Electronic Supplementary Material (ESI) for Analytical Methods.

Electronic Supplementary Information (ESI)

Baseline Correction for Raman Spectra Using Improved Asymmetric Least Squares

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Choosing of suitable values for parameters. For each pair of parameters (p , λ_1 and λ), a baseline was estimated and the *RMSE* of the proposed method was computed. Figure 1S shows that the performance of IAsLS while varying the parameters λ_1 and λ , p keeps unchanged otherwise, say $p = 0.001$. It is found that, when $\lambda_1 \le 10^{-4}$, the *RMSE* performance is affected very little with the choice of parameter λ_1. And then, the *RMSE* reaches its minimum value when the value of λ is up to $\lambda = 10^5$. Finally, the baseline estimated is shown in Figure S2. Figure S3 shows that the performance of IAsLS while varying the parameter p , whereas λ_1 and λ keep unchanged simultaneously, say $\lambda = 10^5$, $\lambda_1 = 10^{-4}$.And the baseline estimated with the more appropriate parameters is shown in Figure S4.The simulation shows that, in order to obtain the optimal performance, the value of p should be set to less than 0.1, and the range of λ value to 10^2 to 10^6, and the range of λ_1 value to less than 10^{-4}.

Abbreviations: IAsLS, Improved asymmetric least square; AsLS, Asymmetric least square; RMSE, Root Mean Square Error; JAsLS, Jiang's asymmetric least square baseline correction method

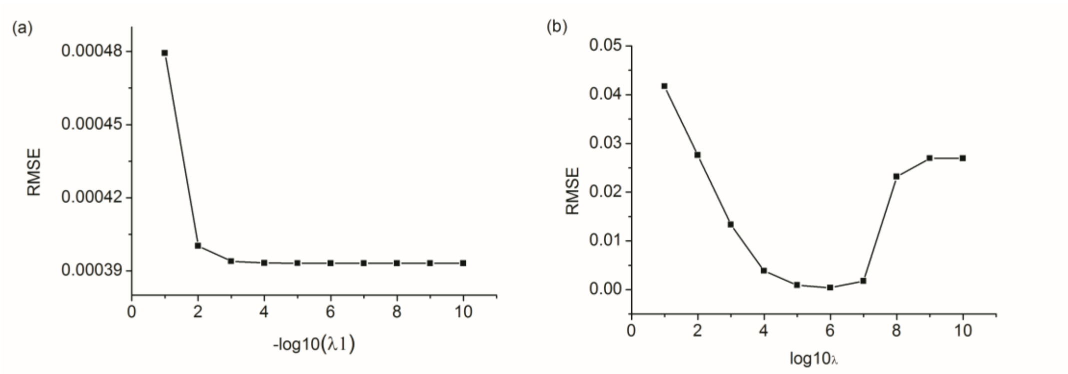


Figure S1 The *RMSE* of the IAsLS method when varying the parameters λ_1 and λ, $p = 0.001$

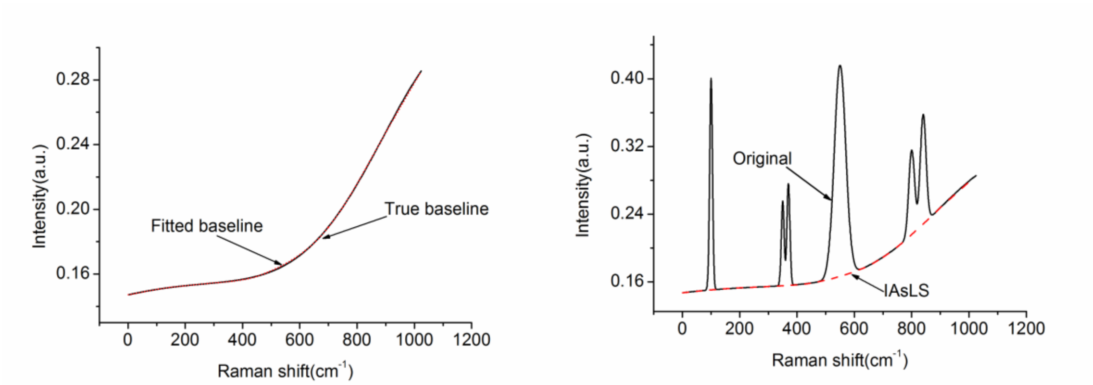


Figure S2 Baseline correction result based on the IAsLS method ($p = 0.001, \lambda = 10^5$, $\lambda_1 = 10^{-4}$, $RMSE = 0.0004$)

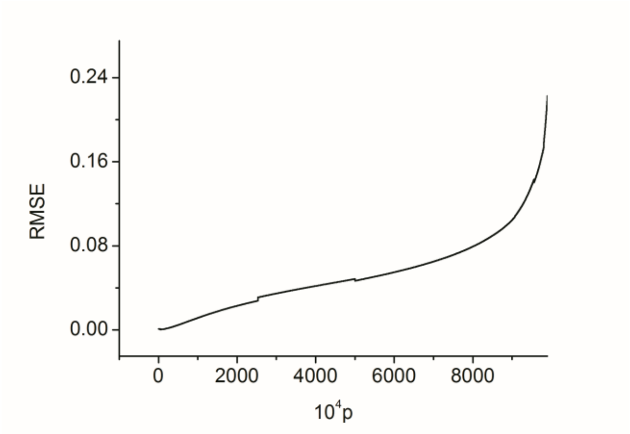


Figure S3 The *RMSE* of the IAsLS method when varying the parameter p, $\lambda = 10^5$, $\lambda_1 = 10^{-4}$

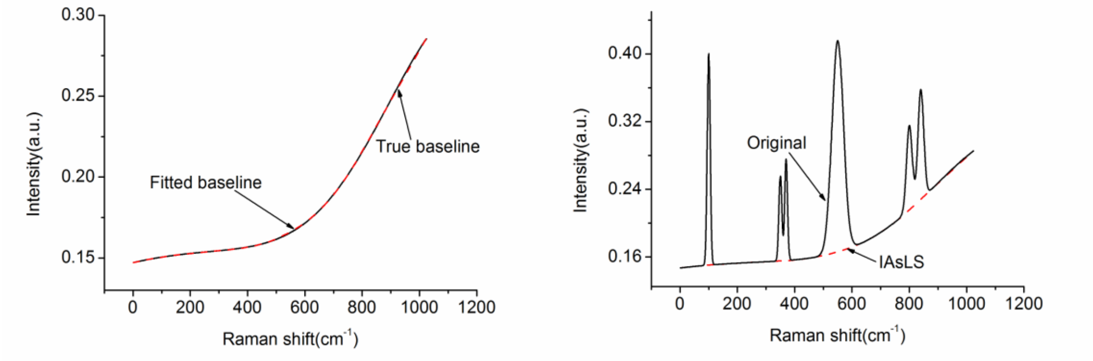
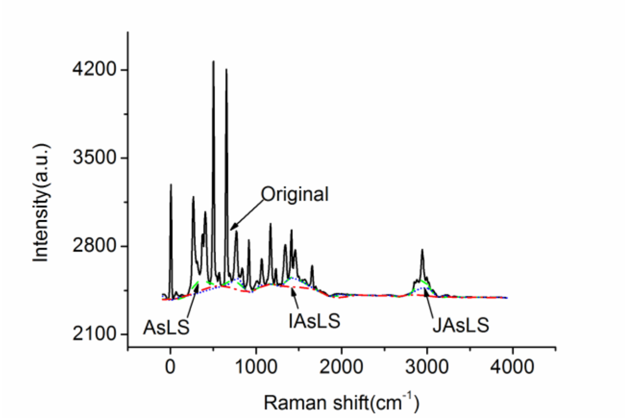


Figure S4 Baseline correction result based on the IAsLS method ($\lambda = 10^5$, $\lambda_1 = 10^{-4}$, $p = 0.0043$, $RMSE = 0.00036$)

Results for the three baseline correction methods. Figure S5 and Figure S6 show that the effect of the three baseline correction methods on spectra for dimethoate solution and solid Rhodamine6G respectively. The results show that IAsLS is able to remove the fluorescence signal better comparing with the other two methods (Figure S5-S6), but not over-fitted. Above all, both of these irrelevant spectral disturbances can be removed well by the IAsLS baseline correction.



FigureS5 Original spectrum and the results of baseline correction methods for dimethoate solution ($\lambda = 10^2$, $\lambda_1 = 10^{-5}$, $p = 0.001$)

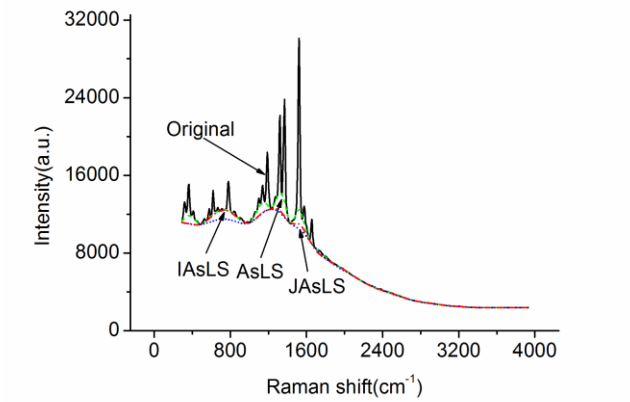


Figure S6 Original spectrum and the results of baseline correction methods for solid Rhodamine6G ($\lambda = 10^2$, $\lambda_1 = 10^{-5}$, $p = 0.01$)