Optimization methods in chromatography and capillary electrophoresis

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Abstract

Many methods have been developed in order to optimize the parameters of interest in either chromatography or capillary electrophoresis. In chemometric approaches experimental measurements are performed in such a way that all factors vary together. An objective function is utilized in which the analyst introduces the desired criteria (selectivity, resolution, time of analysis). Simplex methods and overlapping resolution maps are declining. Factorial designs and central composite designs are more and more popular in electrodriven capillary separations since the number of parameters to master is much larger than in either GC or LC. The use of artificial neural networks is increasing. The advantage of chemometrics tools is that no explicit models are required, conversely the number of experiments to perform may be high and boundaries of the domain are not straightforward to draw and the approach does more than is required. When models are available optimization is easier to perform by regression methods. Computer assisted methods in RPLC are readily available and work well but are still in infancy in CE. Linear solvation energy relationships seem a very valuable tool but estimates of coefficients still require many experiments.
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