EVALUATION OF RUGGED AND OPTIMAL ANALYSIS CONDITIONS IN MICELLAR LIQUID CHROMATOGRAPHY BY USING INTERPRETATIVE OPTIMIZATION STRATEGY AND DERRINGER’S DESIRABILITY FUNCTION

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The development of every liquid chromatographic method consists of several steps concerned with selection of acceptable polarity of mobile and stationary phase, evaluation of optimal separation conditions by interpretative or sequential optimization procedure and method validation, which includes estimation of ruggedness of a method, i.e. stability of main chromatographic parameters such as resolution and peak tailing to changes of mobile phase composition and column temperature. In our opinion, ruggedness of chromatographic method should be determined during optimization procedure as one of the parameters of response function based on multi-criteria decision making process (MCDM).

In this work the new chemometrics approach is proposed for simultaneous evaluation of rugged and optimal conditions in micellar liquid chromatography (MLC, see ref. [1] for detailed description of method). In this procedure the retention of each solute is modeled by earlier proposed simple retention equation [2]. Then, in each point of parametric space the global resolution is estimated by normalized by the mean resolution product, and the time of analysis by the retention of last eluted peak. The ruggedness is quantified as area around each point on the basis of regularities obtained for dependences of retention factor uncertainty on the values of retention factor [3]. As a result the response function is constructed by using one of the MCDM procedures - Derringer’s desirability function. The proposed approach was successfully tested on retention data of 14 preservatives eluted with mobile phases that contained the sodium dodecylsulfate (0.025-0.1 M), 1-pentanol (0.5-2.0 %, v/v) and trifluoroacetic acid (0.1 %, v/v). All separations were performed on liquid chromatograph Hewlett-Packard 1050 with spectrophotometric detector. The optimal and rugged chromatographic conditions of 14 preservatives was used to develop validated analytical method.

This work was supported by INTAS YSF Award No. 06-1000019-5962.