

Packed Columns for Supercritical Fluid Chromatography

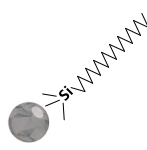
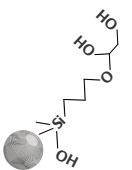
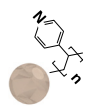
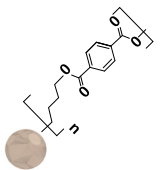
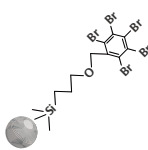
Shim-pack UC^{series} 6 Columns Set for Method Screening

CoreFocus



A set of six columns with a wide variety of stationary phases for separating all sorts of compounds

Shim-pack™ UC series offer a wide variety of stationary phases, providing different retention mechanisms (normal phase, reversed phase or mixed-mode). SFC uses a mixture of sub/supercritical carbon dioxide and a modifier (an organic solvent such as methanol) regardless of the stationary phase used. Therefore, the same mobile phase composition can be used for serial analysis through all columns. Column scouting is effective by using the following set of 6 columns, each providing a different separation selectivity.

	6 columns set					
	UC-ODS	UC-Sil II	UC-Diol II	UC-PolyVP	UC-PolyBT	UC-PBr
Chemistry						
Features	The separation mode is reverse phase. Retention is provided through hydrophobic interaction.	A versatile phase suitable for various applications	The separation mode is normal phase. This inhibits non-specific interactions.	A favorable peak shape is obtained even without acid-base additives.	This is excellent for resolving aromatic compounds through π - π interactions.	The separation mode is mixed-mode, using both polar and non-polar interactions.

For method scouting use a 3.0 μ m, 3.0 x 150 mm column. Corresponding 5.0 μ m, 4.6 x 250 mm columns are also available.

Column name	3 μ m, 3.0x150 mm	5 μ m, 4.6x250 mm
Shim-pack UC-ODS	227-32608-04	227-32608-05
Shim-pack UC-Sil II	227-32607-09	227-32607-02
Shim-pack UC-Diol II	227-32606-09	227-32606-02
Shim-pack UC-PolyBT	227-32501-13	227-32503-12
Shim-pack UC-PolyVP	227-32507-13	227-32509-12
Shim-pack UC-PBr	227-32602-09	227-32602-02

For additional Shim-pack UC information, please see the Shim-pack UC series brochure.



SFC columns Shim-pack UC Series (C190-E251)



SWIFT Methodology Overview

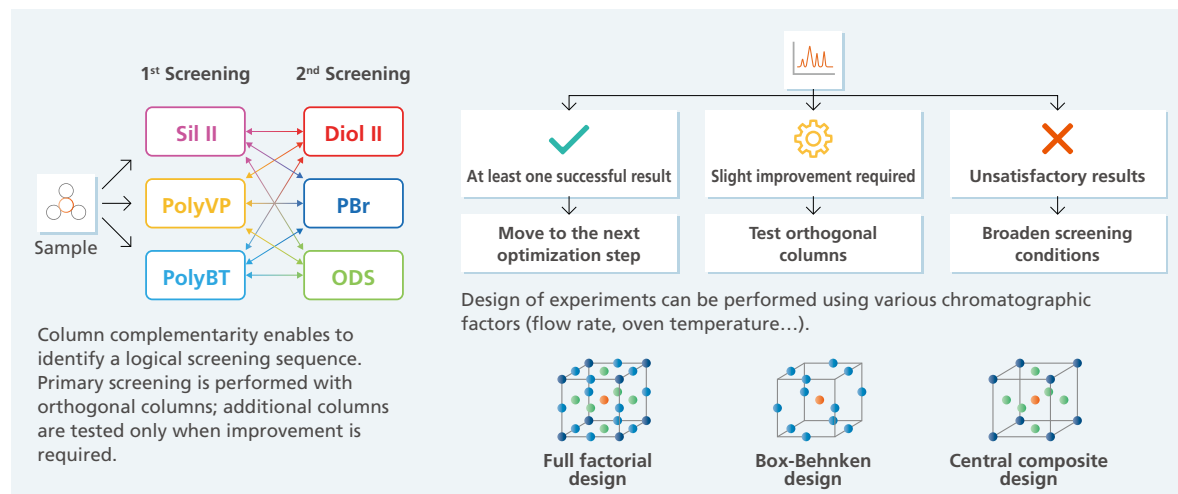
Shimadzu offers "SWIFT (SFC Workflow for Intelligent and Fast Tuning)" to facilitate SFC method development.

SWIFT simplifies screening by combining complementary columns with a decision-tree workflow.

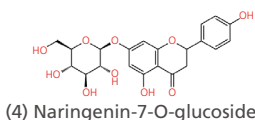
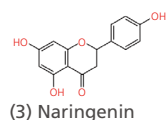
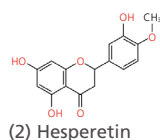
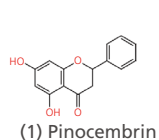
Complementarity-based screening sequence for Shim-pack UC columns Supported by LabSolutions MD for screening evaluation and DoE-based optimization.



LabSolutions MD



Flavanones case study



Method Development Workflow

Step 1.
Column screening

Step 2.
Co-solvent adjustment

Step 3.
Gradient optimization

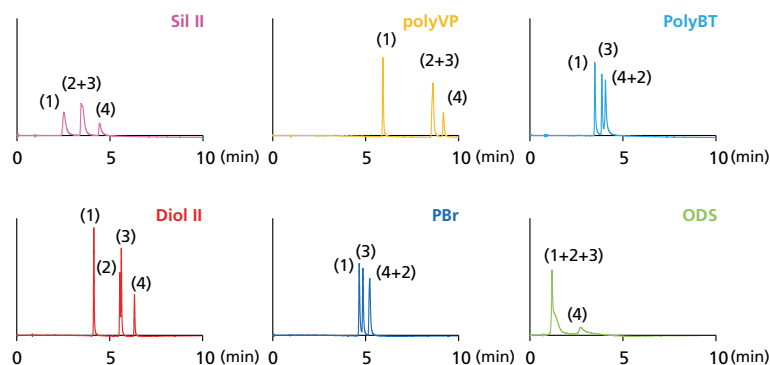
Step 1. Column screening

1st Screening on Sil II, PolyVP and PolyBT:

- Flowrate: 1.2 mL/min
- Gradient: 5 to 100 % B
- Co-solvent (B): MeOH-H₂O (95-5) + 20 mmol/L ammonium formate
- Oven temp.: 25 °C
- Back-pressure: 150 bar

Slight improvement is required
→ Test orthogonal columns

2nd Screening on Diol II, PBr and ODS



Column	Min. resolution	Peak count	Separated peak count	Evaluation value
Sil II	0.418	4	2	17.67
PolyVP	0.405	4	2	17.62
PolyBT	0.417	4	1	16.61
Diol II	0.985	4	3	19.94
PBr	0.471	4	0	17.22
ODS	0.36	4	0	13.07

Column screening identified UC Diol II as the best column.

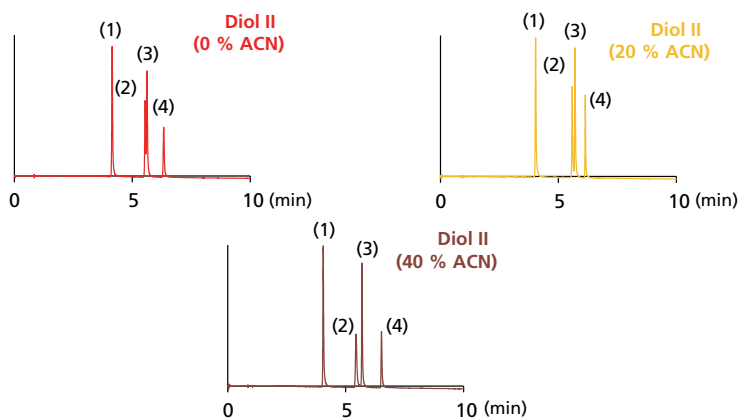
→ Proceed to co-solvent adjustment

Step 2. Co-solvent adjustment

Use the column/gradient combination that gave the highest evaluation value in the column screening step. The additive condition selected during column screening was retained for co-solvent adjustment:

ACN* addition:

- Column: Shim-pack UC Diol II (3.0 × 150 mm, 3 μm)
- Flowrate: 1.2 mL/min
- Gradient: 5 to 100 % B
- Co-solvent (B):
 - MeOH-H₂O (95-5) + 20 mmol/L ammonium formate
 - MeOH-ACN-H₂O (75-20-5) + 20 mmol/L ammonium formate
 - MeOH-ACN-H₂O (55-40-5) + 20 mmol/L ammonium formate
- Oven temp.: 25 °C
- Back-pressure: 150 bar
- *ACN: Acetonitrile



Co-solvent	Min. resolution	Separated peak count	Evaluation value
0 % ACN	0.985	3	19.94
20 % ACN	1.662	2	22.65
40 % ACN	2.681	4	24.00

Positive impact on chromatographic performance

→ Proceed to gradient optimization

Step 3. Gradient optimization

Focus gradient test:

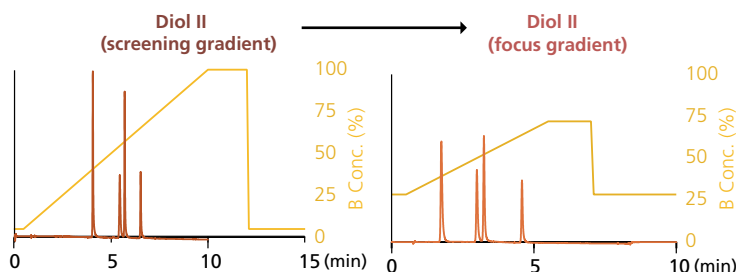
- Column: Shim-pack UC Diol II (3.0 × 150 mm, 3 μm)
- Flowrate: 1.2 mL/min
- Gradient: $C_{e \text{ first}} - 7.5 \%$ (28.2 %) to $C_{e \text{ last}} + 7.5 \%$ (67.9 %) of B
- Co-solvent (B): MeOH-ACN-H₂O (55-40-5) + 20 mmol/L ammonium formate
- Oven temp.: 25 °C
- Back-pressure: 150 bar

DoE for gradient optimization:

- Column: Shim-pack UC Diol II (3.0 × 150 mm, 3 μm)
- Flowrate: 1.2 mL/min
- Gradient: initial/final of % B and gradient time optimized by DoE
- Co-solvent (B): MeOH-ACN-H₂O (55-40-5) + 20 mmol/L ammonium formate
- Oven temp.: 25 °C
- Back-pressure: 150 bar

Optimal conditions were obtained with a low C_i , a high C_f and a short gradient time. A confirmation run was performed to confirm the optimal conditions

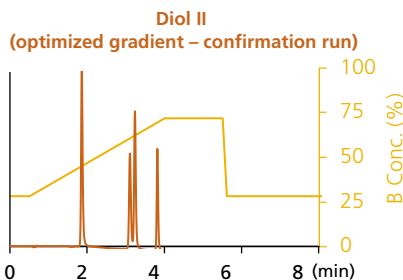
1. Define focused gradient using co-solvent ratio at elution of first ($C_{e \text{ first}}$) and last ($C_{e \text{ last}}$) peaks
2. Check its suitability
3. Optimize the focus gradient using DoE
4. Confirm final conditions



DoE optimization used the following parameters:

Initial concentration (C_i), Final concentration (C_f), Gradient time (t_G)

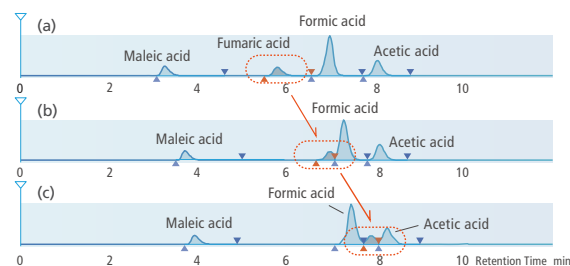
DoE point	Initial Conc. ($C_{e \text{ first}} - x \%$)	Final Conc. ($C_{e \text{ last}} + x \%$)	Gradient time
-1	$C_{e \text{ first}} - 5 \%$	$C_{e \text{ last}} + 5 \%$	2.5 min
0	$C_{e \text{ first}} - 7.5 \%$	$C_{e \text{ last}} + 7.5 \%$	5 min
+1	$C_{e \text{ first}} - 10 \%$	$C_{e \text{ last}} + 10 \%$	7.5 min



LabSolutions MD

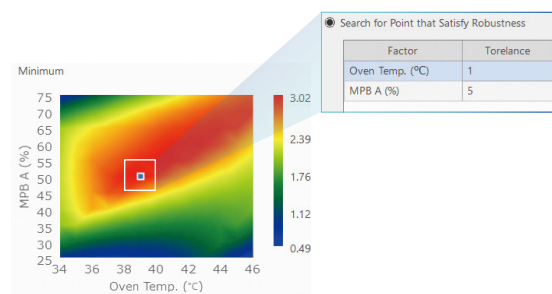
Automatic Tracking of Target Peaks

The figure at right illustrates an example of automatic peak identification for fumaric acid. It highlights how retention time varies with changes in acid concentration and column oven temperature. By filtering out other components based on peak height, the software can automatically detect fumaric acid peaks—even when they elute at different retention times. This enables accurate peak identification through the combined use of multiple parameters.



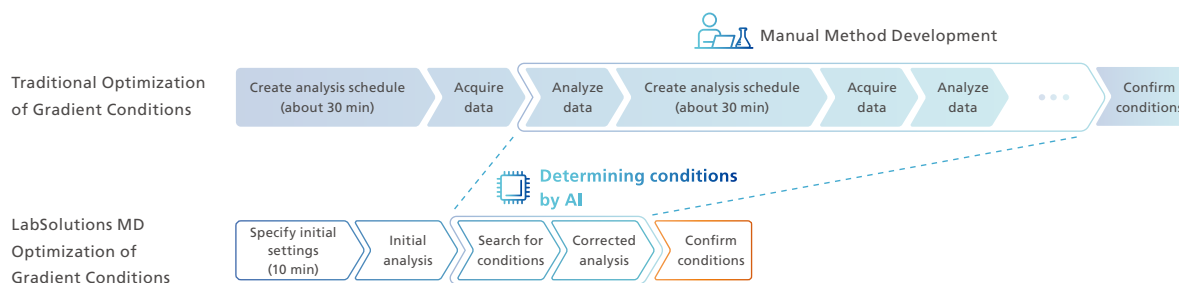
Design Space-Driven Discovery of Optimal Analytical Conditions

During the initial screening phase, samples are analyzed under multiple automatically specified conditions. This data is then used to visually illustrate how variations in each parameter affect separation performance. In the design space shown in the figure on the right—where organic solvent concentration in mobile phase B is plotted on the vertical axis and column oven temperature on the horizontal axis—the results identify 50 % organic solvent and a column oven temperature of 39 °C as the most robust combination of LC parameters.



Automatic Optimization of Gradient Conditions Based on Proprietary AI Algorithm

Shimadzu's proprietary AI algorithm enables automated searching for gradient conditions that meet user-defined separation criteria. Unlike traditional method development—which requires manual creation of analysis schedules and interpretation of results—this AI-driven approach automatically configures subsequent gradient conditions based on acquired data. As a result, optimal gradient conditions can be identified without the need for human intervention.





Shimadzu Corporation

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