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人工神经网络预测离子色谱分离条件

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Prediction of ion chromatographic separation condition by artificial neural network

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摘要 以EDTA为淋洗液,用均匀试验设计法研究了高Cl⁻浓度下Cl⁻与NO₂⁻,NO₃⁻的分离条件.将实验条件和实验结果作为BP神经网络的训练集,同时对网络的结构和训练速率进行筛选和优化.经过2567次训练后,网络训练误差达到10⁻⁵.对训练结果的考察表明,人工神经网络以较少的实验数据成功建立了离子色谱分离条件的预测模型,最大相对误差仅为0.85%.

关键词: 离子色谱法 人工神经网络 训练 相对误差

Abstract: The separation conditions of Cl⁻,NO₃⁻ and NO₂⁻ in high mass concentration of chloride are presented by uniform design.With experimental conditions and results as training collections, the architecture and learning rates of Back-Propagation Artificial Neural Network (BP-ANN) are optimized. Having been trained 2567 times, the errors of the network are in 10⁻⁵ order.The examination for the training results indicates that the artificial neural network sets up successfully the prediction models of ion chromatographic separation with less experimental data than those from general experimental method.The maximum relative error is only 0.85%.

Key words: ion chromatography artificial neural network training relative error

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