用局部拟合主成分回归计算光度分析法测定黄连生物碱

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摘要　针对具有样本数据非无匀分布和非线性特点的光度分析问题，提聘种局部拟合 主成分回归法，用于中药多组分计算测定。该方法根据待测样本与各已知样本光度 分析数据的欧式距离确定相应的权值，将部分权值较大的样本组成校正集，并用分 段线性拟合算法建立待测样本的校正预测模型，将其用于分析黄连的药根碱、巴巴 亭和小檗碱等三种生物碱，所得预测均方根误差分别为0.023,0.0400和0.052，优 于主成分回归法、偏最小二乘法以及人工神经元网络法所得结果。这表明，本方法 用于中药光度分析能获得较为准确的计算分析结果。

关键词　光度法　中药　小檗碱　生物碱　分光光度法

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Determination of Alkaloids of Coptis chinensis by Spectral Analysis Based on Local Fitting Principal Component Regression

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Abstract To determine multi-constituent of Traditional Chinese Medicine (TCM) by spectral analysis, a new method for establishing the calibration model of spectral data which is nonuniform distribution and nonlinear, named local fitting principal component regression (LFPCR), is proposed. The weight of eveiy sample in the known sample set is calculated according to the distance between the test set data and the known sample set data, and then a calibration set is composed of the samples with relatively greater weights. Based on the calibration set, the calibration model can be established by linear fitting of multi- section. Applying the proposed method to determining jtrorrhizine, plmatine and berberine of Coptis chinensis, the root mean square errors of prediction results obtained by LFPCR are 0.023, 0.040 and 0. 052 respectively, which are superior to those obtained by PCR, PLS and ANN. Therefore, the method can be used to determine multi-constituent of TCM at higher accuracy.

Key words　RHOTOMETRY　CHINESE DRUG　BERBERINE　ALKALOID　SPECTROPHOTOMETRY

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