

Supplementary information

1. Corn dataset:

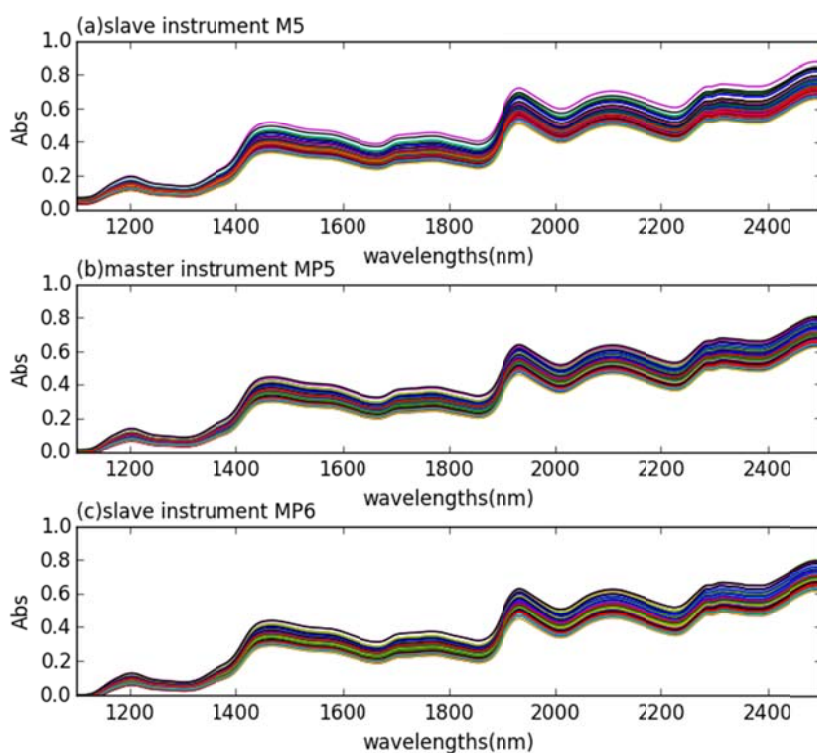


Fig S-1. (a) Spectra of corn samples scanned on M5 instrument; (b) Spectra of corn samples scanned on MP5 instrument. (c) Spectra of corn samples scanned on MP6 instrument.

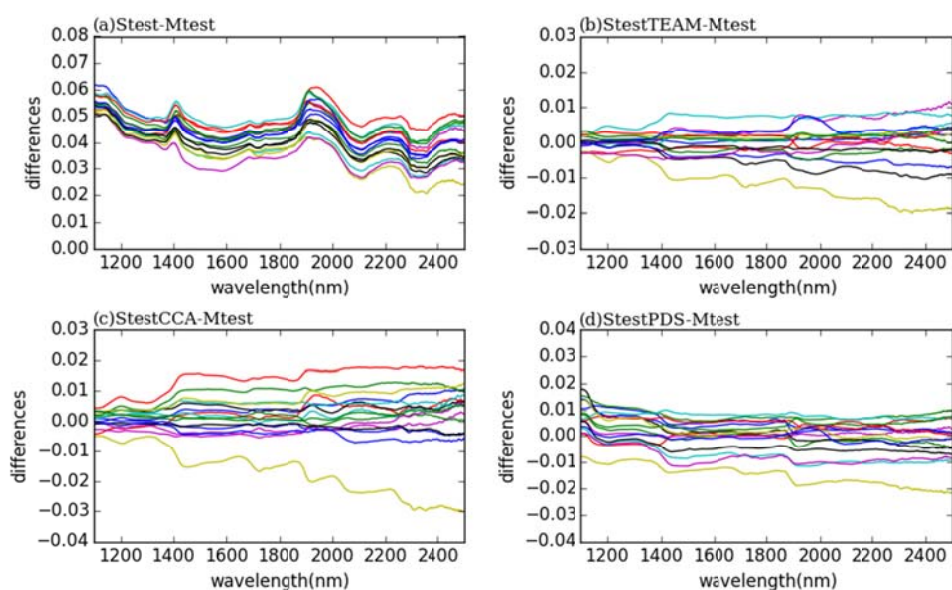


Fig S-2. (a) Spectral differences between the instruments M5 and MP5 of 16 corn samples(N=40); (b) Spectral differences between the transfer spectra by TEAM and MP5; (c) Spectral differences between the transfer spectra by CCA and MP5; (d) Spectral differences between the transfer spectra by PDS and MP5.

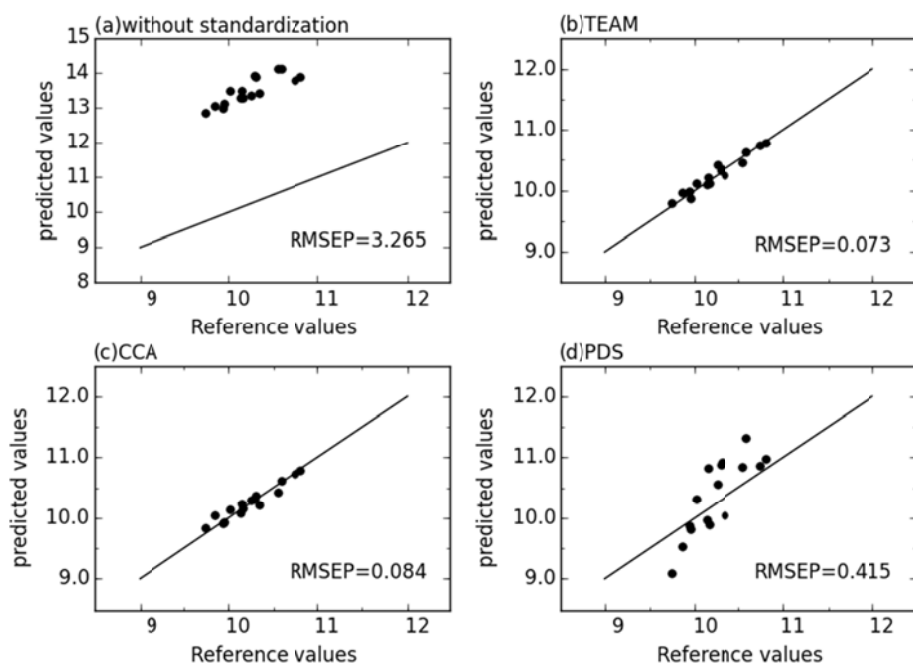


Fig S-3. Scatter plots for prediction of 16 corn samples on M5 instrument with calibration on MP5 instrument(N=40); (a) Without standardization, (b) TEAM standardization, (c) CCA standardization, (d) PDS standardization

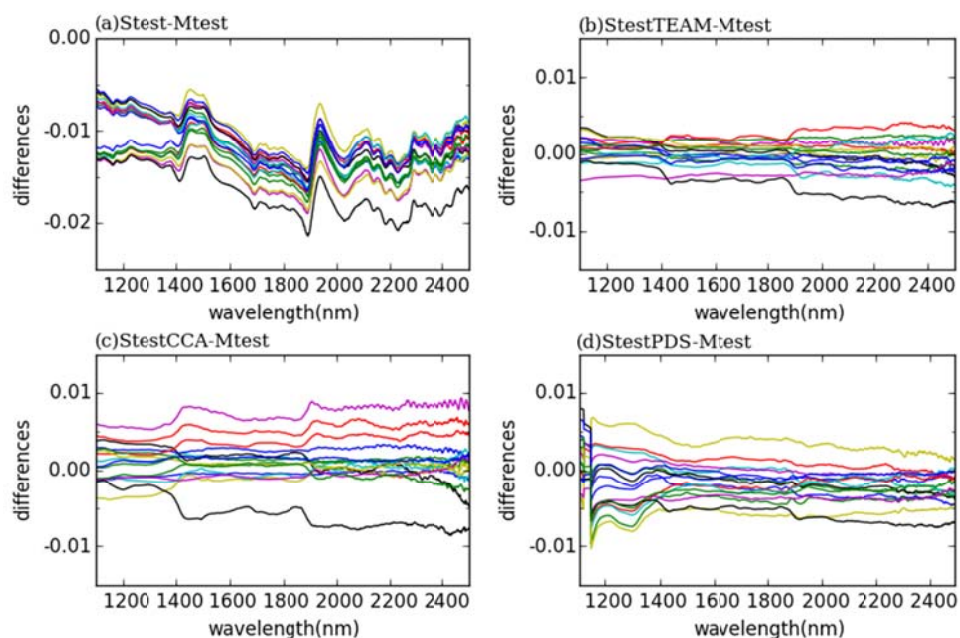


Fig S-4. (a) Spectral differences between the instruments MP6 and MP5 of 16 corn samples(N=40); (b) Spectral differences between the transfer spectra by TEAM and MP5 (c) Spectral differences between the transfer spectra by CCA and MP5; (d) Spectral differences between the transfer spectra by PDS and MP5.

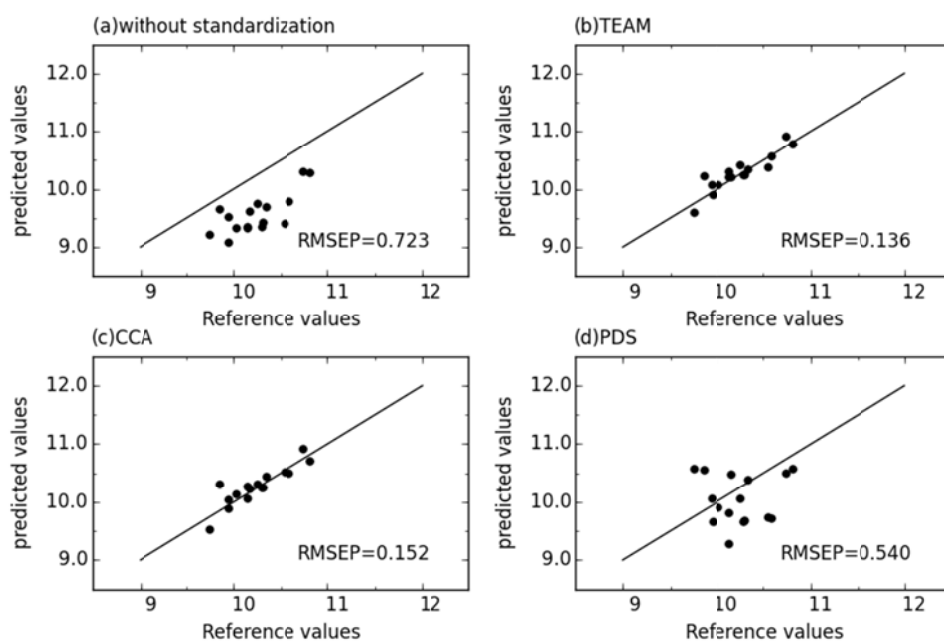


Fig S-5. Scatter plots for prediction of 16 corn samples on MP6 instrument with calibration on MP5 instrument(N=40); (a) Without standardization, (b) TEAM standardization, (c) CCA standardization, (d) PDS standardization

2. Tobacco datasets

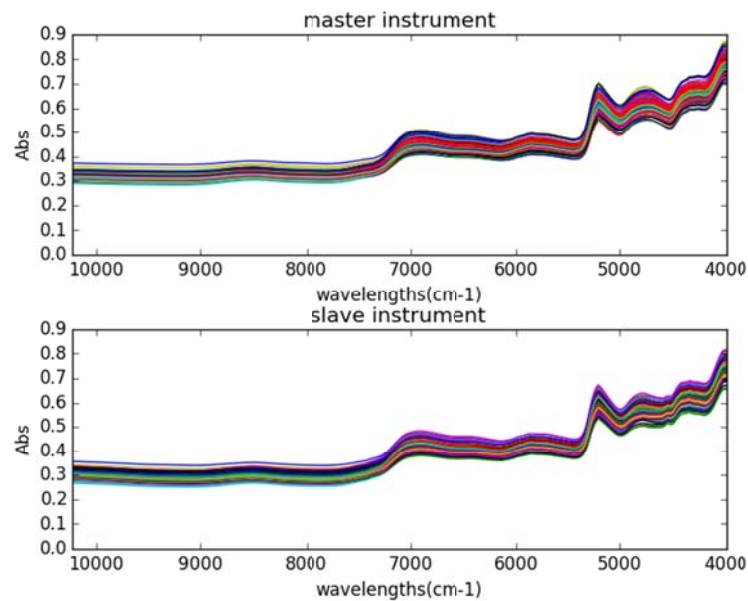


Fig S-6. (a) Spectra of tobacco samples scanned on master instrument M; (b) Spectra of tobacco samples scanned on slave instrument S.

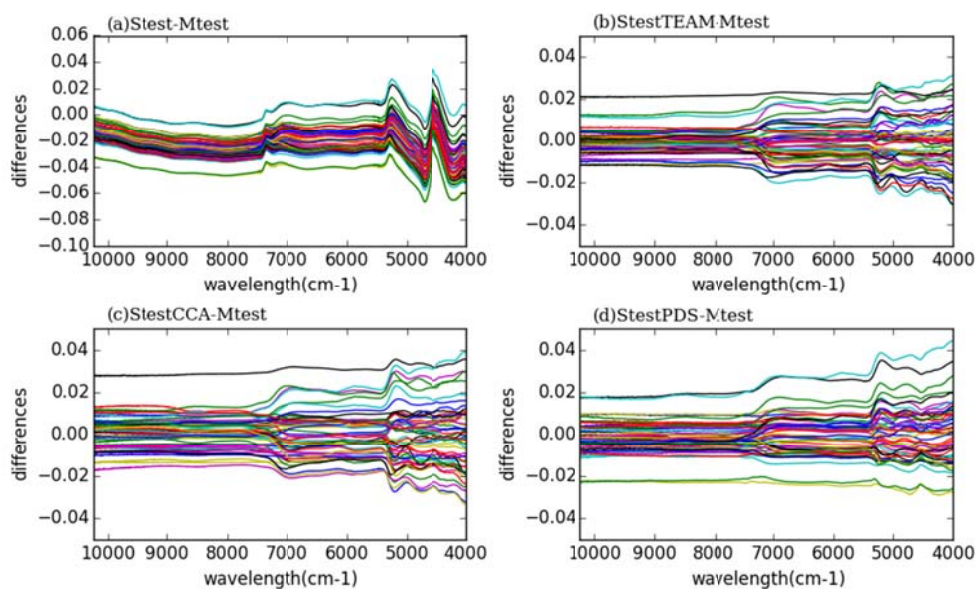


Fig S-7. (a) Spectral differences between the instruments S and M of 52 tobacco

samples(N=40); (b) Spectral differences between the transfer spectra by TEAM and M; (c) Spectral differences between the transfer spectra by CCA and M; (d) Spectral differences between the transfer spectra by PDS and M.

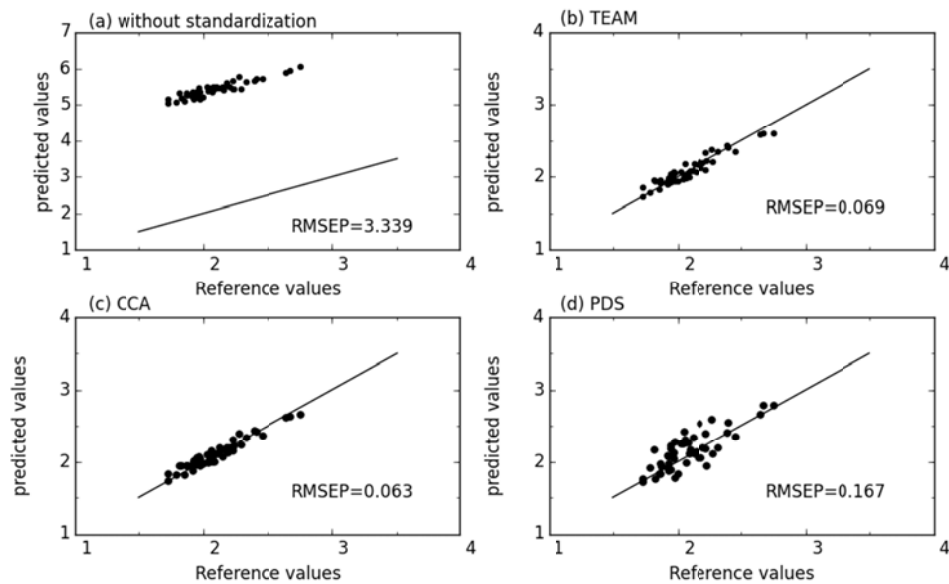


Fig S-8. Scatter plots for prediction of 52 tobacco samples on S instrument with calibration on M instrument(N=40); (a) Without standardization, (b) TEAM standardization, (c) CCA standardization, (d) PDS standardization

3. Pharmaceutical tablets datasets

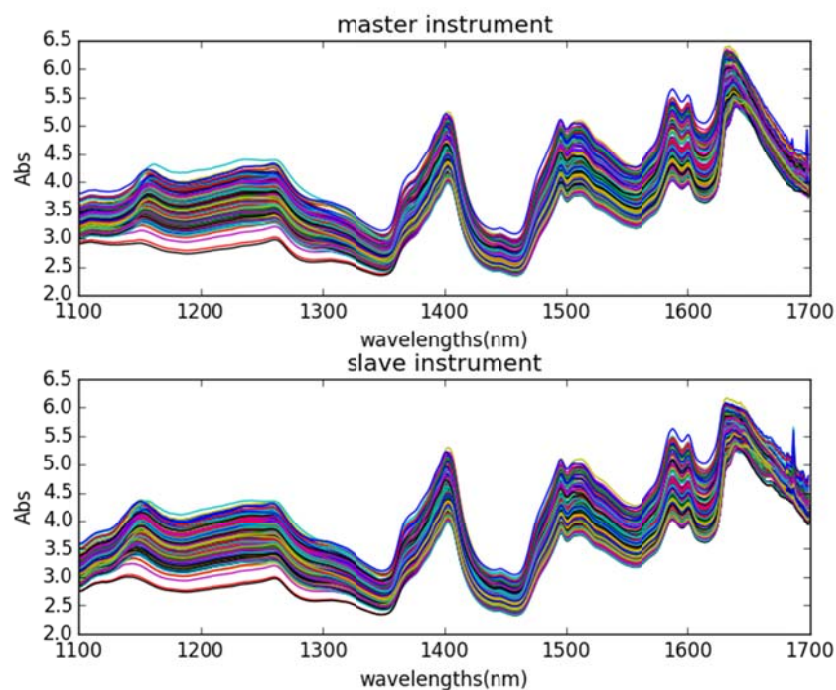


Fig S-9. (a) Spectra of pharmaceutical tablets samples scanned on M instrument; (b) Spectra of corn samples scanned on S instrument.

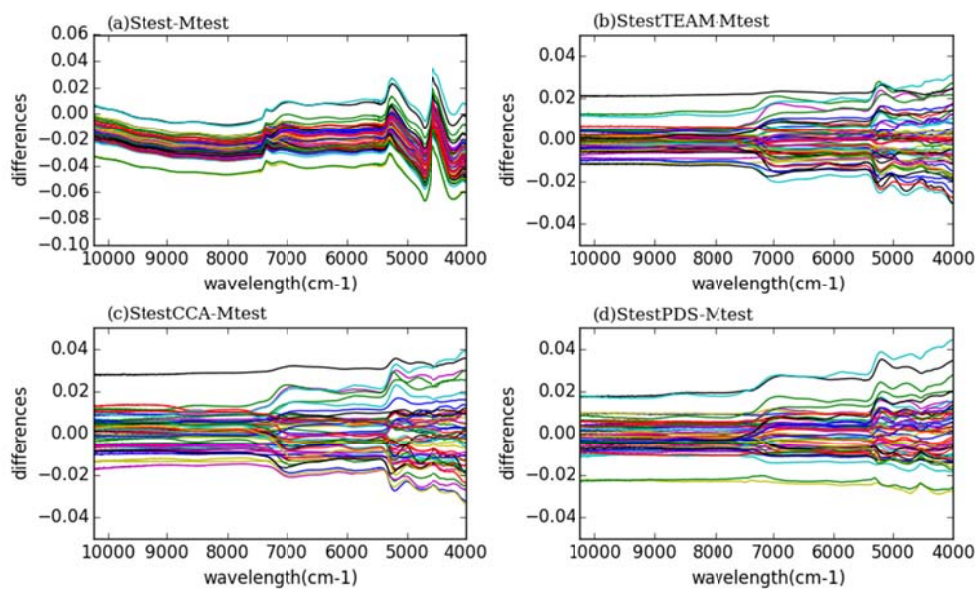


Fig S-10. (a) Spectral differences between the instruments S and M of 155 pharmaceutical tablets samples(N=55); (b) Spectral differences between the transfer spectra by TEAM and M; (c) Spectral differences between the transfer spectra by CCA and M; (d) Spectral differences between the transfer spectra by PDS and M.

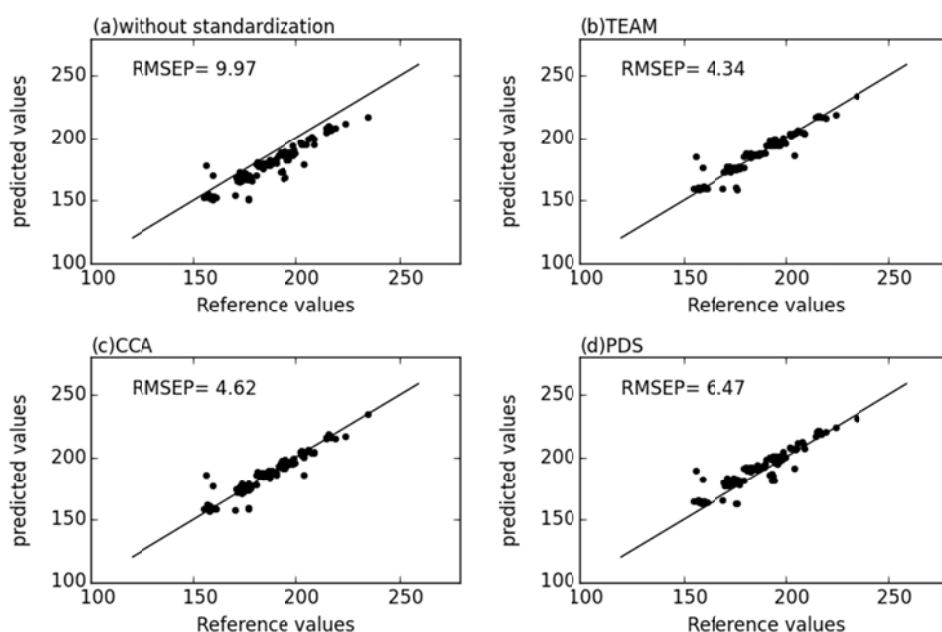


Fig S-11. Scatter plots for prediction of 155 pharmaceutical tablets samples on S instrument with calibration on M instrument(N=55); (a) Without standardization, (b) TEAM standardization, (c) CCA standardization, (b) PDS standardization

4. Stability of ensemble ELM-AEs

In order to show TEAM method is stable, we have trained 2000 ensemble ELM-AEs, for each ELM-AE the weights and biases of the hidden nodes were randomly generated and the number of hidden nodes was randomly selected from 300 to 500 for 10 times. Then the distribution of the RMSEPs of these ELM-AEs can be obtained.

Fig S-12 shows the distribution of the RMSEPs from M5 transfer to MP5 with 30 standardization samples. T-test was performed and at the significance level $\alpha = 0.05$, the mean of RMSEP obtained with TEAM is significantly less than the RMSEP obtained with PDS and CCA. The variance of the distribution is 0.00073.

Fig S-13 shows the distribution of the RMSEPs from MP6 transfer to MP5 with 30 standardization samples. T-test was performed and at the significance level $\alpha = 0.05$, the mean of RMSEP obtained with TEAM is significantly less than the RMSEP obtained with PDS and CCA. The variance of the distribution is 0.00056.

Fig S-14 shows the distribution of the RMSEPs of pharmaceutical tablets dataset with 40 standardization samples. T-test was performed and at the significance level $\alpha = 0.05$, the mean of RMSEP obtained with TEAM is significantly less than the RMSEP obtained with PDS and CCA. The variance of the distribution is 0.00029.

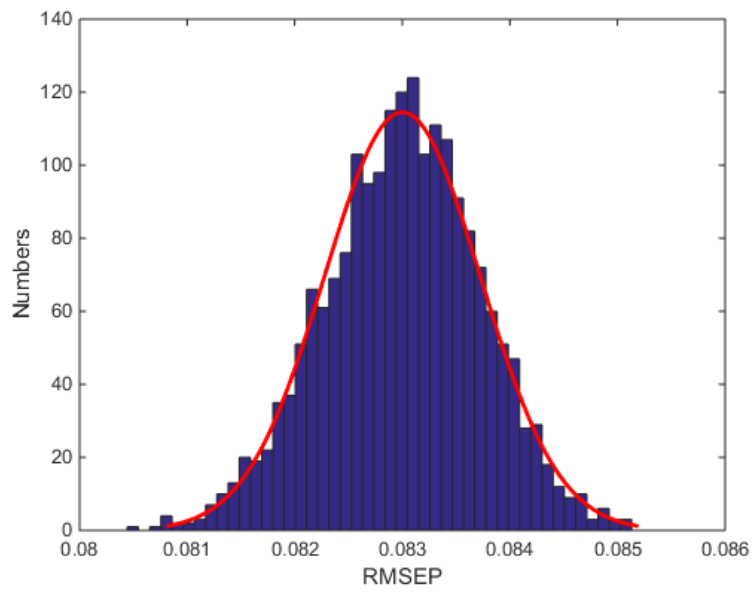


Fig S-12.The distribution of RMSEP from M5 transfer to MP5 with 30 standardization samples for ELM-AEs with different hidden nodes numbers and different weights and biases.

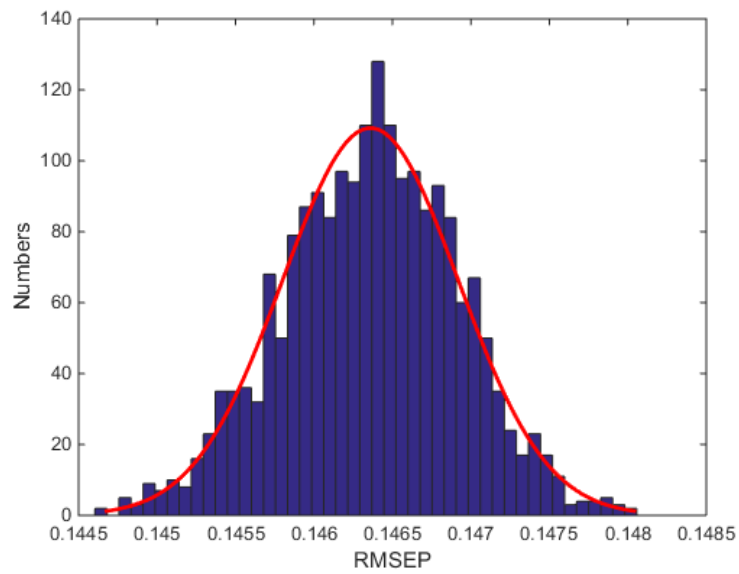


Fig S-13.the distribution of RMSEP from MP6 transfer to MP5 with 30 standardization samples for ELM-AEs with different hidden nodes numbers and different weights and biases.

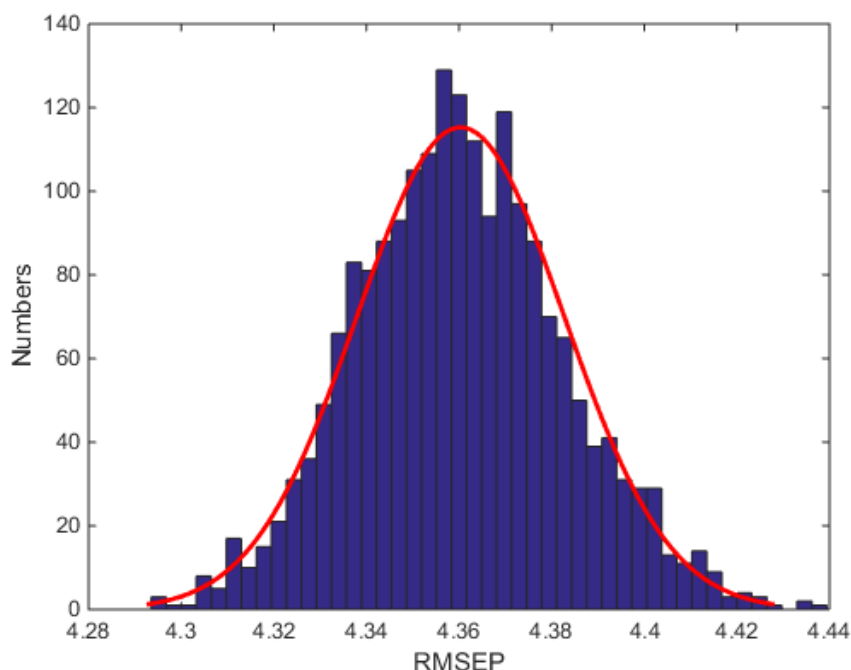


Fig S-14.the distribution of RMSEP of pharmaceutical tablets datasets with 40 standardization samples for ELM-AEs with different hidden nodes numbers and different weights and biases.

5. Optimize the regularization parameter C

FigS-15 and FigS-16 below show the variation trend of RMSEP with the change of C on corn datasets (from MP6 transfer to MP5) and tobacco datasets, with the growth of C, the RMSEP value is decrease and trend to be steady. So, for corn and tobacco datasets, we choose regularization parameter C as 50000. But for pharmaceutical tablets datasets, from the FigS-17, we can find the RMSEP get minimize values when C is 500, so for pharmaceutical tablets datasets, we choose regularization parameter C as 500. But for pharmaceutical tablets datasets, the variation range of RMSEP on validation set is very small, so even choose regularization parameter C as 50000, we can still get good performance for TEAM method on independent test set. So for suggestion, when use TEAM, the default value of regularization parameter C can be set as 50000. But readers can also optimize the regularization parameter C based on the RMSEP value on validation set.

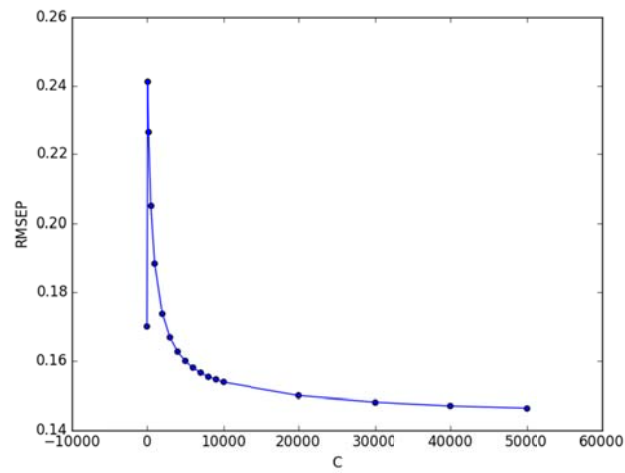


Fig S-15 the variation trend of RMSEP with the change of regularization parameter C of corn (from MP6 transfer to MP5) dataset with 20 standardization samples.

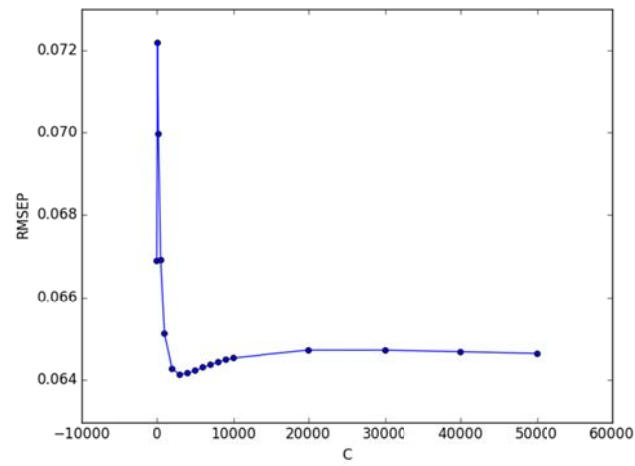


Fig S-16 the variation trend of RMSEP with the change of regularization parameter C of tobacco dataset with 50 standardization samples.

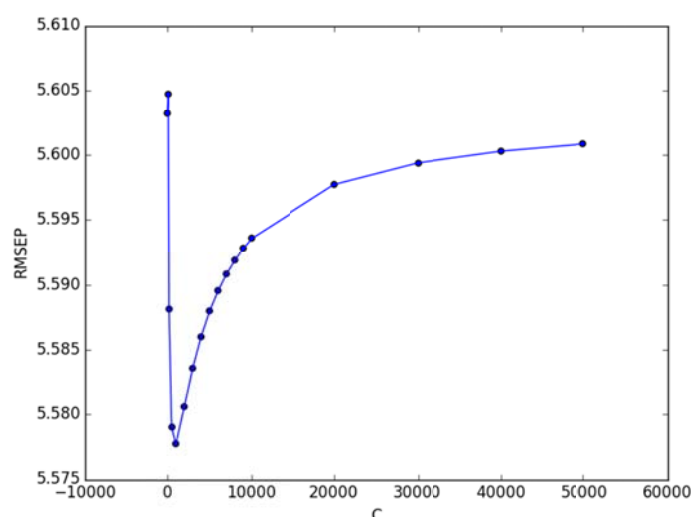


Fig S-17 the variation trend of RMSEP with the change of regularization parameter C of pharmaceutical tablets dataset with 40 standardization samples.

6. Optimize number of hidden neurons and choose a correct interval

In TEAM method, though we select a relatively high number of hidden nodes, but it will not suffer from the over-fitting problem.

In principle, for the process project the input data to hidden layer, this process will not result in overfitting problem, and for the process from hidden layer to output layer, Moore-Pensore generalized inverse was get, in order to prevent overfitting problem a regularization term was added.

To testify it, we select hidden nodes from 0 to 500 on corn samples (from M5 transfer to MP5 (N=25)), for each hidden nodes, train ELMs and one can get the RMSEP values on validation sets. From the Fig S-18 below, when hidden nodes is less than 65, as in ELM-AE the weights and biases of the hidden nodes should be orthogonal to improve the generalization performance, the weights cannot be orthogonalized, so TEAM cannot be implied on lower hidden nodes. And with the growth of hidden nodes, the performance of ELM-AE is tend to stable and after the hidden nodes is large than 300, the RMSEP is fluctuating in a very small range around a stable value about 0.09. So even for each hidden nodes number large than 300, the performance of TEAM is better than other calibration transfer method, but in order to make TEAM be robust, we training multiple ELMs with the hidden nodes range from 300 to 500. Based on each ELM-AE, the transfer spectra can be get, Get the average transfer from a series of transfer spectra which is the transfer spectra from the slave instrument to master instrument.

In TEAM, the dimension of the ensemble is set as 50 which is an empirical value, in fact when we

choose the dimension of the ensemble is 10 or even 1, the performance of TEAM is good, the dimension of the ensemble is not an important parameter that need to be optimized, the only function of it is to make the TEAM be more robust. From the Fig.4 and Fig S-12, Fig S-13, Fig S-14 in article and supplementary information, it shows clearly that TEAM is a stable transfer method when the number of hidden nodes for each ELM-AE is randomly selected from 300 to 500 for 10 times. It demonstrate that the dimension of the ensemble can be selected in large range of options.

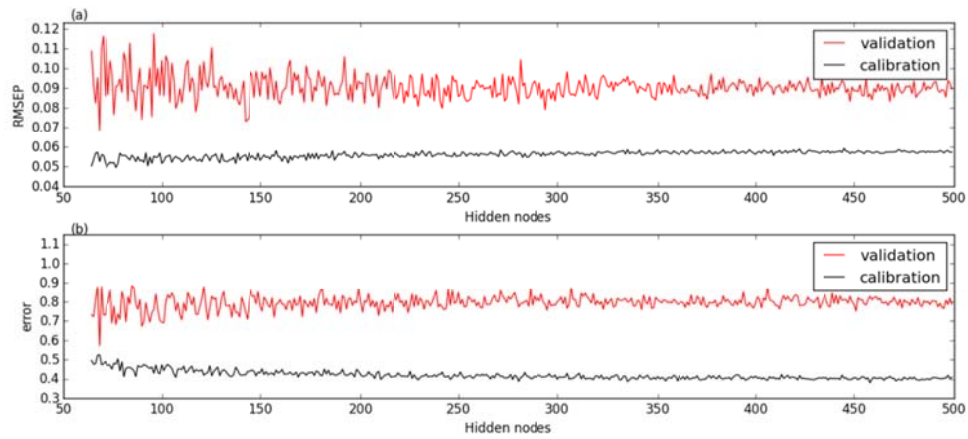


Fig S-18. (a)the variation trend of RMSEP with the change of hidden nodes on corn (from M5 transfer to MP5(N=25)) on validation set and calibration set; (b) the variation trend of error with the change of hidden nodes on validation set and calibration set.