Journal of Planar Chromatography - Modern TLC
Volume 12, Issue 5, September 1999, Pages 365-372

Document Type: Article

View references (22)

Optimization of separation in TLC by use of desirability functions and mixture designs according to the 'PRISMA' method

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Abstract

A computer program has been developed for optimization of mobile phase composition in thin-layer chromatography (TLC). The desirability function technique combined with the 'PRISMA' model was used to enhance the quality of TLC separations. The statistical models for prediction of retardation and band-broadening at different mobile phase compositions obtained by the PRISMA method were examined for cyanobacterial hepatotoxins on normal-phase TLC plates and for phenolic compounds on reversed-phase (RP) layers. The study showed that the relationship between mobile phase composition and retardation of the test mixtures can be expressed with high accuracy by use of quadratic regression models. The retardation was described by k(c) = 1/(R(F) 1) and the band-broadening in terms of the band width at the half-height of the peak (w(h)). The models obtained were used to predict the resolution (R(s)) for different solvent combinations. The desirability function converted the calculated R(s) value into the desirability value (D) and the overall optimum was then defined by the overall desirability. The optimum mobile phase mixtures for the separation were obtained as a contour plot inside the horizontal plane of the PRISMA model and good separation was achieved by use of the optimized solvent combination. Depending on the objective for which the optimum separation is being investigated, the program enables either optimization of critical pairs or determination of the overall optimum in which the intention is reasonable separation of as many compounds as possible.

Author Keywords

'PRISMA' model; Desirability function; Normal phase; Optimization; Reversed phase; TLC

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