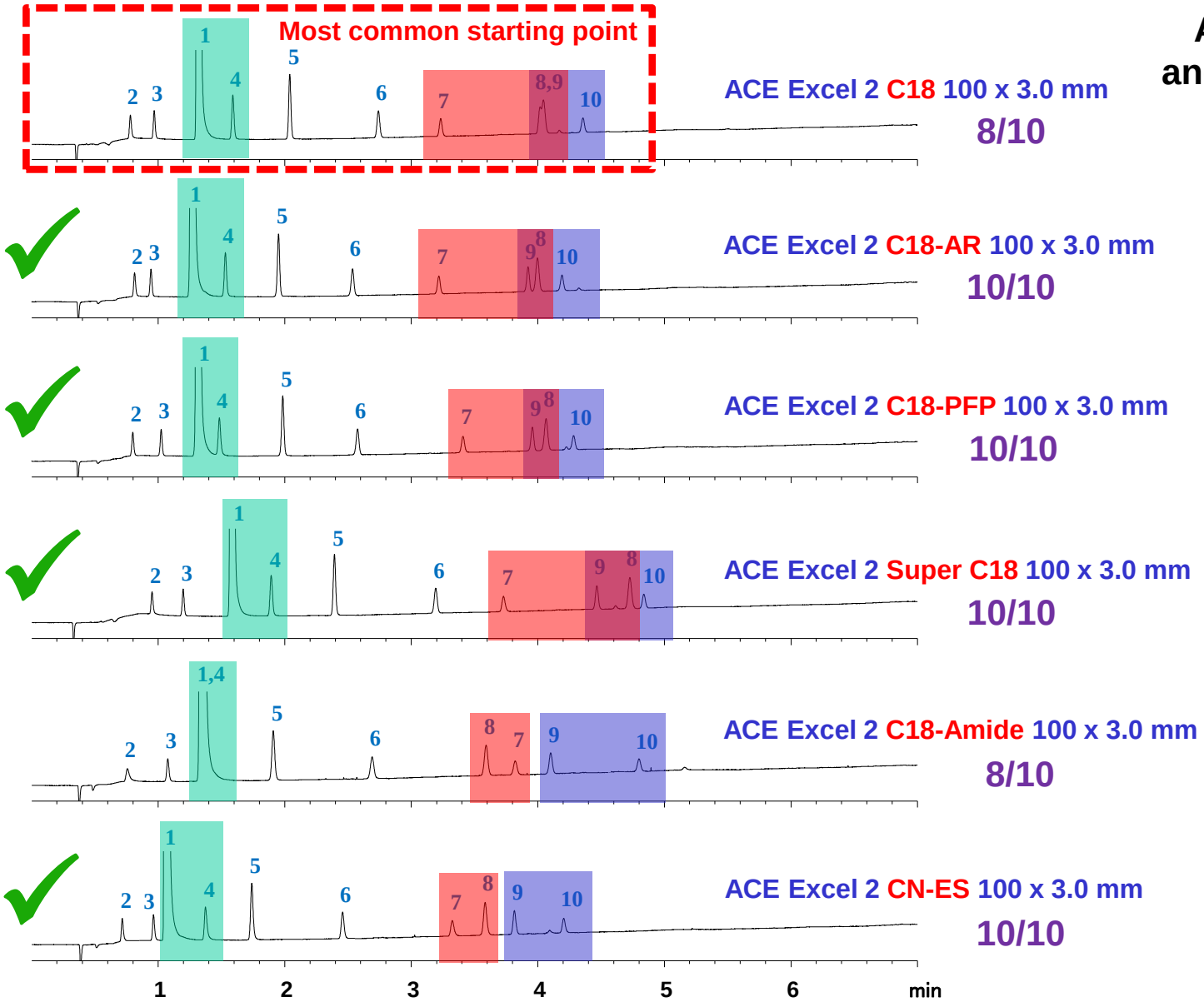
4-chlorophenol
pka = 9.3
LogP = 2.43
LogD 5.5 = 2.43
LogD 7.4 = 2.42

General scouting conditions:
100 x 3.0 mm columns
A: 20 mM Ammonium acetate pH 6.0
B: 20 mM Ammonium acetate pH 6.0 in MeOH or MeCN:H_2O (9:1 v/v)
Gradient: 5 to 95%B in 10 mins
Temp: 40°C, 2µL injection, Flow rate: 1.2 ml/min
Sample: Acetaminophen with rel subs at 0.5% w/w

Total Selectivity, Method Development: Screening Platform

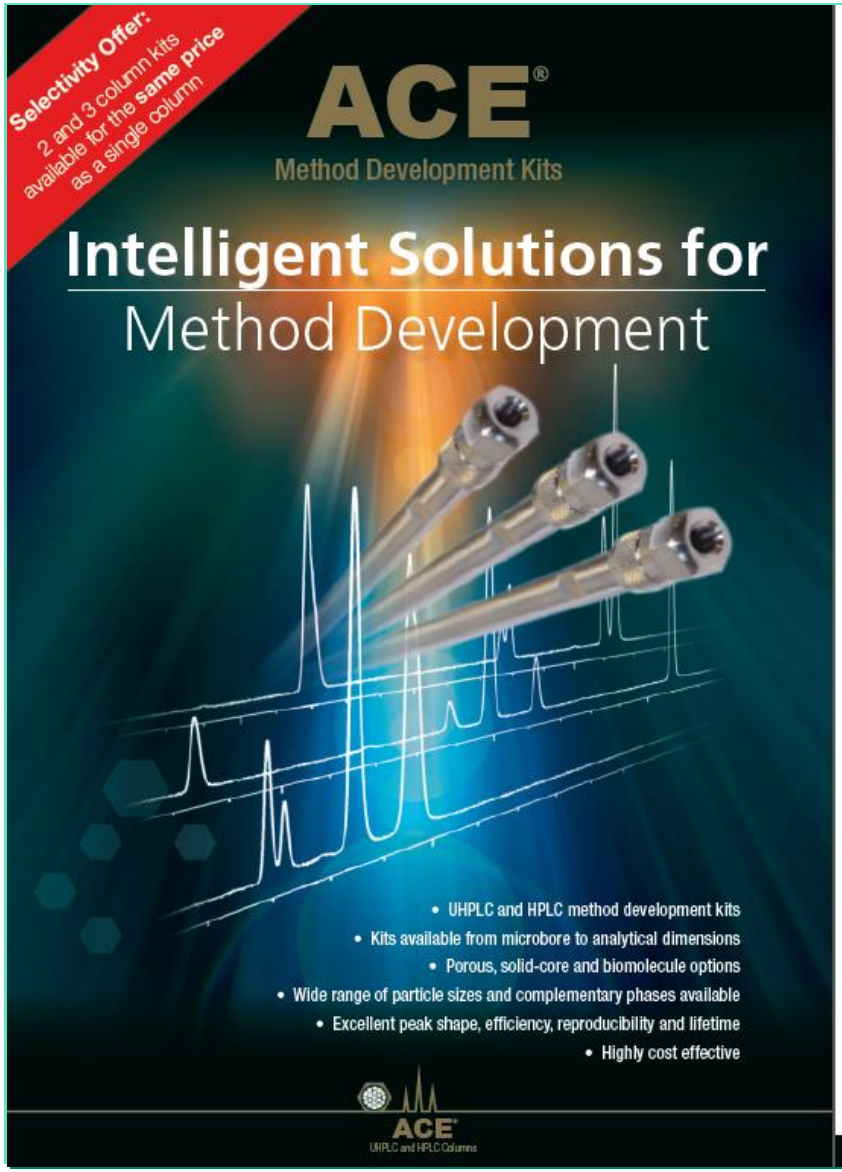


Total Selectivity, Method Development: Screening Platform



Acetaminophen and related analytes

ACE® Method Development Kit Brochure



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!
- 4 different ACE Method Development Kits available from microbore (0.5mm id) through to analytical (4.6mm id) dimensions for rapid, systematic method development.
- Each kit contains carefully selected ACE phases which enables 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 pages 4-7)	ACE C18	****	-	-	*	**
		ACE C18-AR	****	*** (donor)	*	**	***
		ACE C18-PFP	****	*** (acceptor)	****	***	****
2	ACE Extended Method Development Kit (see pages 8-11)	ACE SuperC18	****	-	-	-	**
		ACE C18-Amide	****	-	**	****	**/***
		ACE CN-ES	***	*	***	**	*
3	ACE UltraCore Method Development Kit (see pages 12-14)	ACE UltraCore SuperC18	***	-	-	-	**
		ACE UltraCore SuperPhenylHexyl	**	*** (donor)	*	**	***
4	ACE Bioanalytical 300Å Method Development Kit (see pages 15-17)	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

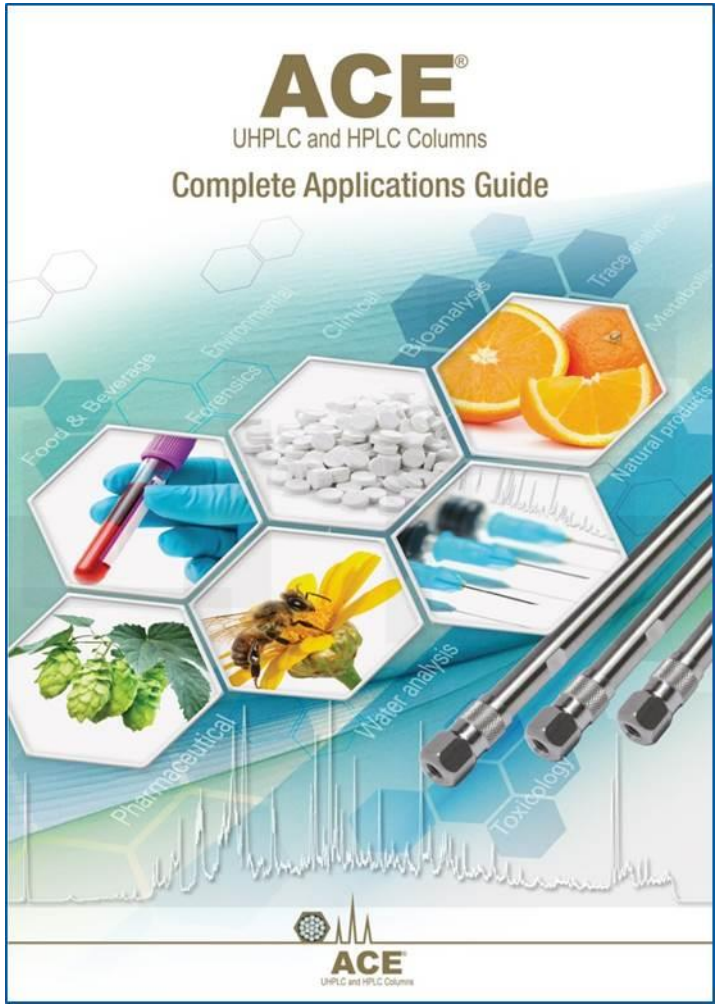
Learn More: www.ace-hplc.com

Overall Conclusions

- **Selectivity** is helpful in chromatography
- **Understanding selectivity** aids method development by focussing efforts on **high impact** variables
- It is possible to **design** stationary phases to **maximize selectivity**
- **Screening columns** with **differing retention mechanisms** is useful for method development
- An **optimized** method development platform **based on selectivity** has been described

ACE Complete Applications Guide

- **Brand new 200 page applications guide with >300 ACE applications**
- **Clinical, forensic, food & beverage, environmental, LC-MS, pharmaceutical all covered**
- **Application and analyte indexes**
- **Request your hardcopy now**



http://mac-mod.com/pdf/application-packets/ACE%20Complete%20Applications%20Guide.pdf

Thank you for your attention

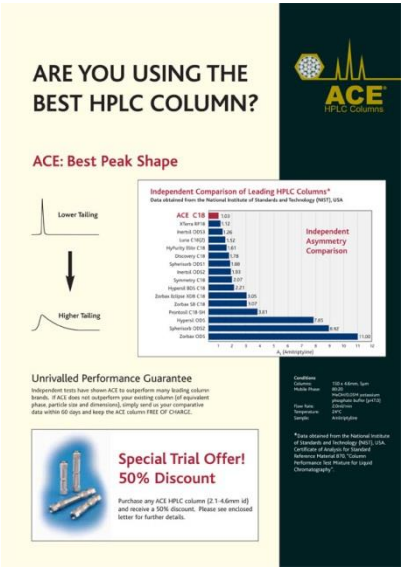
All ACE products are available globally

info@ace-hplc.com

USA: www.mac-mod.com

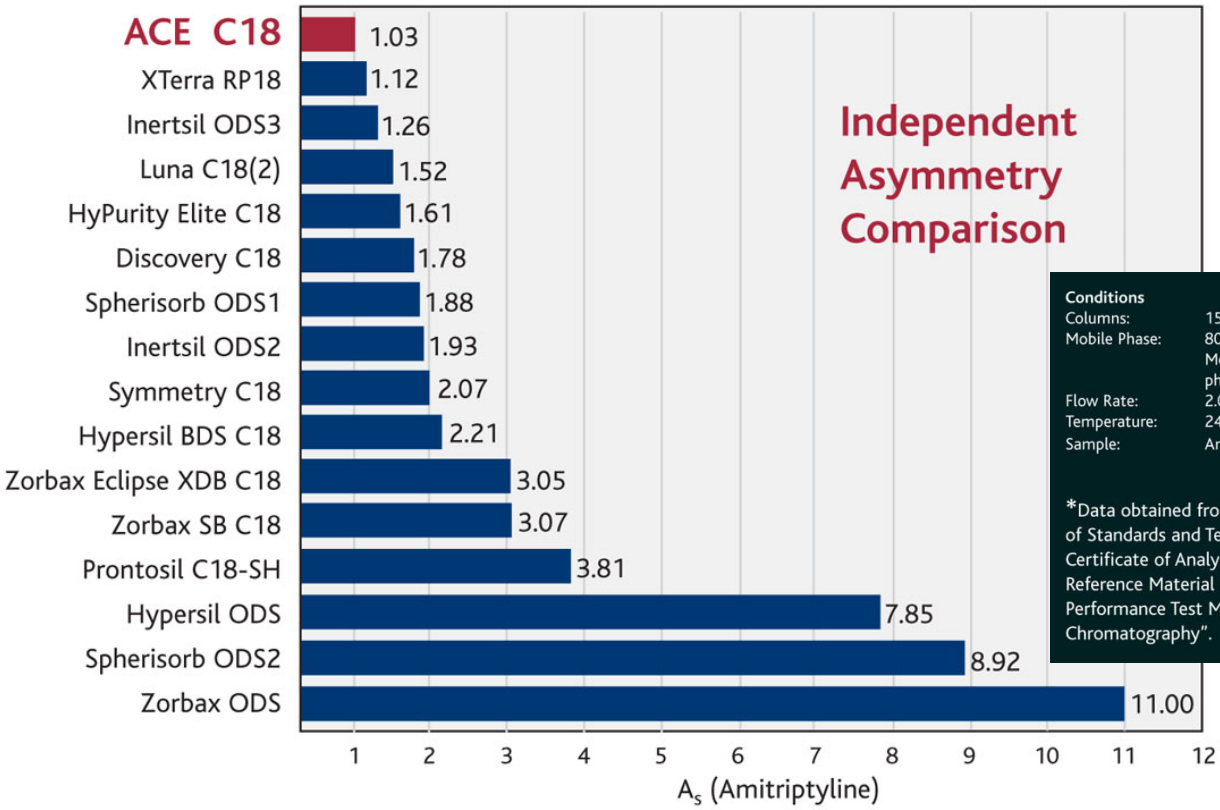
What Do ACE UHPLC / HPLC Columns Offer?

- **Highest Performance Shown from Independent Testing**
- **NIST**



Independent Comparison of Leading HPLC Columns*

Data obtained from the National Institute of Standards and Technology (NIST), USA



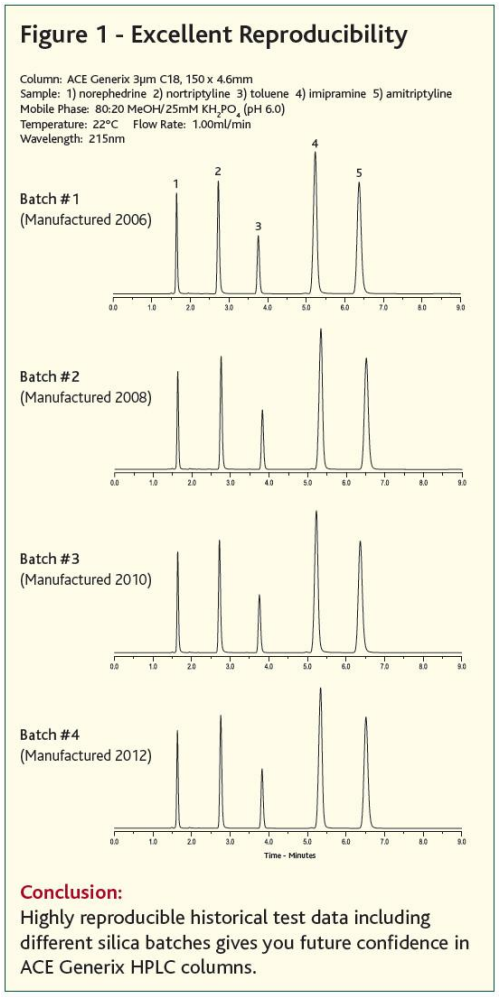
Conditions

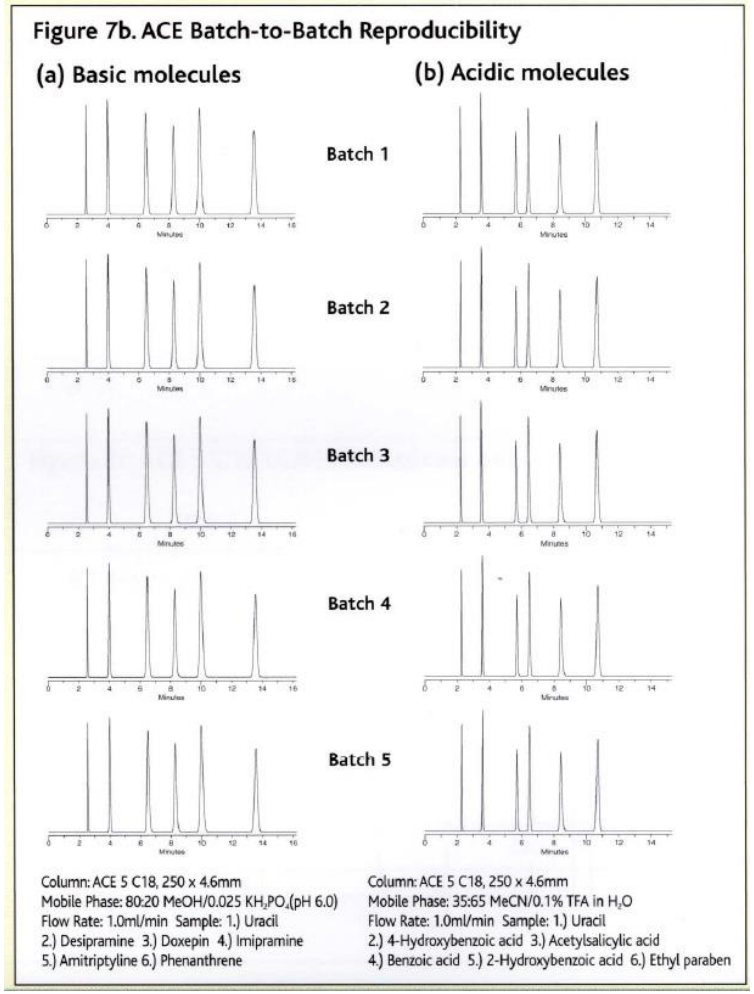
Columns:	150 x 4.6mm, 5µm
Mobile Phase:	80:20 MeOH/0.05M potassium phosphate buffer (pH7.0)
Flow Rate:	2.0ml/min
Temperature:	24°C
Sample:	Amitriptyline

*Data obtained from the National Institute of Standards and Technology (NIST), USA. Certificate of Analysis for Standard Reference Material 870, "Column Performance Test Mixture for Liquid Chromatography".

What Do ACE UHPLC / HPLC Columns Offer?

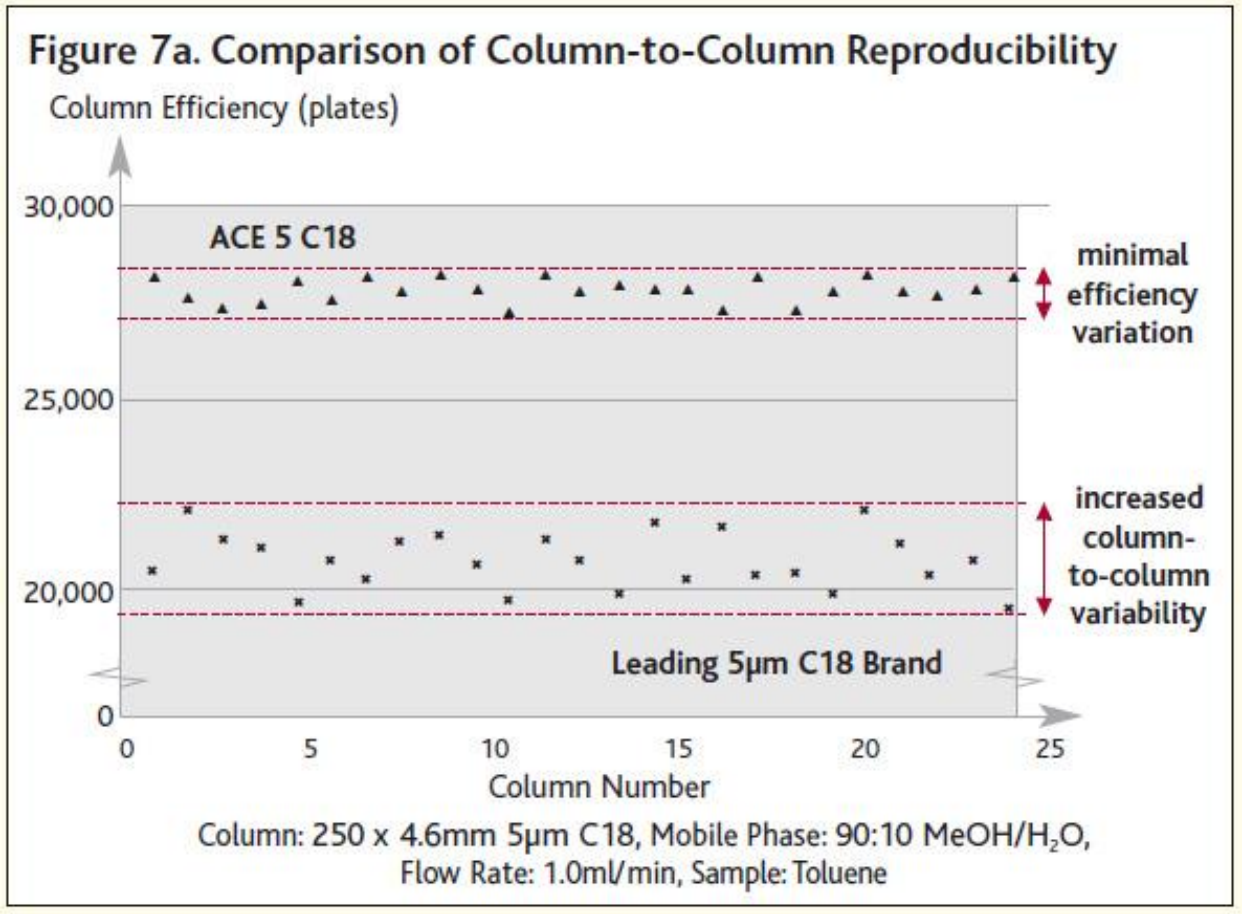
- **Reproducibility, Quality & Performance – guaranteed.**



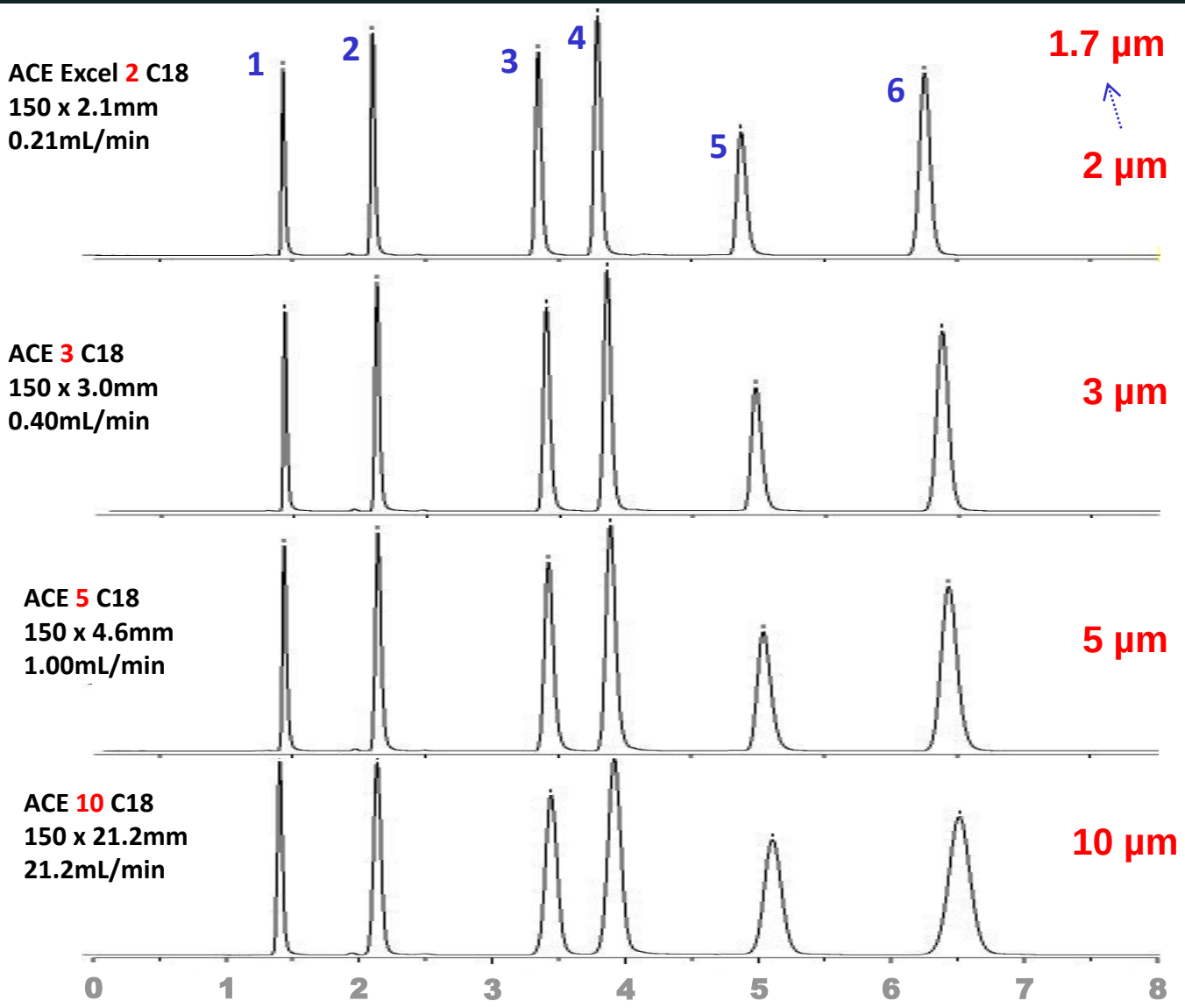


What Do ACE UHPLC / HPLC Columns Offer?

- **Reproducibility, Quality & Performance – guaranteed.**



ACE® Excel ™ UHPLC Columns – Scalability & Reproducibility



UHPLC

HPLC

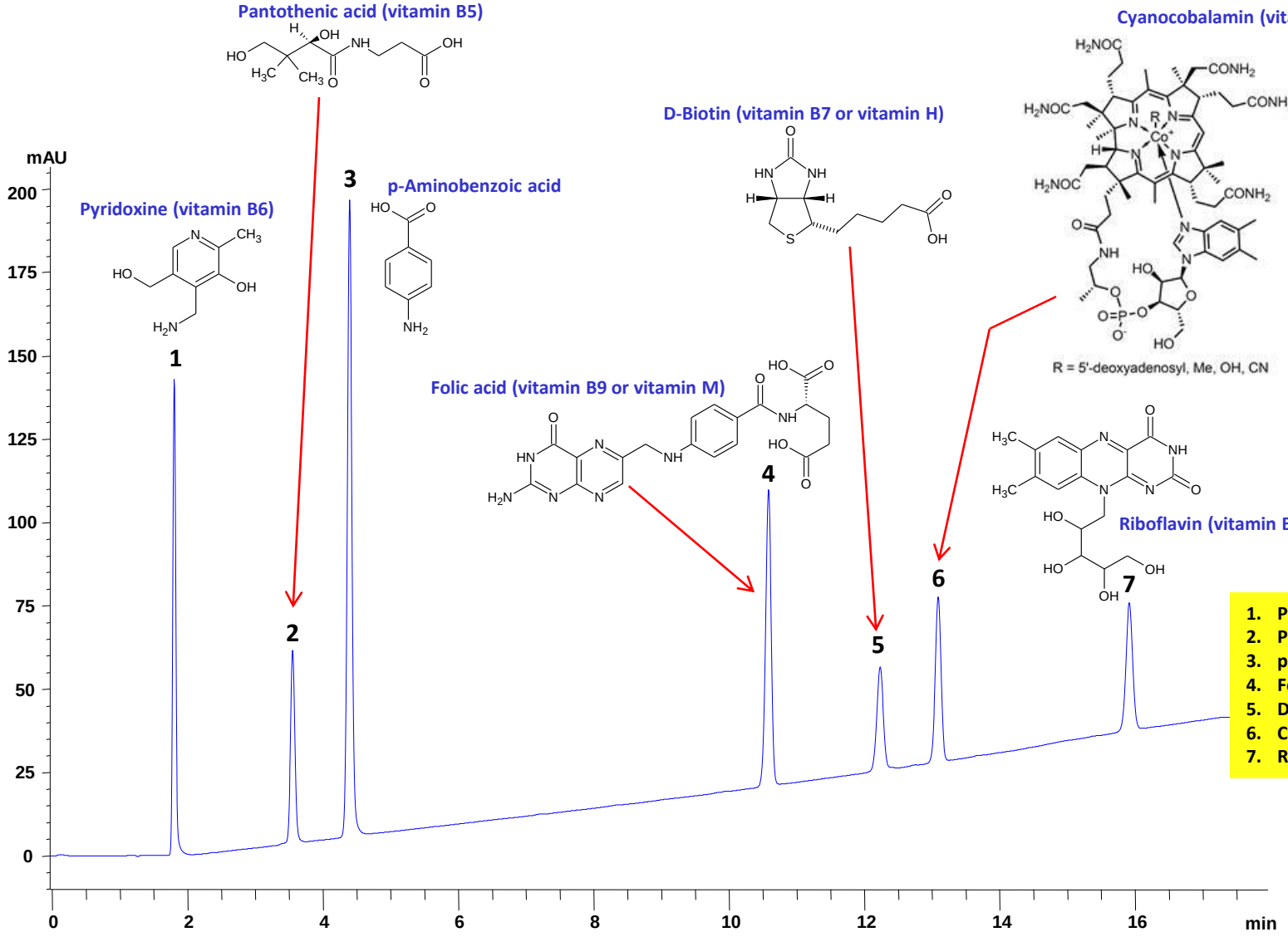
Prep LC

MP: 35:65 v/v MeCN:0.1% TFA (aq); 22C; 254nm; 1. uracil; 2. 4-hydroxybenzoic acid; 3. acetylsalicyclic acid; 4. benzoic acid; 5. 2-hydroxybenzoic acid 6. ethyl paraben

Applications

ACE® C18-AR™: Water Soluble Vitamins

ACE 3 C18-AR



150x4.6mm, 3µm

Gradient analysis

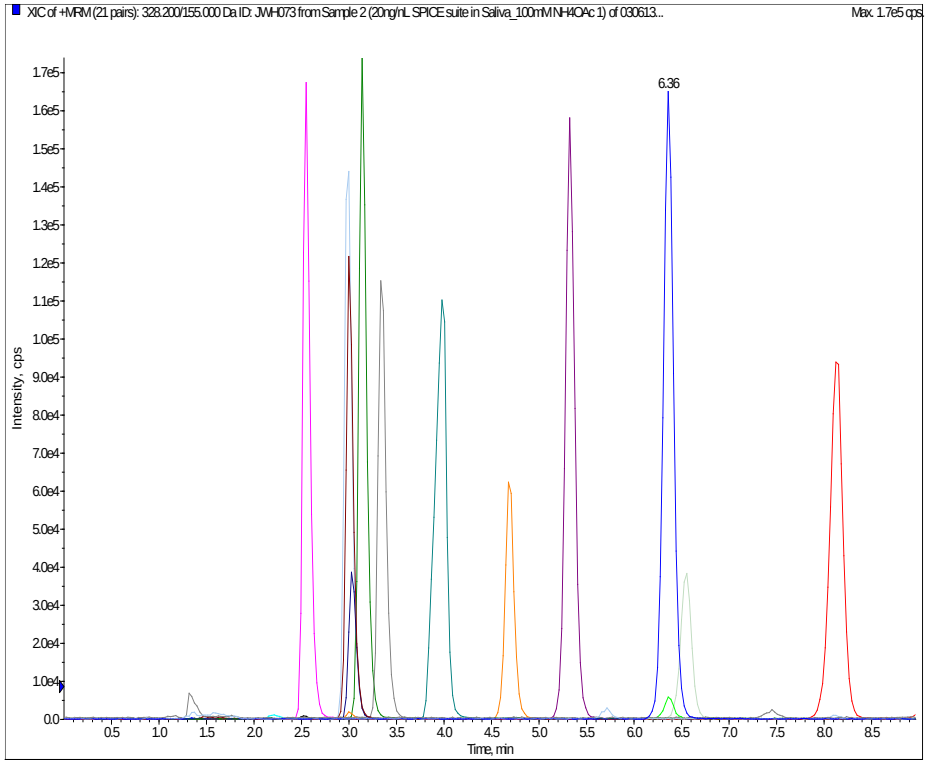
A = 20mM KH_2PO_4, pH 2.83 (aq)
B = 20mM KH_2PO_4, pH 2.83 in 1:1 v/v MeOH:water
40C
205nm
1.5mL/min

T (min)	%B
0	20
15	70

1. Pyridoxine (vitamin B6)
2. Pantothenic acid (vitamin B5)
3. p-Aminobenzoic acid
4. Folic acid (vitamin B9 or vitamin M)
5. D-Biotin (vitamin B7 or vitamin H)
6. Cyanocobalamin (vitamin B12)
7. Riboflavin (vitamin B2)

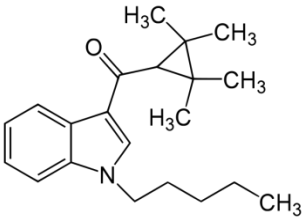
ACE® C18-AR™: Synthetic Cannabinoids (SPICE) From Oral Fluid

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

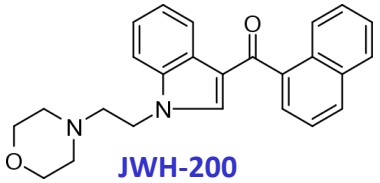


Retention Time (minutes)	Analyte	MRM Transition	Declustering Potential (DP)	Collision Energy (CE)	Cell Exit Potential (CXP)
2.55	JWH-250 N-(5-hydroxypentyl)	352>120.9	40	30	16
2.99	JWH-073 N-(3-hydroxybutyl)	344>155	40	30	16
3.00	UR-144 5-Hydroxy-pentyl	328.5>125	30	35	16
3.03	UR-144 Pentanoic Acid	342.5>125	30	35	16
3.14	d5-JWH-018 N-(4-hydroxypentyl	363.5> 155	40	35	16
3.14	JWH-018 N- (4-hydroxypentyl	358> 155	40	30	16
3.34	JWH-018 5-pentanoic acid	372>155	40	30	16
3.98	JWH-200	385>155	40	30	16
4.69	XLR-11	330>125	30	35	16
5.32	JWH-250	336>121	40	30	16
6.36	JWH-073	328>155	40	30	16
6.37	UR-144 5-Chloro-pentyl	346.9>125	30	35	16
6.55	UR-144	312.5>125	30	35	16
8.14	JWH-018	342>155	40	30	16

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

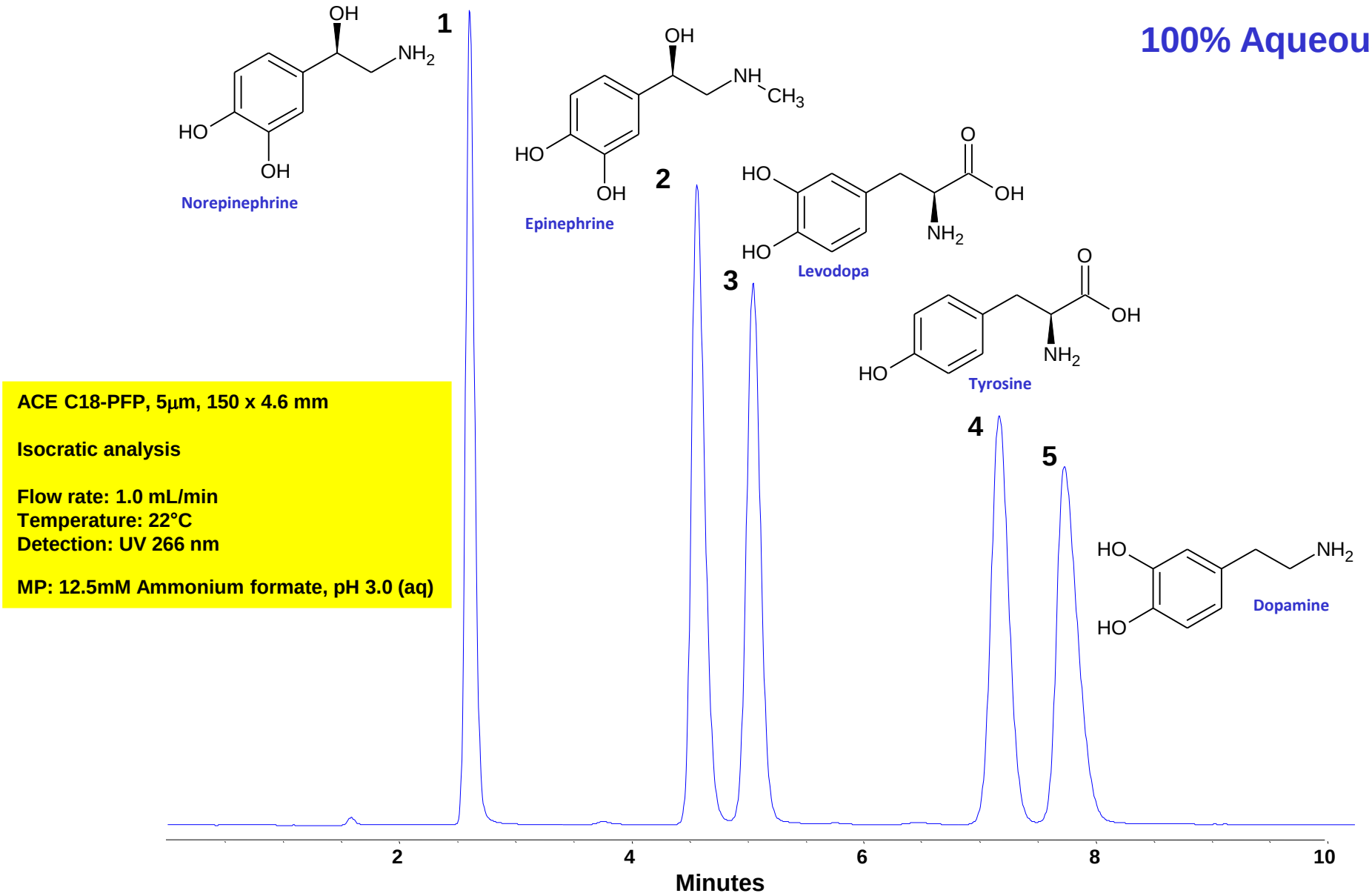


UR-144



JWH-200

ACE® C18-PFP™: Catecholamine Analysis



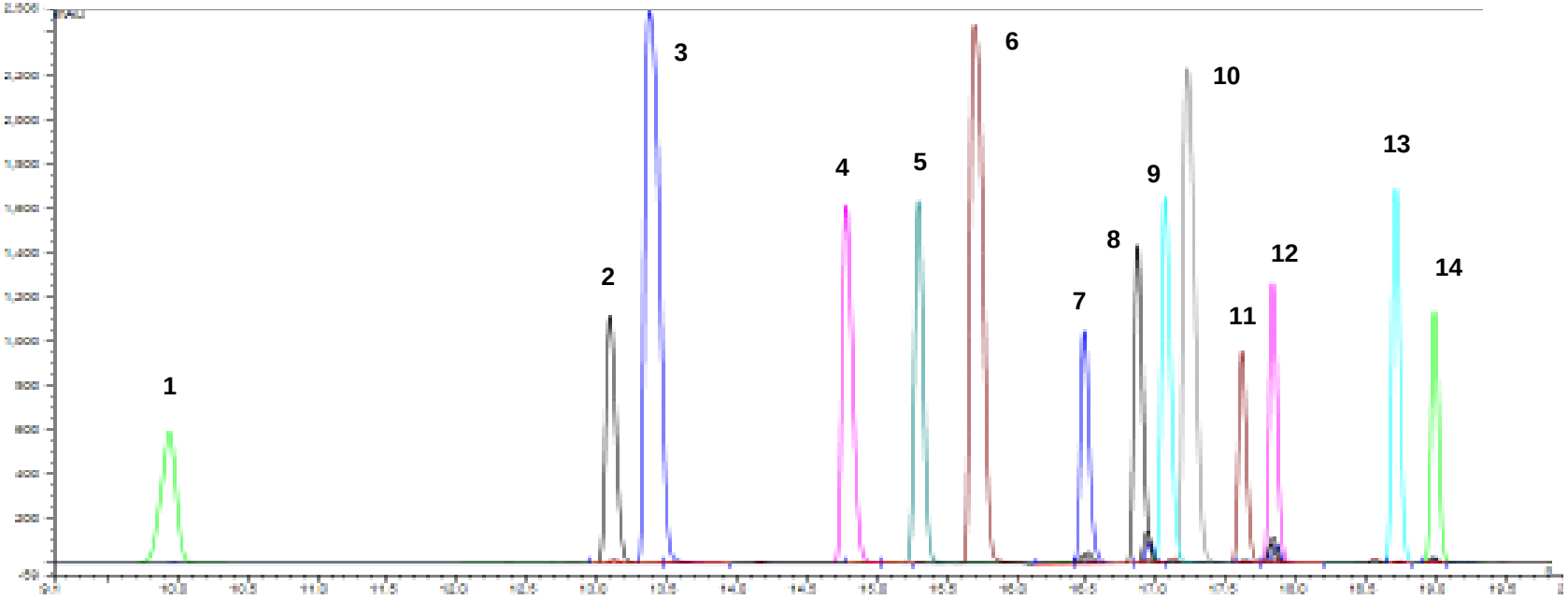
ACE C18-PFP: Phenols and Phenoxy Acids

ACE 3 C18-PFP
3µm, 150 x 4.6mm
Gradient analysis
A = Methanol
B = 0.1% formic acid in water

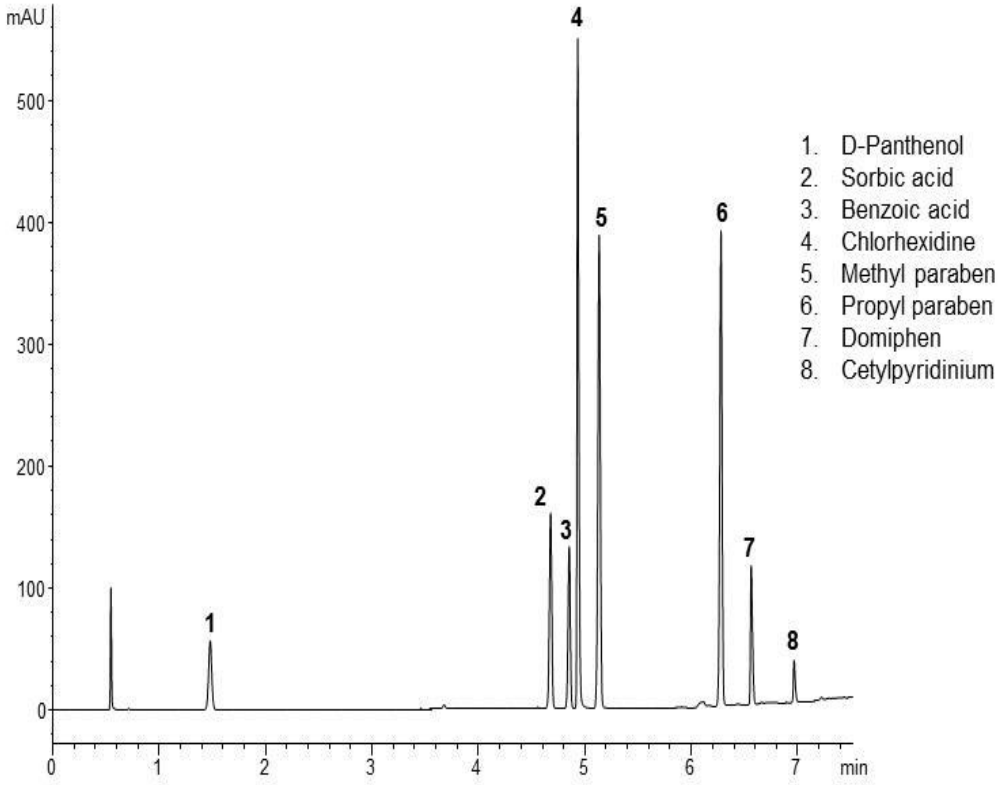
Time (mins)	%B
0	90
20	0

Flow rate: 1ml/min
Column temperature:
Detection: UV, 280nm

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



ACE® C18-Amide™: FMCH, Antiseptics and Preservatives



1. D-Panthenol
2. Sorbic acid
3. Benzoic acid
4. Chlorhexidine
5. Methyl paraben
6. Propyl paraben
7. Domiphen
8. Cetylpyridinium

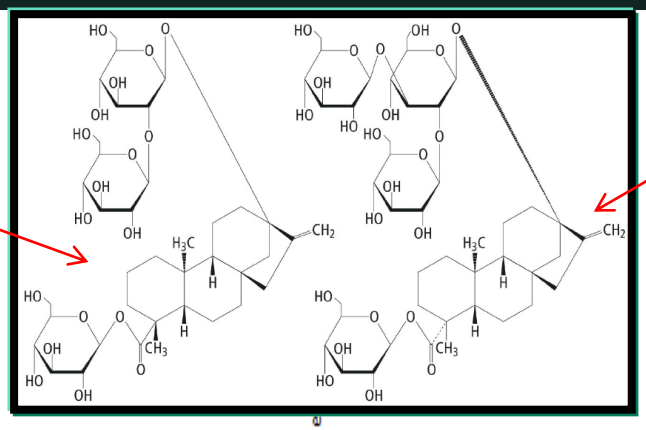
Conditions

Column:	ACE Excel 3 C18-Amide
Dimensions:	100 x 4.6 mm
Part Number:	EXL-1112-1046U
Mobile Phase:	A: 0.1% phosphoric acid in H_2O
	B: 0.1% phosphoric acid in MeCN

Time (mins)	%B
0	5
2	5
8	90
9	90
9.5	5

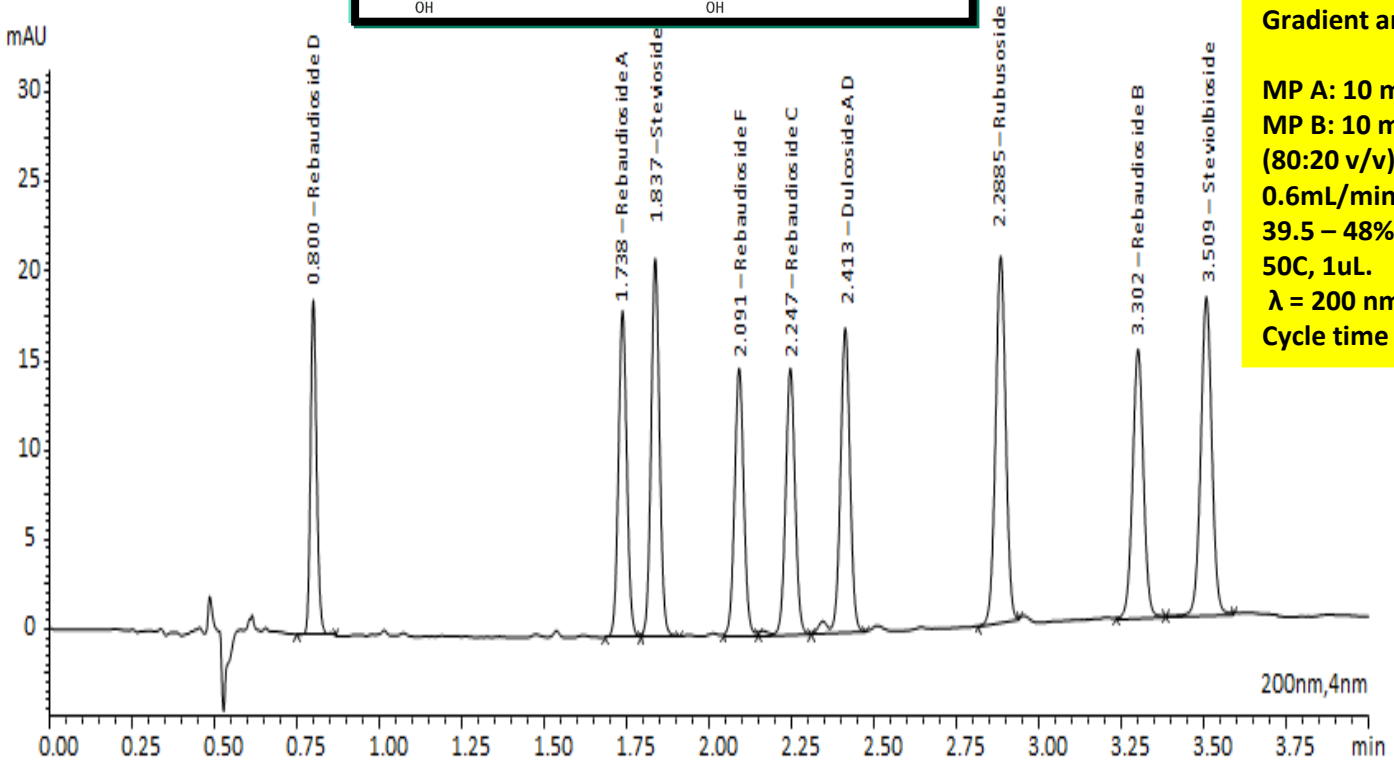
Flow Rate:	2.0 mL/min
Injection:	1 µL
Temperature:	40 °C
Detection:	UV, 210 nm
Instrument:	Chromaster UltraRs

ACE® SuperC18™: Artificial Sweeteners (Stevia Glycosides)



Stevioside
MW = 804.87

Rebaudioside
MW = 967.01



ACE Excel SuperC18, 2um, 150 x 2.1 mm
Gradient analysis

MP A: 10 mM NaH_2PO_4, pH 2.8 in H_2O.
MP B: 10 mM NaH_2PO_4, pH 2.8 in MeCN/H_2O (80:20 v/v).
0.6mL/min
39.5 – 48%B in 4 mins.
50C, 1uL.
λ = 200 nm.
Cycle time = 7 mins.

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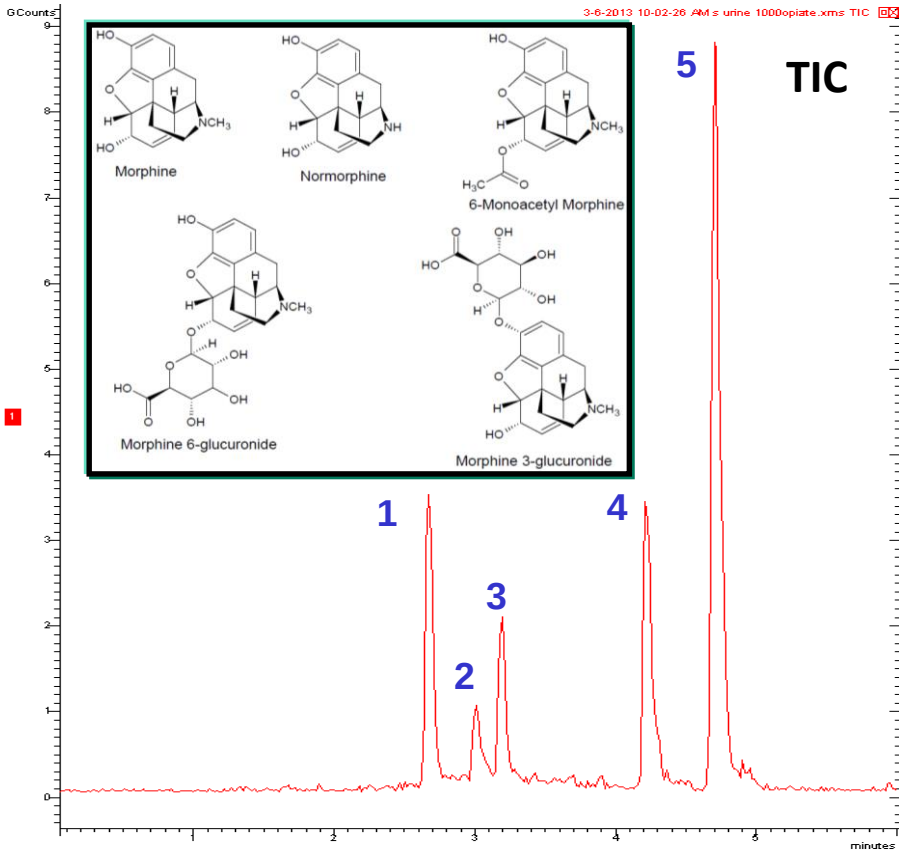
ACE® SuperC18™: Opiates In Urine by LC-MS/MS

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

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



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

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

T	%B
0	5
5	95

60C, 2uL.

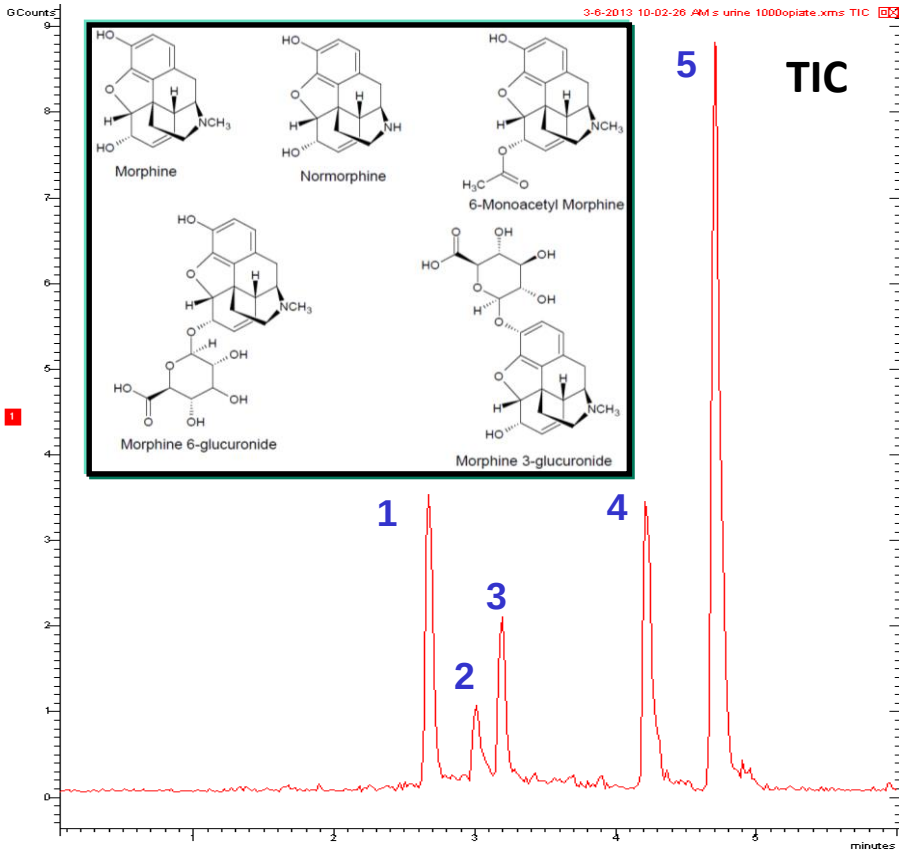
Varian 320 Triple Quadrupole MS
Electrospray voltage: +5 kV
Inlet capillary voltage: 30 V
CID with argon at 1.5 mTorr; Collision cell potential ranges from 5 to 17 V
Drying gas (nitrogen) temperature: 325 C
Nebulizing gas (nitrogen) pressure: 35 psi
Extended Dynamic Range

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

ACE® SuperC18™: Opiates In Urine by LC-MS/MS

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

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



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

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

T	%B
0	5
5	95

60C, 2uL.

Varian 320 Triple Quadrupole MS
Electrospray voltage: +5 kV
Inlet capillary voltage: 30 V
CID with argon at 1.5 mTorr; Collision cell potential ranges from 5 to 17 V
Drying gas (nitrogen) temperature: 325 C
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Extended Dynamic Range

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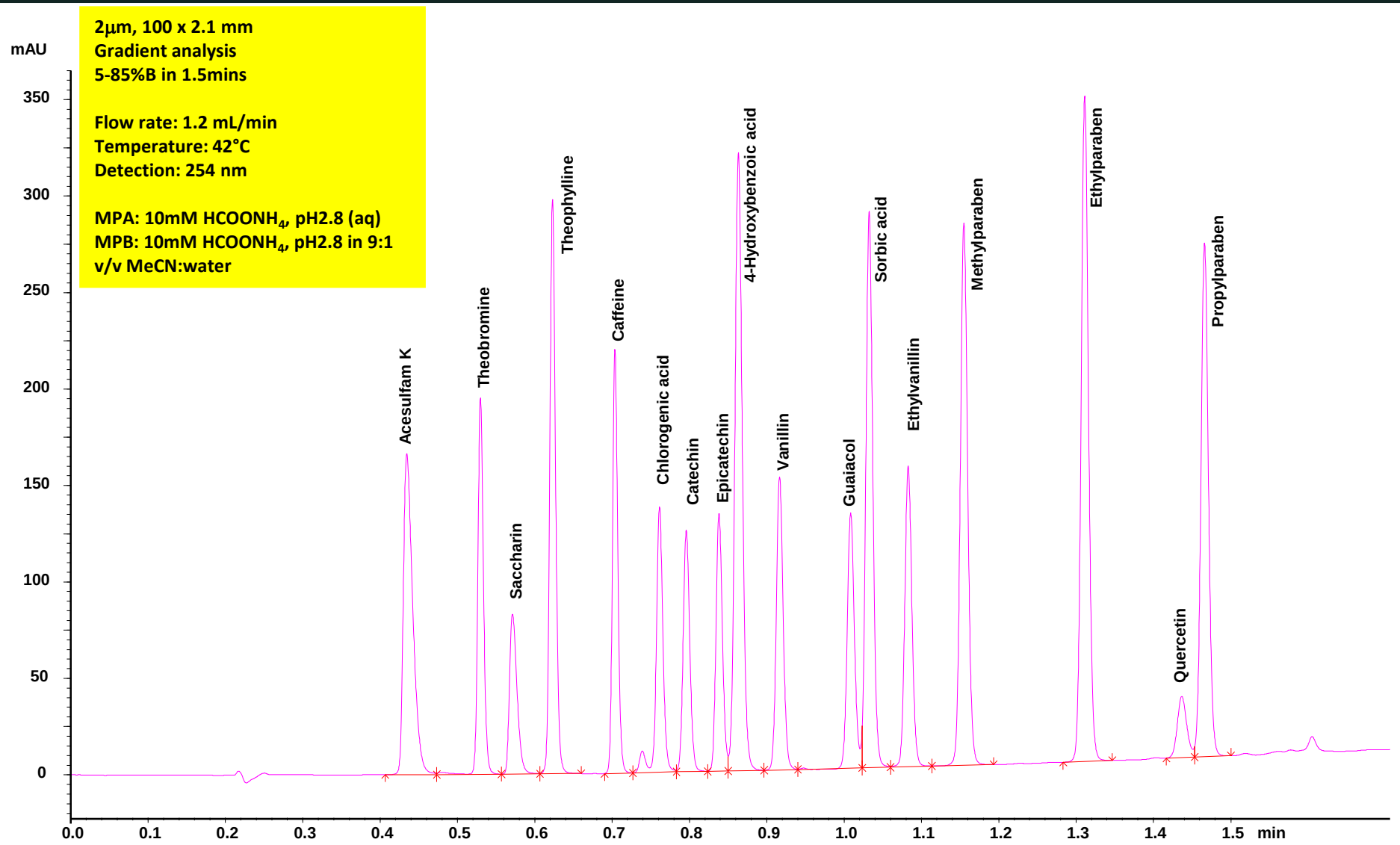
Normorphine	272.0	165.0
morphine 6-β-D glucuronide	462.0	285.9
6-acetylmorphine	328.0	164.9
morphine	286.0	200.9

ACE® Excel C18-Amide™: Chocolate Analysis



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ACE® C18-Amide™: Hair Dye Restricted Components #1

ACE Excel C18-Amide

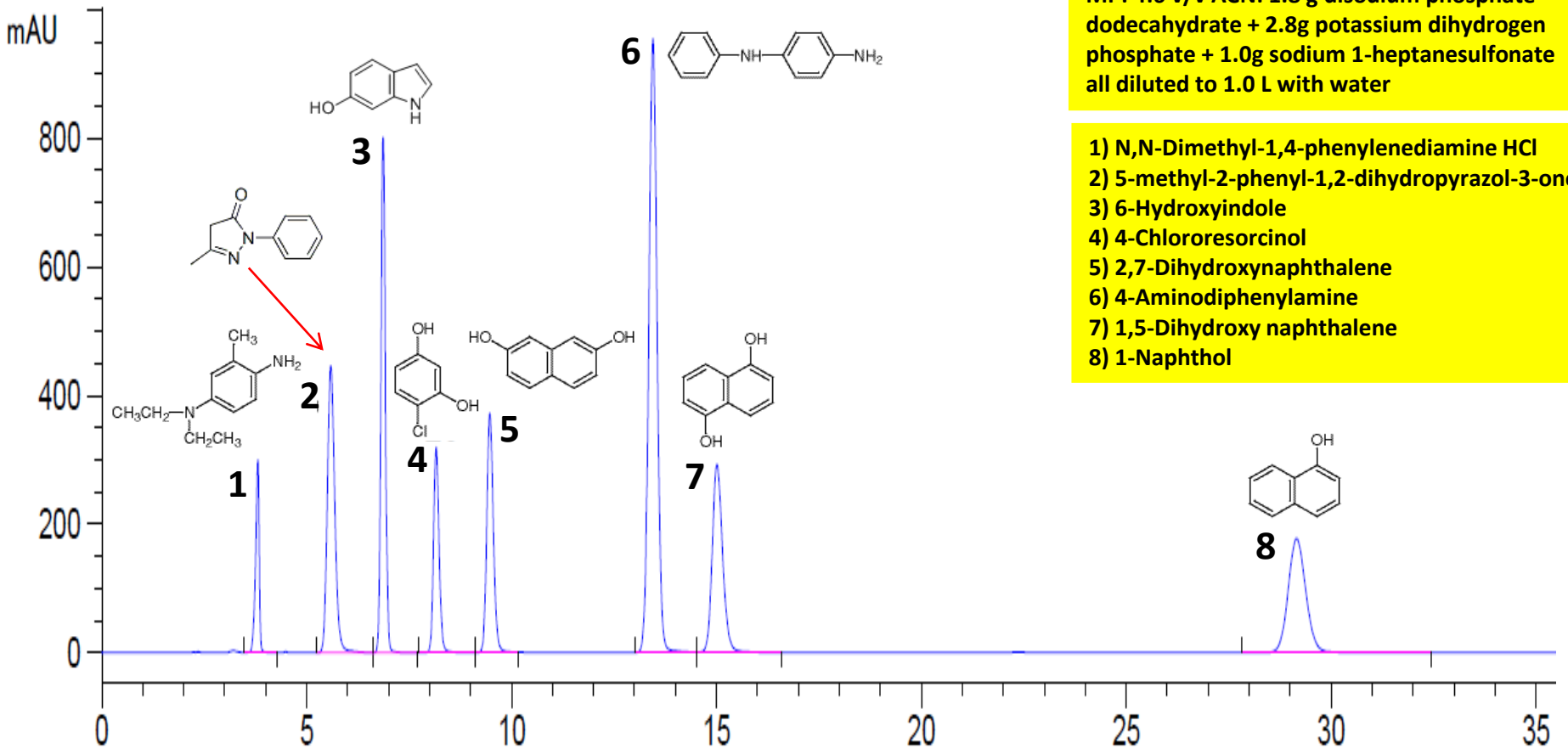
Based on Chinese
National Testing Method

5um, 250 x 4.6 mm
Isocratic analysis

Flow rate: 1.0 mL/min
Temperature: 60°C
Detection: UV 280 nm

MP: 4:6 v/v ACN: 1.8 g disodium phosphate dodecahydrate + 2.8g potassium dihydrogen phosphate + 1.0g sodium 1-heptanesulfonate all diluted to 1.0 L with water

1) N,N-Dimethyl-1,4-phenylenediamine HCl
2) 5-methyl-2-phenyl-1,2-dihydropyrazol-3-one
3) 6-Hydroxyindole
4) 4-Chlororesorcinol
5) 2,7-Dihydroxynaphthalene
6) 4-Aminodiphenylamine
7) 1,5-Dihydroxy naphthalene
8) 1-Naphthol



ACE® C18-Amide™: Hair Dye Restricted Components #2

ACE Excel C18-Amide

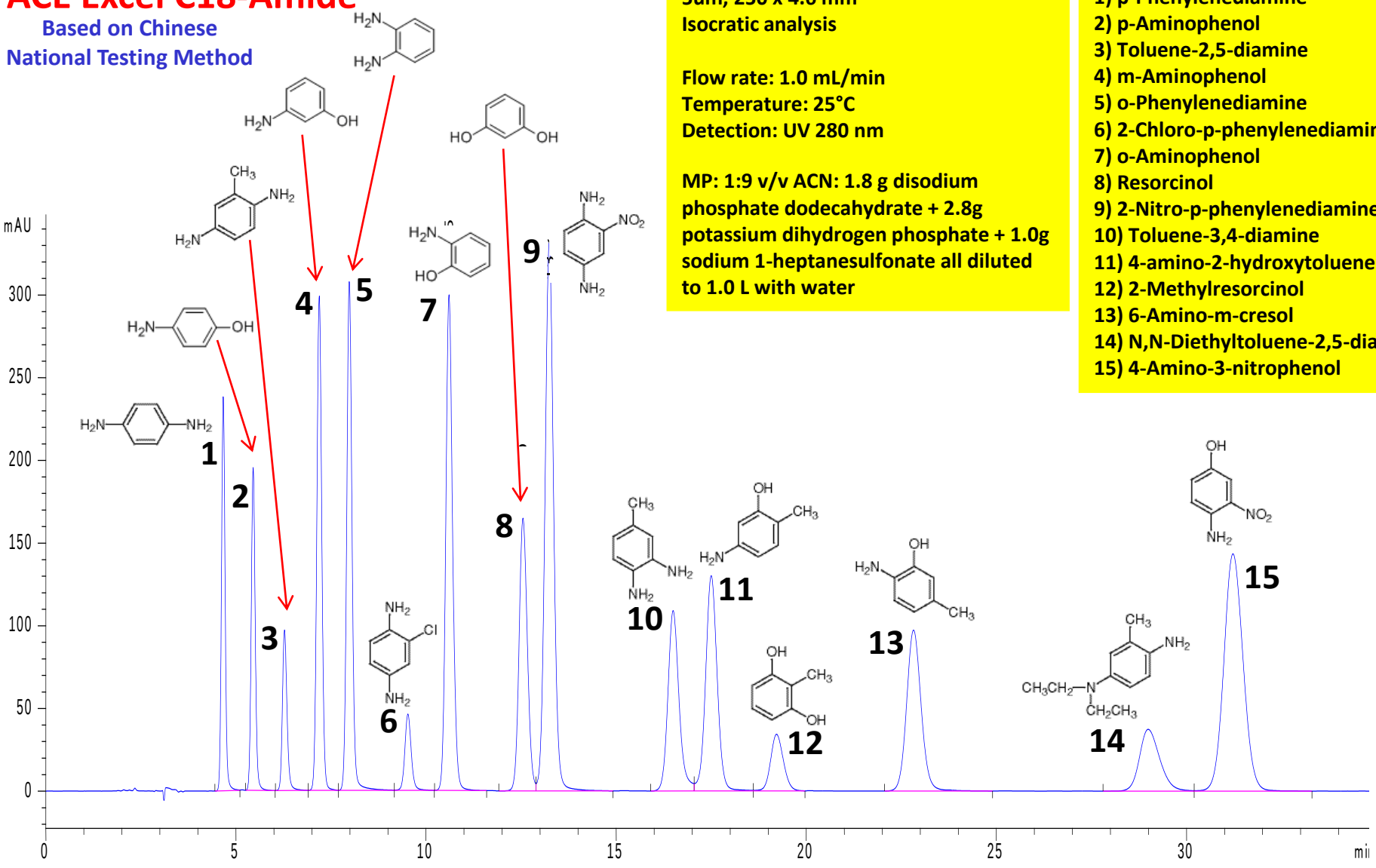
Based on Chinese National Testing Method

5um, 250 x 4.6 mm
Isocratic analysis

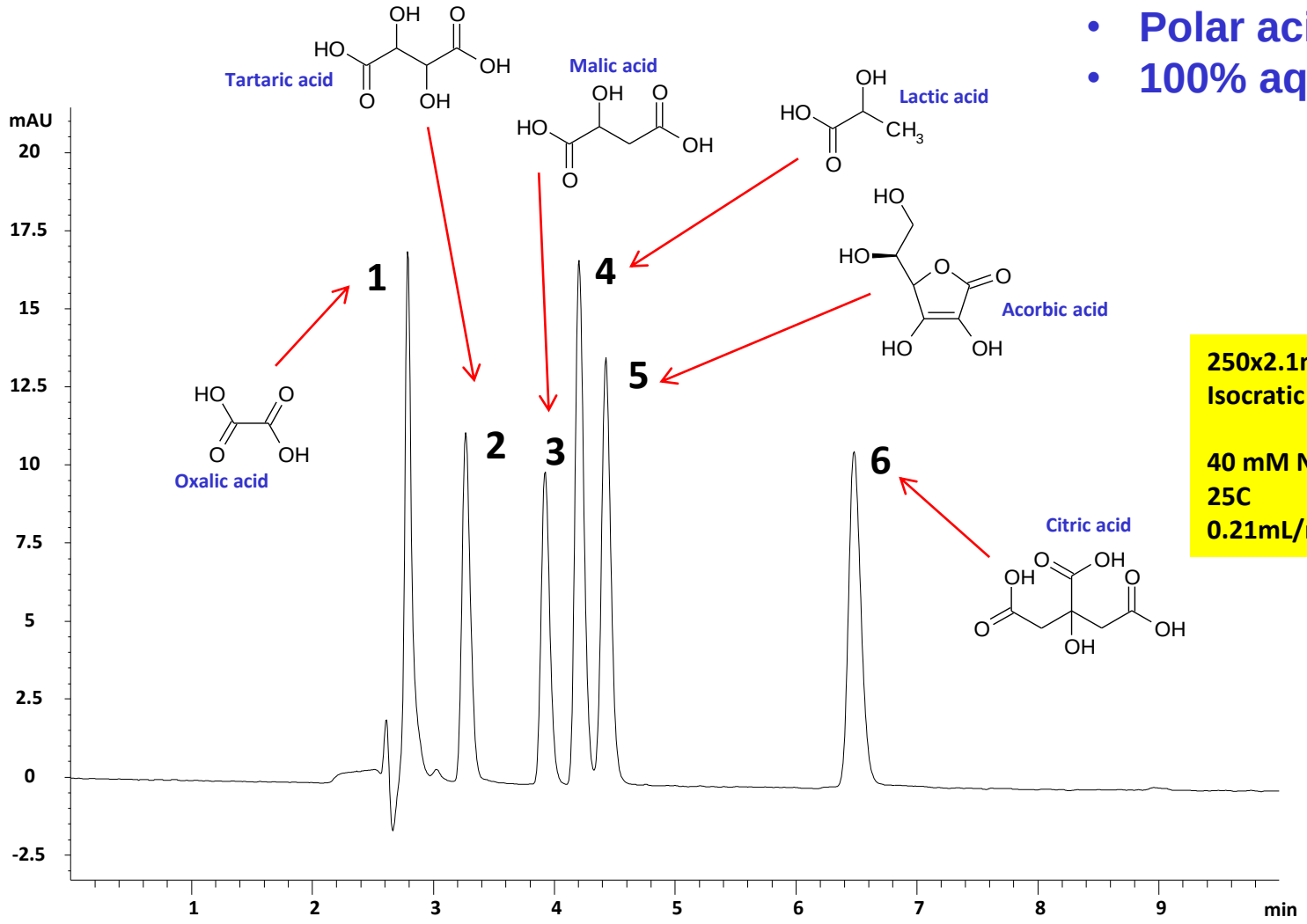
Flow rate: 1.0 mL/min
Temperature: 25°C
Detection: UV 280 nm

MP: 1:9 v/v ACN: 1.8 g disodium phosphate dodecahydrate + 2.8g potassium dihydrogen phosphate + 1.0g sodium 1-heptanesulfonate all diluted to 1.0 L with water

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



ACE® C18-Amide™: Beverage Analysis: Wine Acids

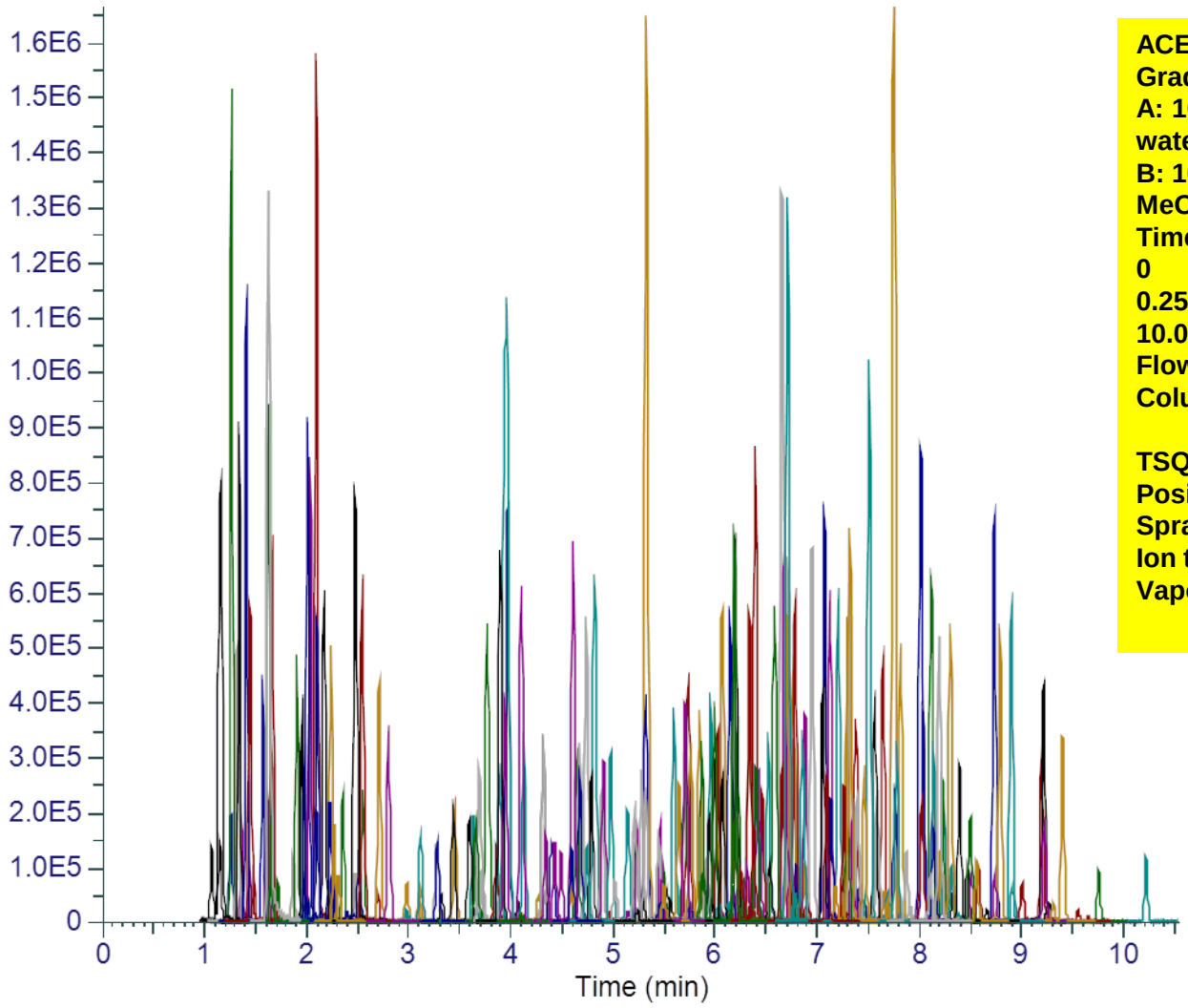


- Polar acid resolution
- 100% aqueous eluent

250x2.1mm, 3µm
Isocratic analysis

40 mM $NH_4H_2PO_4$, pH 2.5 (aq)
25C
0.21mL/min

250 Pesticide Screen using LC-MS/MS (I)



ACE Excel C18 2µm, 100 x 2.1mm
Gradient analysis
A: 10mM amm formate + 0.05% formic acid in water
B: 10mM amm formate + 0.05% formic acid in MeOH

Time (mins)	%B	Time (mins)	%B
0	2	12.0	100
0.25	30	12.5	2
10.0	100	14.5	2

Flow rate: 0.5ml/min
Column temperature: 50°C

TSQ Quantiva triple quad MS
Positive mode HESI
Spray voltage: 3500V
Ion transfer tube temperature: 350°C
Vaporizer temperature: 300°C

250 Pesticide Screen using LC-MS/MS (II)

	RT	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
5-OH Thiabendazole	1.66	[M+H]+	218.0	147.2	191.1
Abamectin	9.45	[M+NH4]+	890.5	305.3	567.5
Acephate	1.26	[M+H]+	184.0	143.1	125.1
Acetamiprid	2.24	[M+H]+	223.1	126.1	90.1
Aldicarb	2.95	[M+NH4]+	208.1	116.1	89.0
Aldicarb Sulfone	1.44	[M+NH4]+	240.1	148.0	86.0
Aldicarb Sulfoxide	1.37	[M+NH4]+	224.1	132	89.1
Allethrin	8.33	[M+H]+	303.2	135.1	123.1
Ametoctradin	7.64	[M+H]+	276.2	149.1	176.2
Atrazine	4.64	[M+H]+	216.1	174.0	104.0
Azinphos Ethyl	6.30	[M+H]+	346.0	132.1	233
Azinphos Methyl	5.14	[M+H]+	318.0	132.0	124.9
Azinphos Methyl OA	2.98	[M+H]+	302.0	132.2	160.0
Azoxystrobin	5.59	[M+H]+	404.1	372.1	344.1
Bendiocarb	3.72	[M+H]+	224.1	167.1	109.1
Benoxacor	5.23	[M+H]+	260.1	134.1	120.1
Bifenazate	6.27	[M+H]+	301.1	198.0	170.1
Bitertanol	7.41	[M+H]+	338.2	269.3	99.1
Boscalid	5.85	[M+H]+	343.0	307.0	140.0
Bupirimate	6.68	[M+H]+	317.2	210.2	237.3
Buprofezin	8.24	[M+H]+	306.1	201.1	106.1
Cadusafos	7.58	[M+H]+	271.1	159.0	131.0
Carbaryl	4.07	[M+NH4]+	219.1	145.1	127.0
Carbendazim	2.10	[M+H]+	192.1	160.1	132.1
Carbofuran	3.77	[M+H]+	222.1	165.2	123.2
Carboxin	3.97	[M+H]+	236.1	143.0	93.0
Carfentrazone Ethyl	6.88	[M+H]+	412.0	346.1	366.0
Chlorantraniliprole	5.24	[M+H]+	484.0	286.0	194.0
Chlorfenvinphos	7.21	[M+H]+	359.0	170.0	99.1
Chlorimuron Ethyl	5.73	[M+H]+	415.1	186.0	83.0
Chlorpyrifos	8.47	[M+H]+	349.9	198.0	97.0
Chlorpyrifos OA	6.65	[M+H]+	334.0	278.0	197.9
Clethodim	7.71	[M+H]+	360.3	164.1	136.1
Clofentezine	7.38	[M+H]+	303.0	138.1	102.0
Cloransulam Methyl	4.13	[M+H]+	430.0	398.1	370.0
Clothianidin	1.99	[M+H]+	250.0	169.1	132.0
Coumaphos	7.07	[M+H]+	363.0	227.1	307.1
Crotoxyphos	5.86	[M+NH4]+	332.1	127.1	193.1
Crufomate	6.77	[M+H]+	292.1	236.1	108.1
Cyantraniliprole	4.33	[M+2+H]+	475.0	286.0	444.1
Cyazofamid	6.52	[M+H]+	325.1	108.1	261.2

	RT	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z
Cyflufenamid	7.42	[M+H]+	413.1	295.1	203
Cymoxanil	2.48	[M+H]+	199.1	128.1	111.1
Cyphenothrin	9.27	[M+NH4]+	393.2	151.2	123.2
Cyprosulfamide	3.30	[M+H]+	375.1	135.1	254.1
Cyromazine	1.15	[M+H]+	167.1	125.2	68.2
DEF	9.20	[M+H]+	315.1	169.0	113.0
Demeton-S Sulfone	2.55	[M+H]+	291.1	235.1	263.1
Dialifos	7.46	[M+H]+	394.0	208.1	181.0
Diazinon	7.12	[M+H]+	305.1	169.1	153.2
Diazinon OA	5.32	[M+H]+	289.1	153.2	233.1
Dichlormid	3.85	[M+H]+	208.0	140.0	81.2
Dichlorvos	3.63	[M+H]+	221.0	109.1	127.0
Dicrotophos	1.87	[M+H]+	238.1	112.2	193.1
Diethofencarb	5.53	[M+H]+	268.2	124.1	180.2
Diflubenzuron	6.66	[M+H]+	311.0	158.0	141.0
Dimethenamid	5.70	[M+H]+	276.1	244.1	168.2
Dimethoate	2.23	[M+H]+	230.1	199.0	125.0
Dimethomorph	5.76, 6.07	[M+H]+	388.1	301.0	165.1
Dinotefuran	1.36	[M+H]+	203.1	129.1	114.2
Dioxacarb	2.26	[M+H]+	224.1	123.1	167.1
Dioxathion	8.10	[M-C4H10O2PS2]+	271.1	97.0	125.0
Disulfoton Sulfone	4.59	[M+H]+	307.0	261.1	125.0
Disulfoton Sulfoxide	4.49	[M+H]+	291.0	185.1	213.1
Diuron	4.82	[M+H]+	233.0	72.1	160.0
DMST	3.90	[M+H]+	215.1	106.1	151
Dodine	7.56	[M+]+	228.3	186.3	60.1
Emamectin	8.57	[M+H]+	886.5	158.1	126.1
Ethiofencarb	4.27	[M+H]+	226.1	107.1	169.1
Ethiofencarb Sulfone	1.90	[M+NH4]+	275.1	107.1	201.1
Ethiofencarb Sulfoxide	1.98	[M+H]+	242.1	107.1	185.0
Ethion	8.31	[M+H]+	385.0	199.1	143.0
Ethion Monoxon	6.73	[M+H]+	369.0	199.0	143.0
Ethiprole	5.77	[M+NH4]+	413.9	351.0	255.0
Ethofumesate	5.55	[M+H]+	287.1	121.1	241.1
Ethoprop	6.46	[M+H]+	243.1	173.0	131.0
Etofenprox	9.75	[M+NH4]+	394.2	177.2	107.1
Etoxazole	8.73	[M+H]+	360.2	141.0	304.2
Famoxadone	7.24	[M+NH4]+	392.2	331.1	238.0
Fenamidone	5.76	[M+H]+	312.1	236.1	92.2
Fenamiphos	6.71	[M+H]+	304.1	217.1	202.0
Fenamiphos Sulfone	4.10	[M+H]+	336.1	266.1	188.1
Fenamiphos Sulfoxide	3.96	[M+H]+	320.1	233.1	171.1

250 Pesticide Screen using LC-MS/MS (III)

	RT	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z
Fenazaquin	9.21	[M+H]+	307.2	161.2	57.2
Fenhexamid	6.39	[M+H]+	302.1	178.0	97.2
Fenobucarb	5.49	[M+H]+	208.1	95.0	152.0
Fenoxaprop Ethyl	8.03	[M+H]+	362.1	288.1	91.1
Fenoxycarb	6.80	[M+H]+	302.1	88.1	116.1
Fenpropimorph	6.42	[M+H]+	304.3	147.2	119.1
Fenpyroximate	8.90	[M+H]+	422.2	366.1	214.1
Fensulfothion	4.89	[M+H]+	309.0	235.0	281.1
Fenuron	2.17	[M+H]+	165.1	72.1	77.1
Flonicamid	1.66	[M+H]+	230.1	203	98.0
Fluazifop P Butyl	8.12	[M+H]+	384.1	282.2	328.2
Fludioxonil	5.76	[M+NH4]+	266.1	158.1	131.0
Flufenoxuron	8.79	[M+H]+	489.0	158.1	141.1
Flufenpyr Ethyl	6.71	[M+H]+	409.1	335.0	307.0
Flumetsulam	2.03	[M+H]+	326.1	129.1	109.0
Flumiclorac Pentyl	8.13	[M+NH4]+	441.1	308.1	354.1
Fluometuron	4.31	[M+H]+	233.1	72.2	46.3
Fluopicolide	6.00	[M+H]+	383.0	173.0	145.0
Fluopyram	6.33	[M+H]+	397.1	173.0	208.0
Fluoxastrobin	6.40	[M+H]+	459.1	427.2	188.1
Fluridone	5.32	[M+H]+	330.1	309.1	290.0
Flusilazole	6.77	[M+H]+	316.1	247.2	165.1
Fluthiacet Methyl	6.88	[M+H]+	404.0	344.0	273.9
Flutolanil	5.95	[M+H]+	324.1	262.0	282.0
Flutriafol	4.74	[M+H]+	302.1	70.1	123.1
Fluxapyroxad	6.02	[M+H]+	382.1	342.1	314.1
Forchlorfenuron	4.78	[M+H]+	248.1	129.1	93.1
Formetanate HCl	1.26	[M+H]+	222.0	165.1	120.0
Fosthiazate	4.40	[M+H]+	284.1	104.1	228.1
Hexaconazole	7.29	[M+H]+	314.1	158.9	70.0
Hexythiazox	8.51	[M+H]+	353.1	228.0	168.0
Imazalil	5.14	[M+H]+	297.1	159.1	255.1
Imazosulfuron	5.28	[M+H]+	413.0	153.0	156.1
Imidacloprid	1.96	[M+H]+	256.1	209.1	175.0
Imiprothrin	6.34	[M+H]+	319.2	151.1	123.1
Indaziflam	6.58	[M+H]+	302.2	158.1	145.1
Indoxacarb	7.75	[M+H]+	528.1	249.0	150.1
Ipconazole	7.81	[M+H]+	334.2	70.1	125.0
Iprovalicarb	6.31	[M+H]+	321.2	119.1	186.2
Isofenphos	7.39	[M+H]+	346.1	217.0	245.1
Isoprocarb	4.67	[M+H]+	194.1	95.1	152.2
Isoproturon	4.79	[M+H]+	207.2	72.2	165.2

	RT	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z
Kresoxim Methyl	6.90	[M+H]+	314.1	267.2	222.1
Lactofen	8.22	[M+NH4]+	479.1	344.1	223.0
Lenacil	4.67	[M+H]+	235.1	153.1	136.1
Leptophos OA	7.75	[M+2+H]+	396.9	155.1	364.9
Linuron	5.46	[M+H]+	249.0	182.1	160.1
Malathion	5.92	[M+H]+	331.0	127.1	285.1
Malathion OA	3.89	[M+H]+	315.1	127.1	99.0
Mandipropamid	5.94	[M+H]+	412.1	328.2	356.2
Mefenpyr Diethyl	7.26	[M+H]+	373.1	327.1	160.0
Mepanipyrim	6.21	[M+H]+	224.1	106.2	77.1
Mesotrione	2.01	[M+H]+	340.1	228.1	104.1
Metaflumizone	8.30	[M+H]+	507.1	178.0	287.1
Metalaxyl	4.91	[M+H]+	280.1	220.1	192.1
Metaldehyde	2.02	[M+NH4]+	194.1	62.2	45.3
Metconazole	7.32	[M+H]+	320.2	70.1	125.0
Methamidophos	1.16	[M+H]+	142.0	94.2	125.1
Methidathion	4.97	[M+NH4]+	320.0	145.1	85.1
Methiocarb	5.64	[M+H]+	226.1	169.2	121.1
Methiocarb Sulfone	2.35	[M+NH4]+	275.0	122.1	201.1
Methiocarb Sulfoxide	2.10	[M+H]+	242.1	185.1	122.1
Methomyl	1.61	[M+H]+	163.1	106.1	88.1
Methoxyfenozide	6.04	[M+H]+	369.2	149.1	313.1
Metolcarb	3.28	[M+H]+	166.1	109.1	94.1
Metribuzin	3.59	[M+H]+	215.1	187.1	131.1
Mevinphos	2.70	[M+NH4]+	242.1	193.1	127.1
Monocrotophos	1.71	[M+H]+	224.1	193.0	127.0
Monolinuron	4.16	[M+H]+	215.1	126.1	148.1
Myclobutanil	6.15	[M+H]+	289.1	125.0	70.1
Nicosulfuron	3.45	[M+H]+	411.1	182	213
Norflurazon	4.98	[M+H]+	304.0	160.0	140.0
Norflurazon Desmethyl	4.43	[M+H]+	290.0	179.0	140.0
Omethoate	1.33	[M+H]+	214.0	183.0	125.0
Oxamyl	1.48	[M+NH4]+	237.1	72.0	90.0
Oxamyl Oxime	1.34	[M+H]+	163.1	72.1	90.1
Oxydemeton Methyl	1.57	[M+H]+	247.0	169.1	109.1
Oxydemeton Methyl Sulfone	1.62	[M+H]+	263.0	169.0	109
Parathion Methyl OA	3.10	[M+H]+	248.0	202.0	109.1
Parathion OA	4.61	[M+H]+	276.1	220.1	248.1
Pencycuron	7.50	[M+H]+	329.1	125.1	89.1
Penflufen	6.95	[M+H]+	318.2	234.1	141.0
Penthiopyrad	7.05	[M+H]+	360.1	177.1	276.1
Phenothrin	9.56	[M+H]+	351.2	183.1	168.0

250 Pesticide Screen using LC-MS/MS (IV)

	RT	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z
Phenthoate	6.81	[M+H]+	321.0	247.1	79.1
Phorate OA	5.10	[M+H]+	245.0	75.2	47.2
Phorate OA Sulfone	2.51	[M+H]+	277.0	155.0	127.0
Phorate OA Sulfoxide	2.31	[M+H]+	261.0	153.0	81.0
Phorate Sulfone	4.61	[M+H]+	293.0	114.9	171.0
Phorate Sulfoxide	4.49	[M+H]+	277.0	170.9	199.0
Phosalone	7.35	[M+H]+	368.0	182.0	111.1
Phosmet	5.21	[M+H]+	318.0	160.1	133.1
Phosmet OA	3.12	[M+H]+	302.0	160.0	133.0
Phosphamidon	3.43	[M+H]+	300.1	127.1	174.1
Phoxim	7.25	[M+H]+	299.1	77.2	129.1
Picoxystrobin	6.79	[M+H]+	368.1	145.0	115.0
Pirimicarb	4.24	[M+H]+	239.2	182.1	72.0
Pirimicarb Desmethyl	2.71	[M+H]+	225.1	168.2	72.1
Pirimiphos Methyl	7.34	[M+H]+	306.1	164.2	108.1
Prallethrin	7.69	[M+H]+	301.2	133.0	151.2
Prochloraz	7.39	[M+H]+	376.0	308.1	70.1
Profoxydim	7.71,9.00	[M+H]+	466.2	280.0	180.0
Promecarb	5.88	[M+H]+	208.1	109.0	151.1
Propamocarb	1.41	[M+H]+	189.1	102.0	144.0
Propaquizafop	8.21	[M+H]+	444.1	299.2	371.2
Propargite	8.74	[M+NH4]+	368.2	231.2	175.1
Propetamphos	6.13	[M+H]+	282.1	138.1	156.1
Propoxur (S)	3.69	[M+H]+	210.1	168.2	111.1
Prosulfuron	5.29	[M+H]+	420.1	167.1	141.1
Pymetrozine	1.44	[M+H]+	218.1	105.1	78.1
Pyraclostrobin	7.30	[M+H]+	388.1	163.1	194.1
Pyraflufen Ethyl	7.13	[M+H]+	413.0	339.0	253.1
Pyrazophos	7.31	[M+H]+	374.1	222.2	194.1
Pyridaben	9.22	[M+H]+	365.1	309.0	147.1
Pyridalyl	10.21	[M+2+H]+	492.0	110.9	164
Pyrimethanil	5.45	[M+H]+	200.1	107.1	168.1
Pyriproxyfen	8.39	[M+H]+	322.1	96.0	227.1
Quinalphos	6.78	[M+H]+	299.1	163.1	147.1
Quinoxyfen	8.50	[M+H]+	308.0	197.1	214.1
Quizalofop Ethyl	8.01	[M+H]+	373.1	299.2	255.1
Resmethrin	9.40	[M+H]+	339.2	128.1	171.1
Rimsulfuron	3.94	[M+H]+	432.1	182.1	139.0
Rotenone	6.71	[M+H]+	395.2	213.2	192.1
Saflufenacil	5.32	[M+H]+	501.1	349.1	198.0
Sedaxane	6.20, 6.54	[M+H]+	332.2	159.0	139.0
Sethoxydim	8.03	[M+H]+	328.2	178.0	220.1

	RT	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z
Simazine	3.66	[M+H]+	202.1	104.1	132.1
Spinetoram	8.14	[M+H]+	748.5	142.1	203.1
Spinosad A	7.69	[M+H]+	732.5	142.1	98.0
Spinosad D	8.10	[M+H]+	746.5	142.1	98.0
Spirodiclofen	8.91	[M+H]+	411.1	313.1	71.1
Spiromesifen	8.66	[M+NH4]+	388.1	273.1	187.0
Spiromesifen Alcohol	5.01	[M+H]+	273.2	187.1	179.1
Spirotetramat	6.38	[M+H]+	374.2	302.3	216.2
Spiroxamine	5.95	[M+H]+	298.3	144.2	100.2
Sulfoxaflor	2.39	[M+NH4]+	295.2	174.1	154.1
Sulprofos	8.56	[M+H]+	323.0	219.1	139.1
TCMTB	5.48	[M+H]+	239.0	180.0	136.0
Tebufenozide	6.78	[M+H]+	353.2	133.0	104.8
Tebufenpyrad	8.19	[M+H]+	334.2	117.1	145.1
Tebuthiuron	3.89	[M+H]+	229.1	172.0	116
Tepraloxydim	4.10, 6.19	[M+H]+	342.2	250.1	166.1
Terbufos Sulfone	5.46	[M+H]+	321.0	115.0	143.0
Terbufos Sulfoxide	5.49	[M+H]+	305.1	97.0	187.0
Terbuthylazine	5.71	[M+H]+	230.1	174.1	104.1
Tetrachlorvinphos	6.86	[M+2+H]+	366.9	127.1	206.0
Tetramethrin	7.91, 8.10	[M+H]+	332.2	164.1	135.1
Thiabendazole	2.48	[M+H]+	202.0	175	131.1
Thiacloprid	2.55	[M+H]+	253.0	126.1	99.1
Thiamethoxam	1.65	[M+H]+	292.0	211.1	181.1
Thifensulfuron Methyl	3.28	[M+H]+	388.0	167.1	205.0
Thiobencarb	7.46	[M+H]+	258.1	125.0	89.0
Thiodicarb	4.34	[M+H]+	355.1	163.2	88.1
Thionazin	4.74	[M+H]+	249.1	193.1	97.0
Topramezone	1.63	[M+H]+	364.1	334.1	125.1
Triadimefon	6.07	[M+H]+	294.1	197.0	225.0
Triadimenol	6.25	[M+H]+	296.1	70.2	99.0
Triazophos	6.19	[M+H]+	314.1	162.1	119.1
Tribenuron Methyl	4.59	[M+H]+	396.1	155.1	181.1
Trichlorfon	2.26	[M+H]+	256.9	109.0	221
Tricyclazole	2.80	[M+H]+	190.0	163.1	136.1
Trifloxystrobin	7.78	[M+H]+	409.1	186.2	206.2
Triflumizole	7.87	[M+H]+	346.1	278.0	73.0
Triforine	5.23	[M+2+H]+	434.9	213.0	98.2
Zoxamide	7.09	[M+H]+	336.0	187.0	159