ChromSword Method Development Kits



ACE[®] ChromSword 2 Method Development Kits

Intelligent Solutions for Method Development

Better Method Development Solutions

Solve HPLC method development challenges systematically and efficiently – using ACE columns and ChromSword 2 method development software. The ACE ChromSword Method Development Kit includes 6 alternative selectivity ACE phases, a copy of ChromSword 2 offline with a 6-month activation licence and a wealth of technical information and support – the perfect combination to introduce an improved method development protocol for your laboratory.

What the ChromSword Method Development Kit Contains:

- 1 x ACE C18 column, 1 x ACE C18-AR column, 1 x ACE C18-PFP column, 1 x ACE CN-ES column, 1 x ACE C18-Amide column and 1 x ACE SuperC18 column kits with various dimensions are available. (All columns in the kit are the same dimensions).
- ChromSword 2 Offline version with a 6-month activation licence key. (ChromSword 2 requires Windows XP or later)
- USB containing useful information and examples from ChromSword and Advanced Chromatography Technologies Limited.
- On-going help and advice from our specialist technical support group simply contact info@ace-hplc.com

ChromSword 2 Offline

ChromSword have been developing new and innovative software solutions to support liquid chromatographers with their method development for over 20 years and are experts in this field. The ChromSword 2 Offline software in these method development kits is a baselevel, introductory version of ChromSword, offering an extremely cost effective opportunity to explore the many benefits of the ChromSword 2 software.

ChromSword 2 is designed to help you develop and optimise HPLC separations more effectively and more efficiently. On the basis of only a few experiments you can use the power of ChromSword to simulate numerous possible chromatographic solutions, looking at various columns and method conditions. This data can then be reviewed to identify and then optimise the separation most suitable to your needs. Typical method variables include organic modifier concentration, gradient profile, temperature, pH and much more. This empirical method development approach will provide you with the best possible separation for your analytes.

Furthermore, the 6 ACE columns in the kit have all been pre-calibrated by ChromSword and the data is stored within the library provided. This, together with data on physical chemistry properties, which is also provided, enables some predictive modelling (using the physical chemical properties of the molecular structures of your analytes) to be carried out. Elucidation of a purely theoretical chromatogram is therefore possible with this approach, and although it will be less precise than the hands-on, empirical approach, it may provide a quick indication of the direction in which to focus your efforts. However, whatever a theoretical approach may indicate, it is always recommended that various column selectivities are screened. With these kits, you have a choice of up to 6 different ACE column selectivities to explore!

The ChromSword licence included with the kit will provide you with a full 6 months of method development investigation time. Save hours of frustration and wasted effort in the lab with a new ACE ChromSword 2 Method Development Kit!

Intelligent Solutions for Method Development

ChromSwordAuto 5 vs ChromSword 2 Offline

The ChromSword 2 Offline software contained in the method development kit is a base-level, introductory version of ChromSword, which allows you to explore the benefits of computer simulated method development for an extremely modest investment. A fully automated version, ChromSwrod Auto 5 – the first ever"chromatography method development data system" is also available. ChromSwordAuto 5 bridges the gap between the LC instrument and the method development software by allowing direct control of the HPLC system by ChromSwordAuto 5 in order to fully automate the method development process (figure 1). This is a genuine leap forward for liquid chromatography method development.

ChromSwordAuto 5 provides a complete portfolio of fully automated procedures and tools to cover all steps of a typical method development process from screening to optimisation, through to robustness testing (see figure 2).



Fig 1: ChromSwordAuto 5 bridges the gap between LC instrument and method development software



Fig 2: Typical method development procedure using ChromSwordAuto 5

ChromSwordAuto 5 is based solidly on the theory of liquid chromatography, combined with the newest computing technologies and more than 20 years of practical experience in HPLC method development. It combines automated instrument control and data exchange with mathematical optimisation procedures and artificial intelligence decision making after each run. This extremely powerful combination enables ChromSwordAuto 5 to automatically search for optimal separation conditions and provide you with the answers you need! To discuss options to upgrade to ChromSwordAuto 5 and to discover more about how ChromSwordAuto 5 together with ACE columns can help you develop a Fully Automated Method Development strategy, please contact us at **info@ace-hplc.com**.

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ACE® Advanced Phases for Method Development

Intelligent Solutions for Method Development

The ACE Range of UHPLC/HPLC Columns

The ACE range of UHPLC/HPLC columns offers chromatographers an extremely powerful and reliable approach to UHPLC and HPLC method development. ACE columns are based upon an ultra-inert, high efficiency silica and incorporate the latest developments in LC stationary phase design to provide chromatographers with more choices for alternative selectivity, without compromising stability or robustness.



ACE[®] Stationary Phases Virtually Eliminate the Negative Effects of Silanols on UHPLC & HPLC Separations

ACE Method Development Kits

ACE Method Development Kits are designed to maximise selectivity – the key to resolution in chromatography. A comprehensive range of ACE Method Development Kits for all requirements is available, including kits featuring porous, solid-core, HILIC and bioanalytical 300 Å particle columns, and all offering superb value for money. This ACE ChromSword Method Development Kit contains a range of 6 ACE phases offering alternative selectivities (ACE C18, ACE C18-AR, ACE C18-PFP, ACE CN-ES, ACE C18-Amide and ACE SuperC18), together with base-level introductory version of ChromSword 2 Offline making this kit an ideal tool to investigate method development.



Why Use **ACE**[®] Columns and **ACE**[®] Method Development Kits?

- ACE UHPLC/HPLC columns have a well-deserved reputation for delivering excellent efficiency, reproducibility and lifetime.
- ACE Method Development Kits group together columns with different mechanisms of interaction to maximise selectivity and improve the likelihood of separating difficult or closely related analytes in mixtures.
- Screening columns containing different bonded phases under the same mobile phase conditions can help you achieve your desired separation more quickly, therefore increasing productivity.
- ACE Method Development Kits are highly cost effective, allowing you to explore various selectivities at a reduced cost and facilitating an intelligent approach to method development activity.

ACE[®] ChromSword Method Development Kits

Intelligent Solutions for Method Development

- Contains ACE C18, ACE C18-AR, ACE C18-PFP, ACE CN-ES, ACE C18-Amide and ACE SuperC18 phases
- Ideal for new method development
- Available with 2.1 mm id through to 4.6 mm id and lengths from 50 mm to 250 mm
- Available with 1.7, 2, 3 and 5 µm particle sizes

Phase	Functional Group	Endcapped	Particle Size (µm)	Pore Size (Å)	Surface Area (m²/g)	Carbon Load (%)	Recommended pH Range	100% Aqueous Compatible	USP Listing
ACE C18	Octadecyl (C18)	Yes	1.7, 2, 3, 5	100	300	15.5	2.0-8.0 ^b	No	L1
ACE C18-AR	C18 with integral Phenyl	Yes	1.7, 2, 3, 5	100	300	15.5	2.0-8.0 ^b	Yes	L1
ACE C18-PFP	C18 with integral PFP	Yes	1.7, 2, 3, 5	100	300	14.3	2.0-8.0 ^b	Yes	L1
ACE SuperC18	Octadecyl (C18)	Encapsulated bonding	1.7, 2, 3, 5	90	400	14.8	1.5-11.5ª	No	L1
ACE C18-Amide	C18 with integral amide polar group	Yes	1.7, 2, 3, 5	100	300	16.4	2.0-8.0 ^b	Yes	L1/L60
ACE CN-ES	CN with propri- etary extended alkyl spacer	Yes	1.7, 2, 3, 5	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 <u>www.ace-hplc.com</u>.

^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 <u>www.ace-hplc.com</u>

ACE C18

ACE C18-AR

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.

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

ACE C18-Amide

ACE CN-ES

ACE SuperC18

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

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

Fig 3: Overview of the six ACE columns in the ACE ChromSword Method Development Kit

ACE Columns Provide Alternative Selectivity

According to the resolution equation, selectivity is the most powerful parameter for adjusting analyte resolution. The six phases in the ACE ChromSword Method Development Kit are designed to maximise selectivity and provide a wide range of separation mechanisms, enabling you to identify the best column for your particular analytes.

		Separation Mechanism and Relative Strength						
	Bonded Phases	Hydrophobic Binding	π-π Interaction	Dipole- Dipole	Hydrogen Bonding	Shape Selectivity		
ACE ChromSword	ACE C18	****	-	-	*	**		
Method Development	ACE C18-AR	****	*** (donor)	*	**	***		
	ACE C18-PFP	****	*** (acceptor)	****	***	****		
	ACE SuperC18	****	-	-	-	**		
	ACE C18-Amide	****	-	**	****	**/***		
	ACE CN-ES	* * *	*	***	**	*		

Fig 3: Separation mechanisms for the six ACE columns in the ACE ChromSword Method Development Kit

ACE ChromSword Method Development Kits

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Column Screening with ACE® Phases

Intelligent Solutions for Method Development

Screening a sample on multiple columns under identical conditions using a generic scouting gradient is a powerful tool for method development and allows a suitable column to be quickly identified for a separation. This approach can be extended by screening two different mobile phase organic modifiers to give a more comprehensive, information rich approach. When a column screening approach is combined with the power of ChromSword you have all the tools at your disposal to solve HPLC method development challenges systematically and efficiently. ACE phases and ChromSword are the perfect combination for introducing an improved method development protocol to your laboratory.

As seen in the example (Figure 4) the most common column starting position for much method development (a C18 column) would fail to separate all 10 compounds with either MeCN or MeOH as the mobile phase. However, using the 6 ACE columns provided in the ACE ChromSword Method Development Kit there are 6 possible options to choose from that will separate all 10 analytes; 4 using MeCN as the mobile phase and 2 using MeOH as the mobile phase. All the analyst needs to do now is select the preferred choice and use the power of ChromSword to fully optimise the method quickly and simply.



A: 20 mM Ammonium acetate pH 6.0

B: 20 mM Ammonium acetate pH 0.0 B: 20 mM Ammonium acetate pH 6.0 in MeOH:H₂O or MeCN:H₂O (9:1) v/v)

Gradient: 5 to 95% B in 10 mins, Temp: 40 °C, 2 μ L injection, Flow rate: 1.2 mL/min

Fig 5: An example of column screening using the 6 ACE columns

To discover more about how ChromSword and **ACE**[®] columns can help you develop a successful method development strategy, please contact our support specialists at info@ace-hplc.com

ACE® ChromSword Method Development HPLC/UHPLC Column Kits

(Contains 6 columns: ACE C18, ACE C18-AR, ACE C18-PFP, ACE CN-ES, ACE C18-Amide and ACE SuperC18 of specified dimensions, ChromSword 2 Offline with 6-month activation license and USB drive containing information and examples).

(HPLC/UHPLC hardware format with 1,000 bar/15,000 psi pressure limit)						
Column Dimensions	1.7 µm	2 µm	3 µm	5 µm		
2.1 x 50 mm	MDKCS-17-0502U	MDKCS-2-0502U	MDKCS-3-0502U	MDKCS-5-0502U		
2.1 x 75 mm	MDKCS-17-7502U	MDKCS-2-7502U	MDKCS-3-7502U	MDKCS-5-7502U		
2.1 x 100 mm	MDKCS-17-1002U	MDKCS-2-1002U	MDKCS-3-1002U	MDKCS-5-1002U		
2.1 x 125 mm	-	MDKCS-2-1202U	MDKCS-3-1202U	MDKCS-5-1202U		
2.1 x 150 mm	_	MDKCS-2-1502U	MDKCS-3-1502U	MDKCS-5-1502U		
2.1 x 250 mm	-	-	MDKCS-3-2502U	MDKCS-5-2502U		
3.0 x 50 mm	MDKCS-17-0503U	MDKCS-2-0503U	MDKCS-3-0503U	MDKCS-5-0503U		
3.0 x 75 mm	MDKCS-17-7503U	MDKCS-2-7503U	MDKCS-3-7503U	MDKCS-5-7503U		
3.0 x 100 mm	MDKCS-17-1003U	MDKCS-2-1003U	MDKCS-3-1003U	MDKCS-5-1003U		
3.0 x 125 mm	-	MDKCS-2-1203U	MDKCS-3-1203U	MDKCS-5-1203U		
3.0 x 150 mm	-	MDKCS-2-1503U	MDKCS-3-1503U	MDKCS-5-1503U		
3.0 x 250 mm	-	-	MDKCS-3-2503U	MDKCS-5-2503U		
4.6 x 50 mm	-	MDKCS-2-0546U	MDKCS-3-0546U	MDKCS-5-0546U		
4.6 x 75 mm	-	MDKCS-2-7546U	MDKCS-3-7546U	MDKCS-5-7546U		
4.6 x 100 mm	_	MDKCS-2-1046U	MDKCS-3-1046U	MDKCS-5-1046U		
4.6 x 125 mm	-	MDKCS-2-1246U	MDKCS-3-1246U	MDKCS-5-1246U		
4.6 x 150 mm	_	MDKCS-2-1546U	MDKCS-3-1546U	MDKCS-5-1546U		
4.6 x 250 mm	-	-	MDKCS-3-2546U	MDKCS-5-2546U		

Your decision has lasting effects.



Ultra-Inert Base-Deactivated UHPLC/HPLC Columns For Performance, Selectivity and Guaranteed Reproducibility

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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