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现代应用光学

可见-近红外光谱测定血红蛋白的等效波段选择

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摘要： 将可见-近红外光谱和改进的移动窗口偏最小二乘(MWPLS)方法应用于人类血红蛋白(HGB)无试剂快速检测的高精度波段优选。为了避免模型评价失真,提出了一种新的模型评价体系。首先,从全体205个样品中随机抽取70个作为检验集,余下的135个作为建模集,并划分为具有相似性的定标集(80个样品)和预测集(55个样品)共50次;其次,对每一次划分都分别建模和优化,使得模型具有稳定性;最后,利用检验集对优选出的模型进行再次检验。实验结果表明:可见-短波近红外波段400~1100 nm可以作为人体全血HGB的信息波段;进一步采用MWPLS方法从400~1100 nm中选出全局最优波段为492~890 nm,并得到包含77个等效波段的模型空间。以492~890 nm为例,检验效果预测均方根偏差(V-SEP)、预测相关系数(V-RP)和相对预测均方根偏差(V-RSEP)分别为2.58 g L^{-1}、0.988和1.97%,得到的样品的HGB预测值与临床实测值吻合精度很高,可望应用于临床。

关键词： 人类全血 血红蛋白 VIS-NIR光谱 波段选择 等效模型空间

Equivalent waveband selection of VIS-NIR spectroscopic measurement for hemoglobin

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Abstract: The VIS-NIR spectroscopy combined with the improved Moving Window Partial Least-square (MWPLS) method was applied to a high accurate waveband selection for the rapid no-reagent determination of Hemoglobin (HGB) in human whole blood. A new modeling evaluation system was proposed to avoid the evaluation distortion. First, seventy samples were randomly selected from a total of 205 samples as the validation set,the remaining 135 samples were used as the modeling set, and the modeling set was divided into similar calibration (80 samples) and prediction (55 samples) sets for a total of 50 times.Then, modeling and optimization were performed in each division to get stable model. Finally, the optimized model was validated again using the validation set. Experimental results indicate that the VIS-short NIR region 400-1 100 nm can be used as the information waveband of HGB in human whole blood, the global optimal waveband 492-890 nm is further selected from 400-1100 nm with MWPLS method, and a model space including 77 equivalent wavebands is obtained. By taking the 492-890 nm for an example, validation effects V-SEP, V-RP, and V-RSEP are 2.58 g L^{-1}, 0.988, and 1.97%, respectively. It concludes that HGB prediction values of the samples are highly close to the clinic measured values, which may be used in clinical diagnosis.

Keywords: human blood hemoglobin VIS-NIR spectroscopy waveband selection equivalent model space

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