Optimal Partner Wavelength Combination Method Applied to NIR Spectroscopic Analysis of Human Serum Globulin

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Yun Han
Guangdong Ocean university

hanyun0539@163.com*Corresponding Author*

Yun Zhong
Zhanjiang No.2 High School Hai Dong

Huihui Zhou
Guangdong Ocean University

Xuesong Kuang
Guangdong Ocean University

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Abstract

Human serum globulin (GLB), which contains various antibodies in healthy human serum, is of great significance for clinical trials and disease diagnosis. In this study, the GLB in human serum was rapidly analyzed by near infrared (NIR) spectroscopy without chemical reagents. Optimal partner wavelength combination (OPWC) method was employed for selecting discrete information wavelength. For the OPWC, the redundant wavelengths were removed by repeated projection iteration based on binary linear regression, and the result converged to stable number of wavelengths. By the way, the convergence of algorithm was proved theoretically. Moving window partial least squares (MW-PLS), a well-performed wavelength selection method, was also performed for comparison.

The optimal models were obtained by the two methods, and the corresponding root-mean-square error of cross validation and correlation coefficient of prediction (SECV, RP,CV) were 0.813 g·L-1 and 0.978 with OPWC combined with PLS (OPWC-PLS), and 0.804 g L-1 and 0.979 with MW-PLS, respectively. The two methods achieved almost the same good results. However, the OPWC only contained 28 wavelengths, so it had obvious lower model complexity. Thus it can be seen that the OPWC-PLS has great prediction performance for GLB and its algorithm is convergent and rapid. The results provide important technical support for the rapid detection of serum.

Full Text

Due to technical limitations, full-text HTML conversion of this manuscript could not be completed. However, the manuscript can be downloaded and accessed as a PDF.

Figures

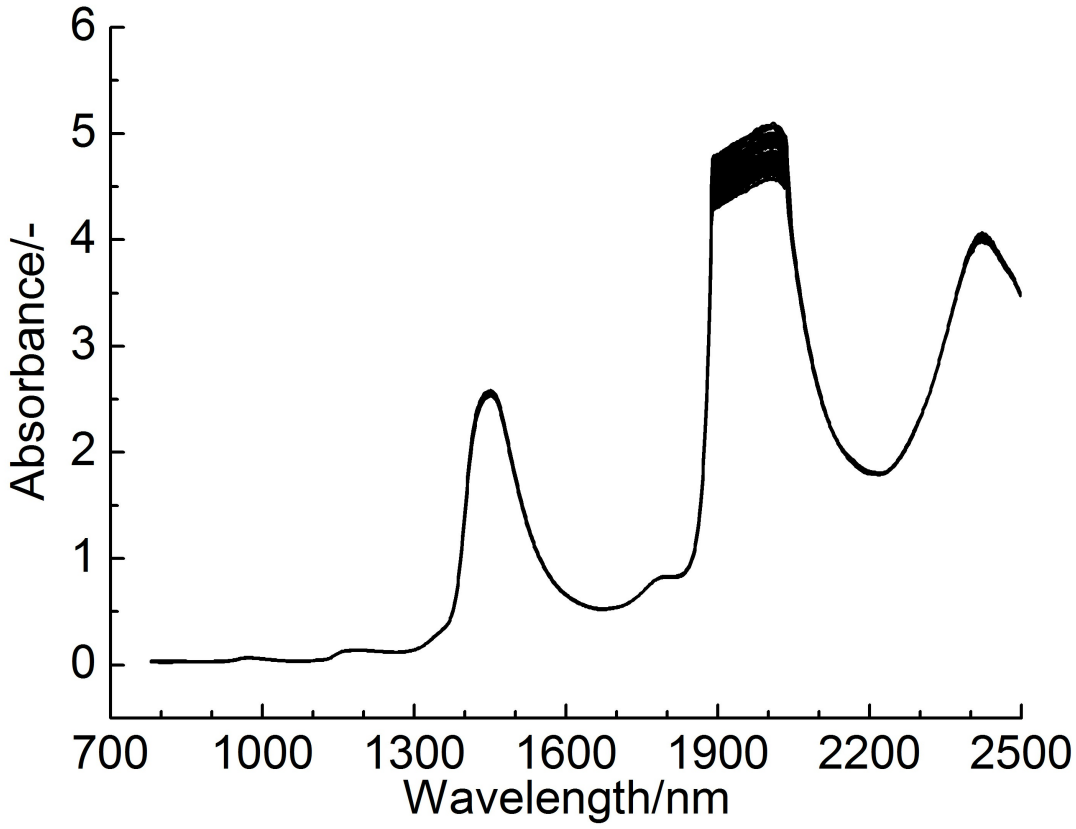


Figure 1

NIR spectra of 230 human serum samples in the scanning area (780-2498 nm).

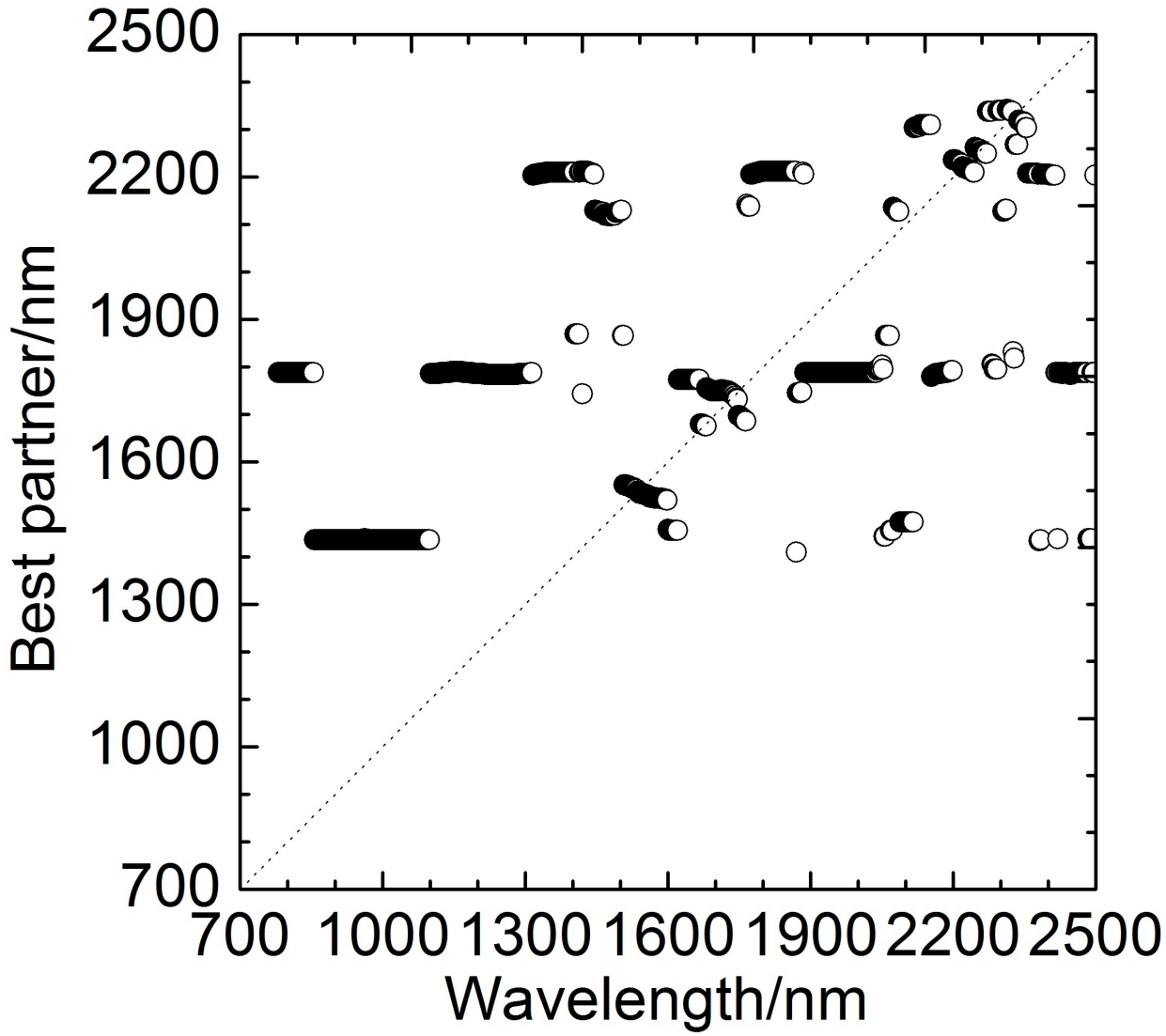


Figure 2

Best partners of 860 wavelengths in the full spectrum region.

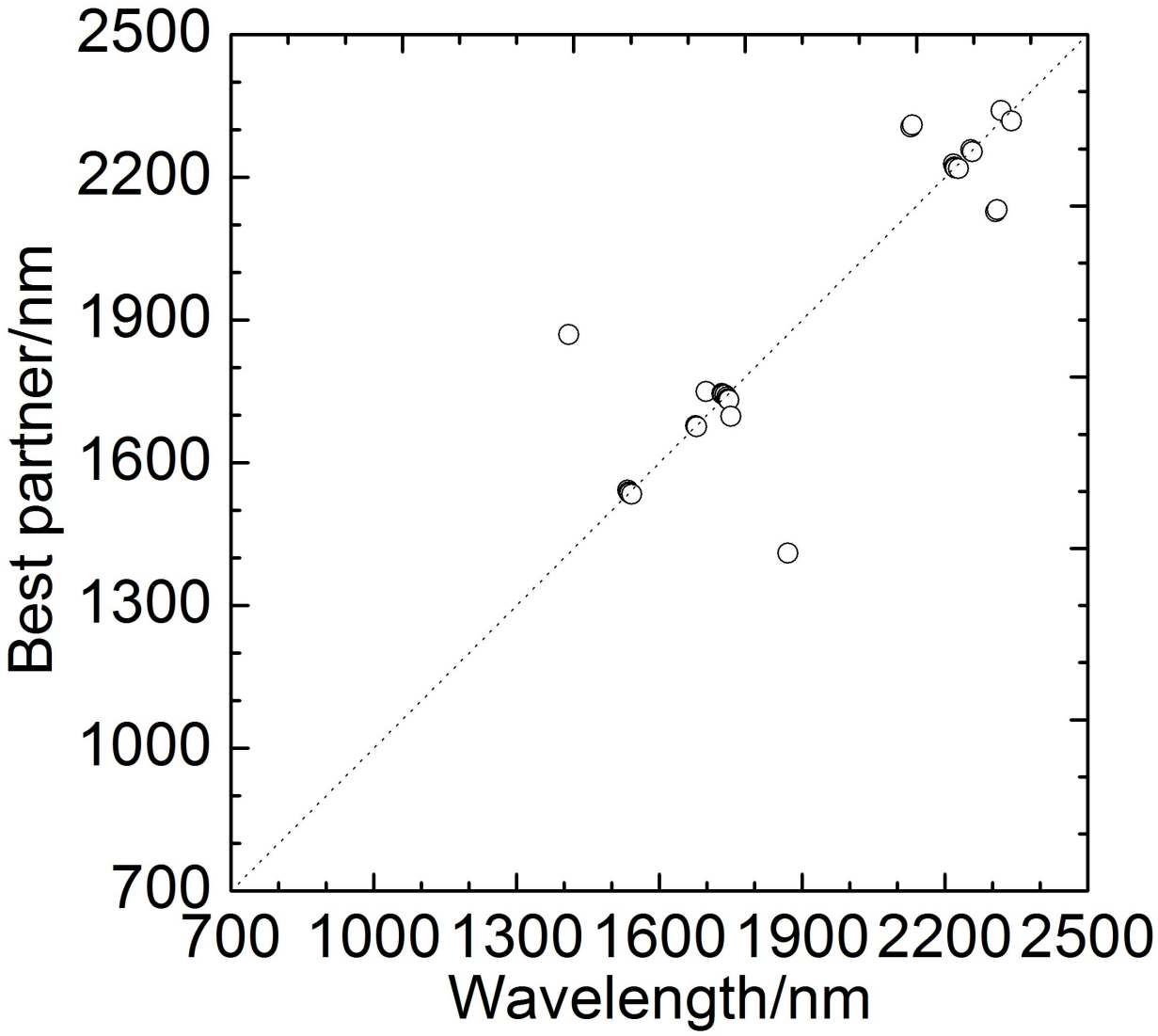


Figure 3

Best partners of the selected 28 wavelengths.

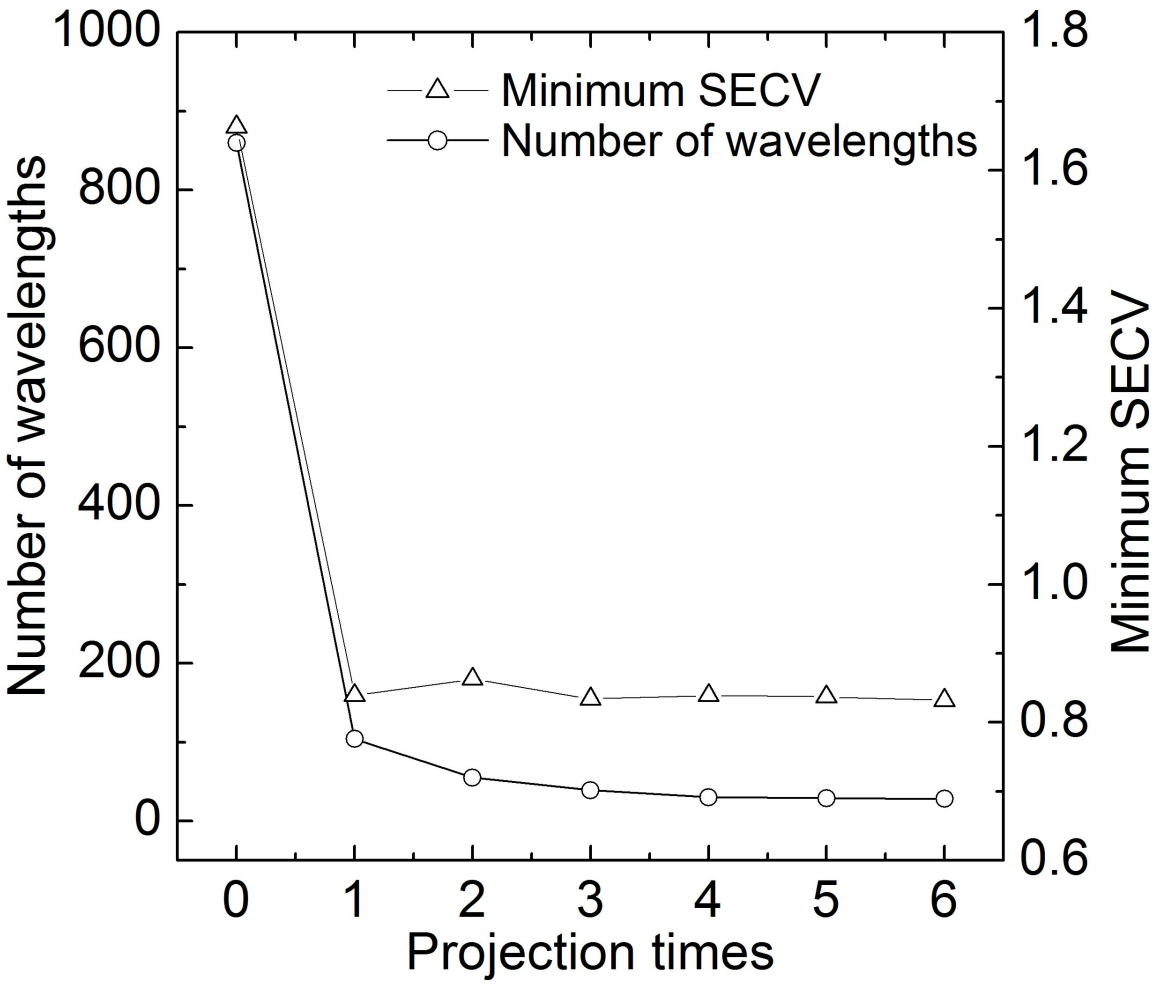


Figure 4

Number of wavelengths and minimum SECV value for each projection.

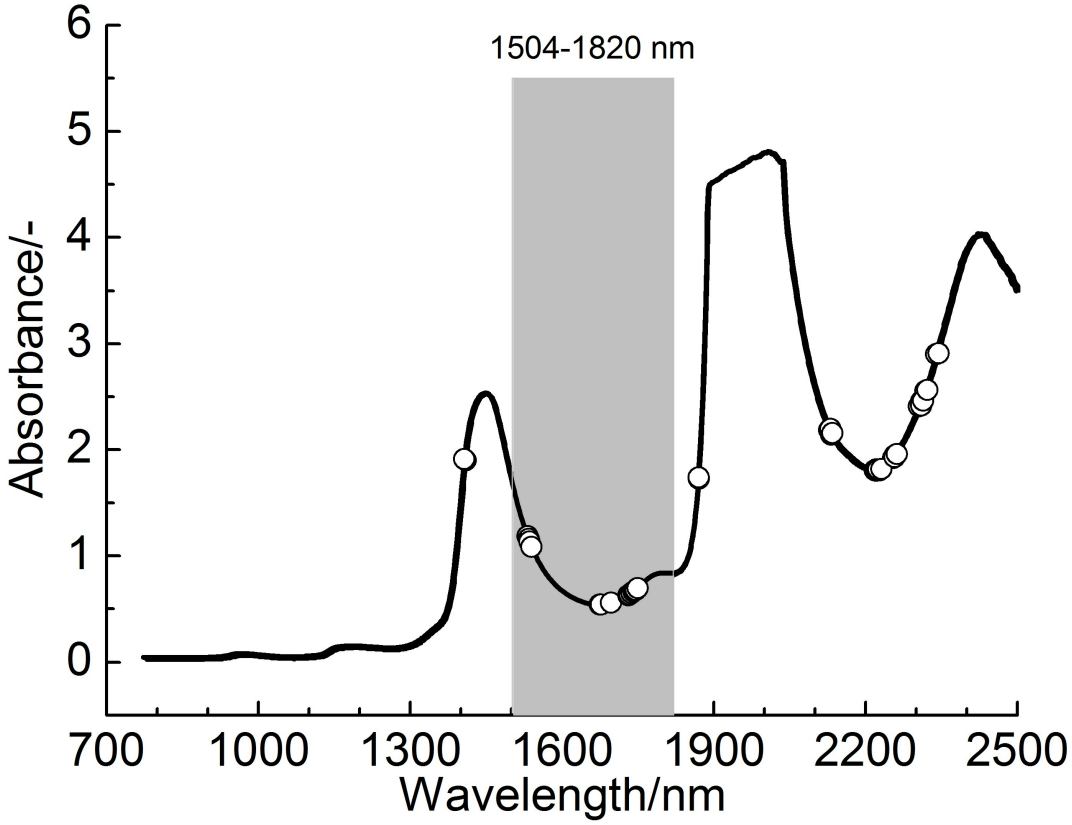
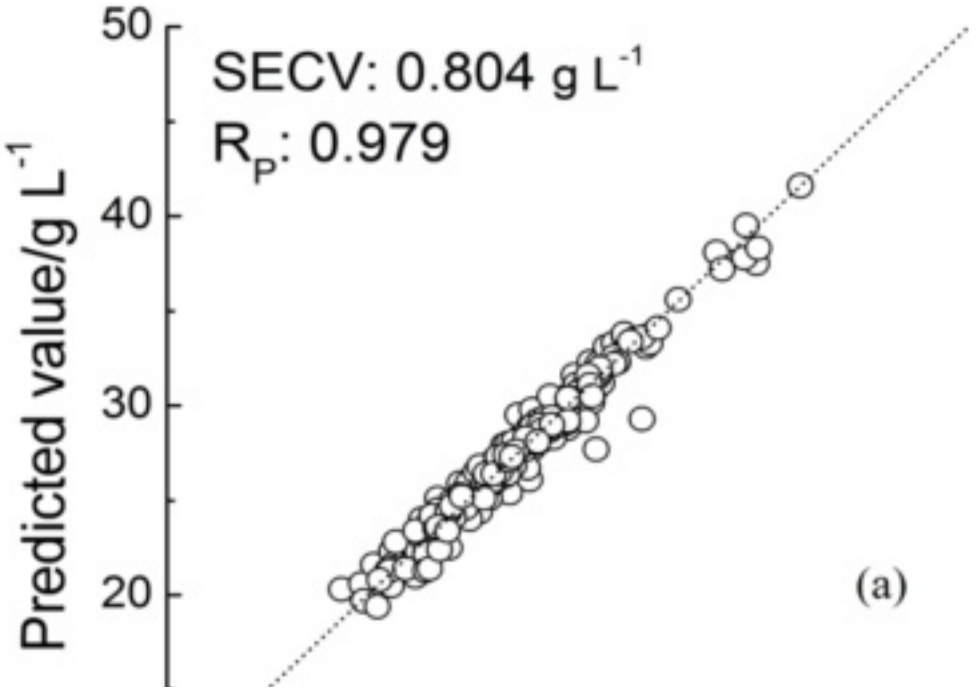


Figure 5

Position of the selected wavelengths with MW-PLS and OPWC-PLS located the average spectrum.



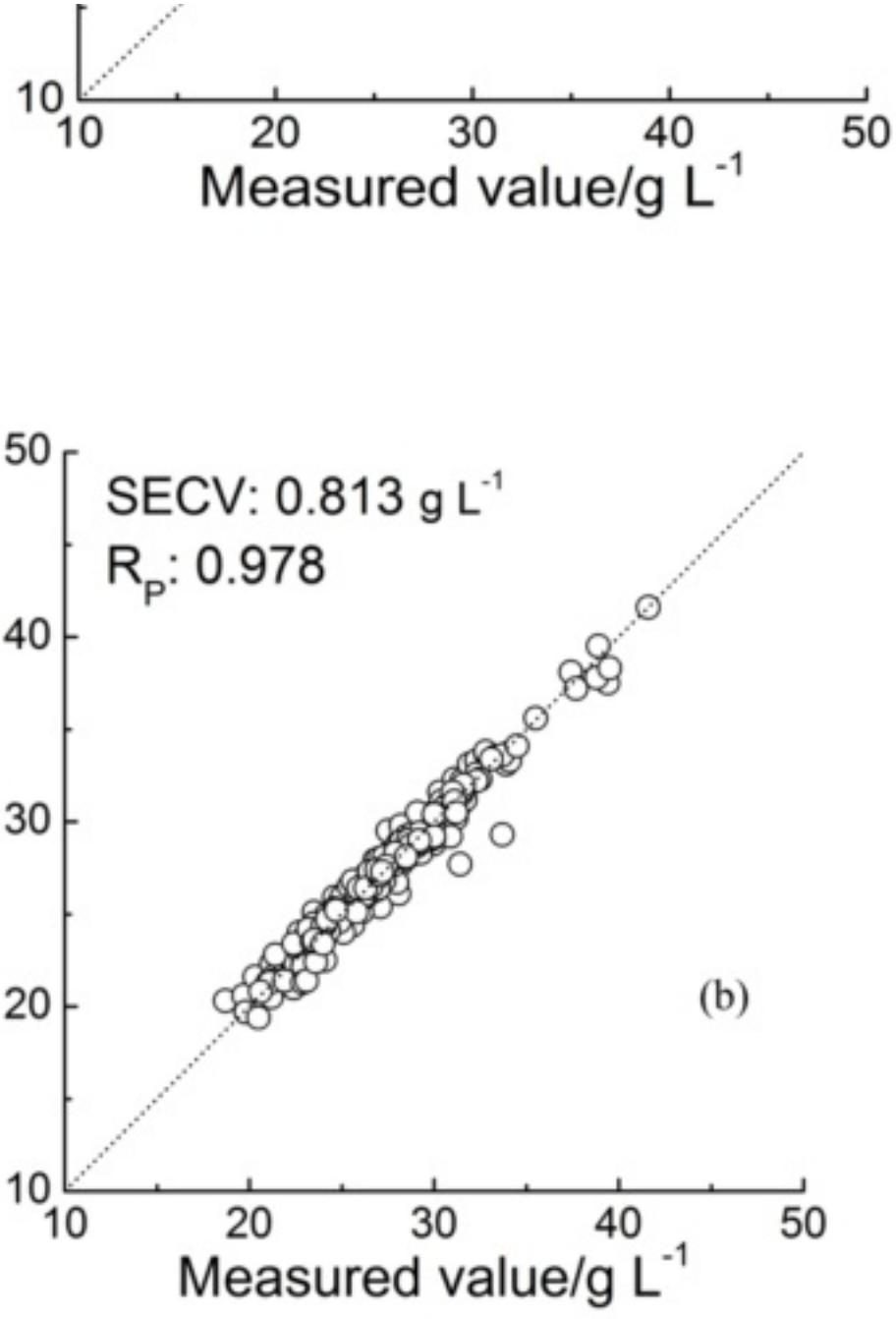


Figure 6

Relationship between the predicted values and measured values of GLB based on (a) MW-PLS and (b) OPWC-PLS methods.