2. Appendix

2.1 Chromatographic Column Parameters

The six chromatographic column parameters are determined experimentally.

2.1.1 Retention factor for pentylbenzene, kPB

A measurement of the surface area and surface coverage (ligand density).

Chromatographic Conditions: MeOH-H_2O (8:2, v/v), 1.0mL/min, 40°C, 5µL injection of pentylbenzene (0.6µg/mL). Injections and flow rates have been scaled for 4.6 mm i.d. columns. The first disturbance of the baseline when injecting methanol has been used as a dead time marker.

2.1.2 Hydrophobicity or hydrophobic selectivity, aCH2

The retention factor ratio between pentylbenzene and butylbenzene, aCH2 = kPB/kBB, is a measure of the surface coverage of the stationary phase as the selectivity between alkylbenzenes differentiated by a single methyl group depends on ligand density.

Chromatographic Conditions: All conditions as for kPB determinations, except individual injections of pentylbenzene (0.6µg/mL) and butylbenzene (0.3µg/mL) are performed.

2.1.3 Shape selectivity, aT/O

The retention factor ratio between triphenylene and *o*-terphenyl, aT/O = kT/kO, is a measure of the shape selectivity, which depends on ligand spacing and the shape/functionality of the silylating reagent.

Chromatographic Conditions: All conditions as for aCH2 determinations, except 5µL injection of o-terphenyl and triphenylene both at 0.05mg/mL.

2.1.4 Hydrogen bonding capacity, aC/P

The retention factor ratio between caffeine and phenol, aC/P = kC/kP, is a measure of the number of available silanol groups and the degree of endcapping.

Chromatographic Conditions: MeOH-H_2O (3:7, v/v), 1.0ml/min, 40°C, individual 5µL of phenol and caffeine (0.5mg/mL).

2.1.5 Total ion-exchange capacity, aB/P pH 7.6

The retention factor ratio between benzylamine and phenol, aB/P pH 7.6 = kB/kP, is a measure of the total silanol activity.

Chromatographic Conditions: 20mM KH_2PO_4, pH 7.6, in 3:7 *v/v* MeOH:H_2O (i.e. 28.6 mM in the aqueous buffer solution), 1.0mL/min, 40°C, individual 5µL injections of phenol and benzylamine HCl both at 0.5mg/mL.

2.1.6 Acidic ion-exchange capacity, aB/P pH 2.7

The retention factor ratio between benzylamine and phenol, aB/P pH 2.7 = kB/kP, is a measure of the acidic activity of the silanol groups.

Chromatographic Conditions: All conditions as for total ion-exchanged determinations above, except using a pH 2.7 KH_2PO_4 buffer.

2.2 Calculation Methods

The Chromatographic Column Selector program contains the above six parameters for 254 chromatographic columns. The mean (µ) and standard deviation (SD) for these six parameters are calculated using all of the 254 columns. For each column, a normalized value (xn_1 to xn_6) is calculated for each of the six parameters, $xn_x = (x_x - \mu_x)/SD$, where x_x is the value raw value for the parameter. The Euclidean distance is then used to calculate the column difference factor (CDF) between the target column and the rest of the columns.

$$CDF = \sqrt{[(xn_{t1}-xn_1)^2 + (xn_{t2}-xn_2)^2 + (xn_{t3}-xn_3)^2 + (xn_{t4}-xn_4)^2 + (xn_{t5}-xn_5)^2 + (xn_{t6}-xn_6)^2]}$$

, where xn_{t1} to xn_{t6} are the normalized values of the six chromatographic parameters for the target column. The CDF values are ranked in ascending order, with the lowest CDF indicating the best column match.

2.3 References

1. Characterization of RPLC columns packed with porous sub-2 µm particles, P. Petersson, M.R. Euerby, J. Sep. Sci., 30 (2007) 2012-2024.

2. Chromatographic classification and comparison of commercially available reversed-phase liquid chromatographic columns containing phenyl moieties using principal component analysis, M.R. Euerby, P. Petersson, W. Campbell, W. Roe, J. Chromatogr. A, 1154 (2007) 138-151.

3. M.R. Euerby, P. Petersson, The Use of Principal Component Analysis for the Characterization of Reversed-Phase Liquid Chromatographic Stationary Phases, in : S. Kromidas (ed.) HPLC made to measure - a practical handbook for optimization, Wiley-VCH, New York, NY, 2006 p.p. 240-255.

4. An evaluation of the robustness of the Tanaka characterization protocol for reversed-phase liquid chromatography columns, P. Petersson, M.R. Euerby, J. Sep. Sci., 28 (2005) 2120-2129.