S450 near infrared spectral instrument model test report

Two grating scanning S450 Near Infrared Spectroscopy Analyzer produced by Shanghai Lengguang Technology Co., Ltd. and an FT near infrared spectrum analyzer are used to collect near infrared spectra of 72 samples of wheat with known crude protein chemical values. Modeling using CAUNIRS software developed by Near Infrared Analysis Laboratory of China Agricultural University. The test items include: spectrogram, instrument model performance contrast, instrument model stability test, different instruments model transfer test, and long term stability of instrument wavelength accuracy.

One.Contrast of spectrogram

With grating instrument and FT instrument repeated measurement of wheat samples two times, the original spectrum and the first derivative spectra comparison as shown in figure 1.
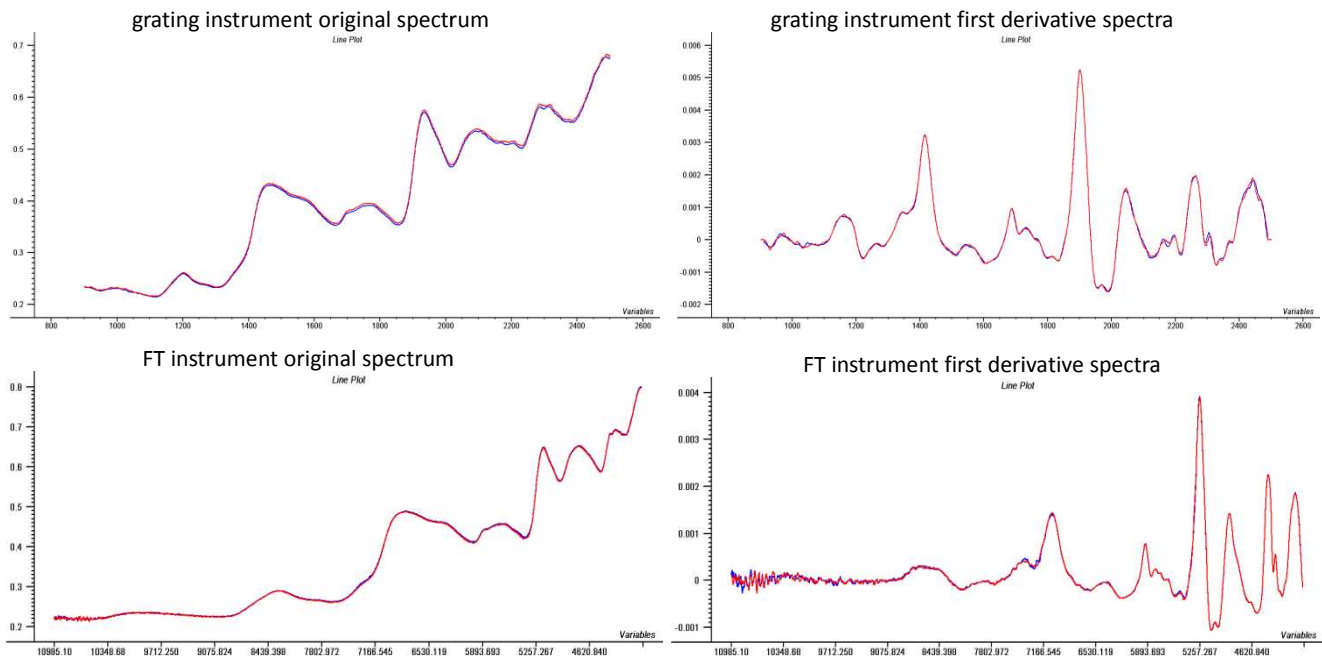

Fig. 1: spectral comparison of grating and FT instruments

Two. Comparison of the performance of instrument modeling

52 wheat samples were used for modeling, and 20 wheat samples were used for model external inspection. The cross validation results of two raster type instruments and a FT instrument model and the external test results of the model are shown in Table 1. The data scatter diagram is shown in Figure 2. The spectral preprocessing methods in the modeling are SNV and FD.

Table 1: results of NIR model of crude protein in three instruments

Instrument number	Cross validation			External test		
	R^2%	SECV	RSD%	R^2	SEP	RSD%
S450 No.1	94.90	0.44	2.93	96.54	0.44	2.90
S450 No.2	94.67	0.44	3.00	95.59	0.48	3.17
FTNIR	95.62	0.40	2.71	97.39	0.36	2.39

Scatter plot of cross validation of wheat crude protein model with grating instrument

Scatter plot of cross validation of wheat crude protein model with FT instrument

Scatter diagram of external validation of wheat crude protein model with grating instrument

Scatter diagram of external validation of wheat crude protein model with FT instrument
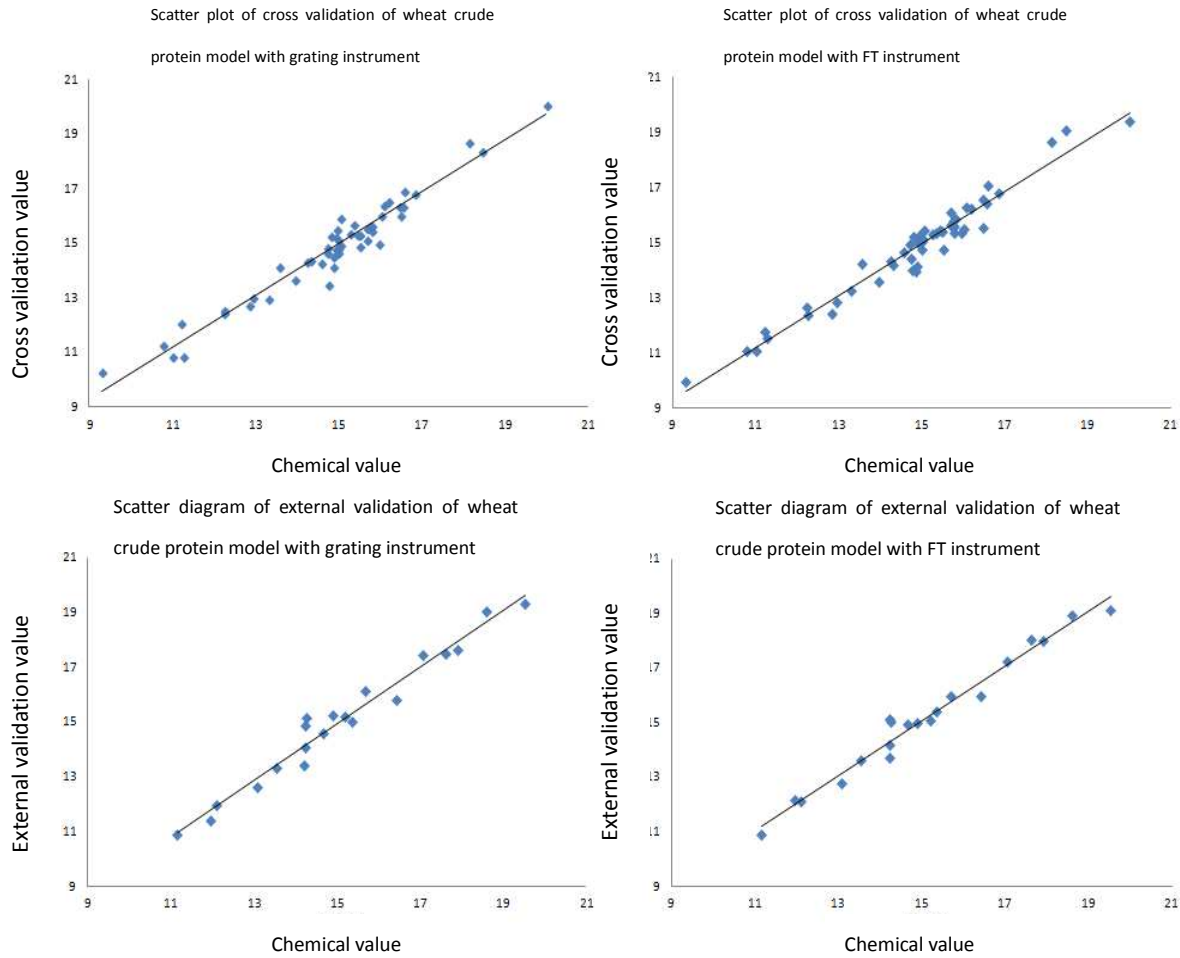
Fig. 2: scatter plot comparison of grating and FT instrument model results

Three. Stability test of instrument model

A wheat sample was selected for 10 repeated spectral scanning tests. The model analysis data were shown in Table 2, and the statistical data are shown in Table 3.

Table 2: repeated test data for wheat crude protein

Serial number	1	2	3	4	5	6	7	8	9	10
S450 No.1	18.98	18.95	19.10	19.16	19.12	19.14	19.20	19.09	19.18	19.21
S450 No.2	19.33	19.38	19.30	19.27	19.27	19.29	19.07	19.23	19.13	19.16

Table 3: instrument model repeatability test

Instrument number	Mean value of crude protein	Std	RSD%
S450 No.1	19.11	0.08	0.44
S450 No.2	19.24	0.09	0.48

Four. Instrument model transfer test

According to Fig. 3, the model of wheat samples was analyzed by different instruments. The difference comparison data were shown in Table 4, and the scatter plot was shown in Fig. 4.
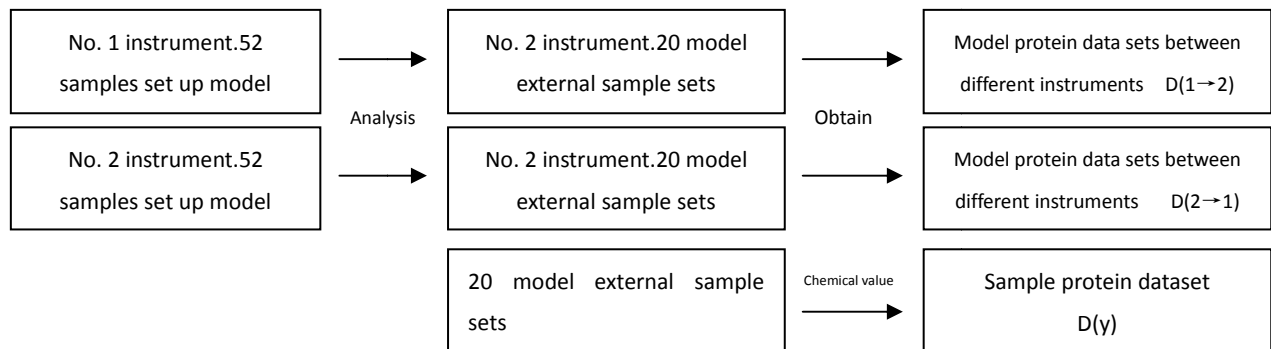
No. 1 instrument.52 samples set up model	→ Analysis	No. 2 instrument.20 model external sample sets	→ Obtain	Model protein data sets between different instruments D(1→2)
No. 2 instrument.52 samples set up model	→	No. 2 instrument.20 model external sample sets	→	Model protein data sets between different instruments D(2→1)
		20 model external sample sets	→ Chemical value	Sample protein dataset D(y)

Figure 3: experimental method

Table 4: error analysis results of different instrument models

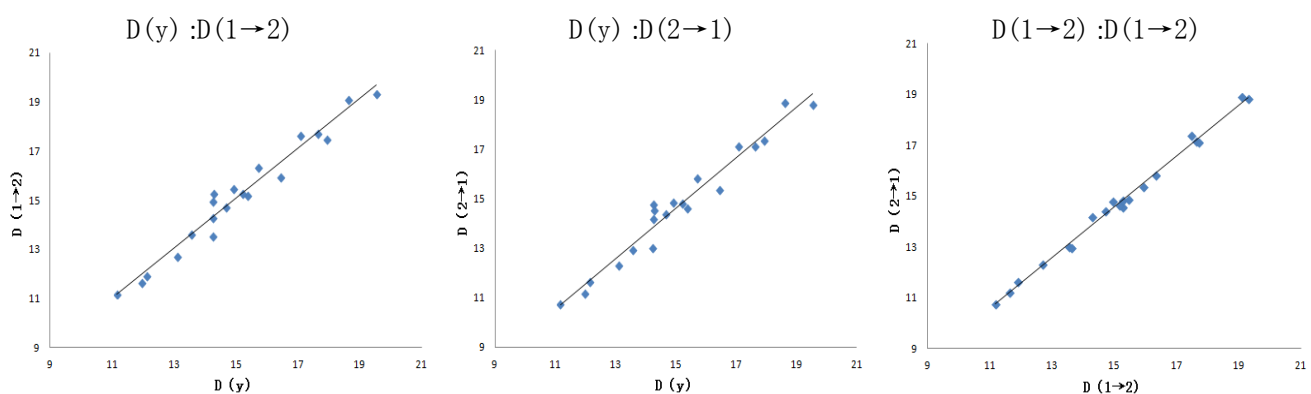| Contrastive data set	R^2%	Std	RSD%
D(y) :D(1→2)	96.15	0.45	2.97
D(y) :D(2→1)	95.95	0.46	3.05
D(1→2) : D(2→1)	99.43	0.17	1.14

Figure 4: scatter plot of deviation analysis of different instrument models

Five. Stability of instrument wavelength accuracy

The wavelength accuracy of spectrometers is easily influenced by ambient temperature. S450 built in polystyrene wavelength standard film ensures the long-term stability of the instrument wavelength accuracy. Using near infrared wavelength standard material (GBW (E) 130551), the accuracy of the wavelength of the test instrument is repeated. Get thousands of spectra in 3 months. The test environment temperature is from 16℃ to 34 ℃, and the accuracy of wavelength is ±0.2nm.
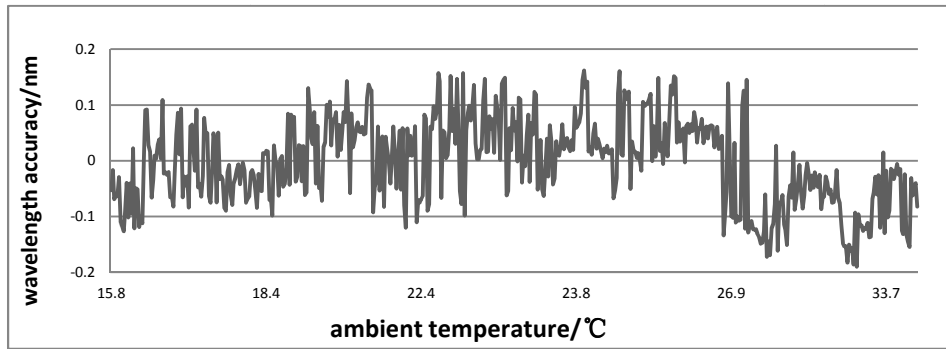
Fig. 5 Relationship between wavelength accuracy and ambient temperature

Six. Summary

- S450 Near Infrared Spectroscopy Analyzer model performance is close to the level of FT instrument.。
- Good transmission capability of instrument model, greatly reducing the workload of modeling in practical application.。
- The long term stability of the wavelength accuracy of the instrument provides an important hardware foundation for establishing a stable and practical near-infrared model.

The S450 Near Infrared Spectroscopy Analyzer combined with the near infrared spectrum analysis software CAUNIRS, the model performance index, stability and transmission capacity can meet the practical application requirements of the near infrared spectroscopy analysis technology.

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parameter	S450 NIR Spectrometer
Measurement method	Integral sphere diffuse reflection sample pool
Spectral bandwidth	12nm
Wavelength range	900nm~2500nm
Wavelength accuracy	≤0.2nm
Wavelength repeatability	≤0.05nm
stray light	≤0.1%
Absorbance noise	≤0.0005Abs
Analysis time	1 minutes (adjustable)
Light source life	More than 5000 hours
Sample quantity	Big cup(Φ90) about 120g,Middle cup(Φ60) about 60g,Small cup(Φ30) about 12g,square cup (50 x 30) about 30g
Calibration technique	quantitative analysis：LPLS qualitative analysis：DPLS
Analysis index number	Unlimited, Support quantitative and qualitative simultaneous analysis
size	540×380×220 (mm)
weight	18Kg