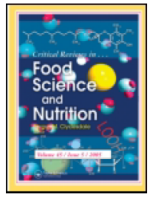
Data preprocessing



Taylor & Francis

Critical Reviews in Food Science and Nutrition

ISSN: 1040-8398 (Print) 1549-7852 (Online) Journal homepage: http://www.tandfonline.com/loi/bfsn20

Applications of Near-infrared Spectroscopy in Food Safety Evaluation and Control: A Review of Recent Research Advances

Jia-Huan Qu, Dan Liu, Jun-Hu Cheng, Da-Wen Sun, Ji Ma, Hongbin Pu & Xin-An Zeng

To cite this article: Jia-Huan Qu, Dan Liu, Jun-Hu Cheng, Da-Wen Sun, Ji Ma, Hongbin Pu & Xin-An Zeng (2015) Applications of Near-infrared Spectroscopy in Food Safety Evaluation and Control: A Review of Recent Research Advances, Critical Reviews in Food Science and Nutrition, 55:13, 1939-1954, DOI: 10.1080/10408398.2013.871693

To link to this article: http://dx.doi.org/10.1080/10408398.2013.871693

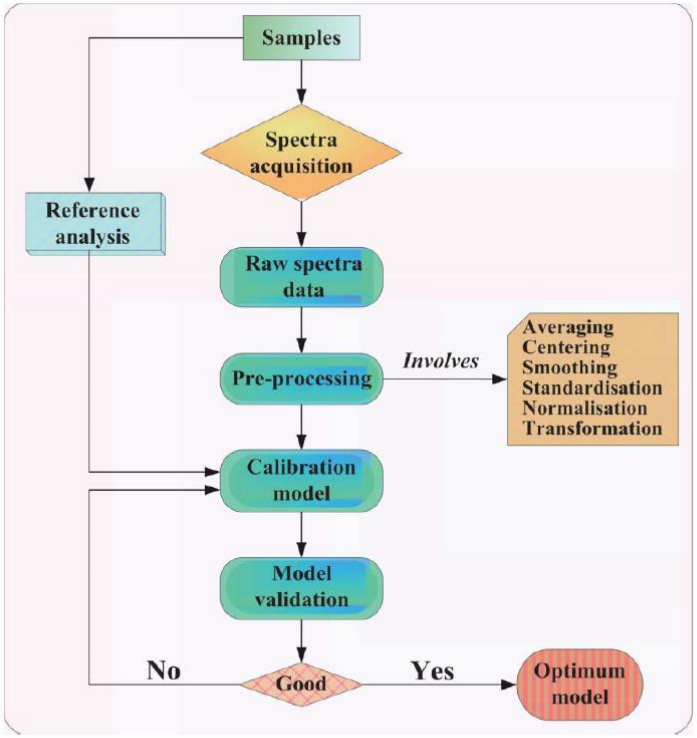


Figure 4 A series of steps in the procedure of NIRS analysis from sampling to an optimal model for prediction.

ผศ.ดร. ศิลา กิตติวัชนะ และคณะนักศึกษา
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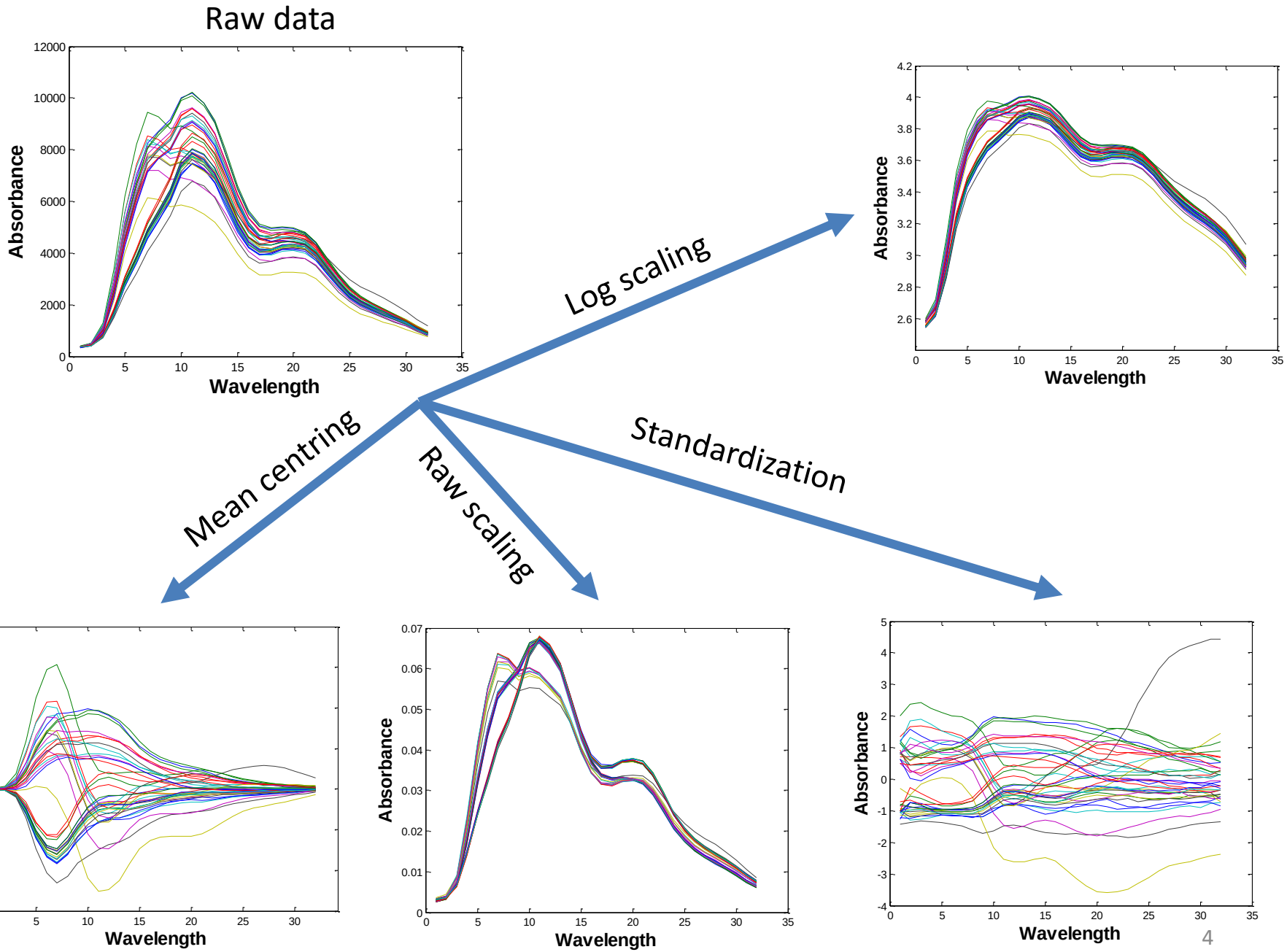
The problems are….

- Data are from different types/scales
- Variation during experiments
- Errors: Systematic and non-systementic errors
- Noise: Homoscedastic and heteroscedastic noise
- Characteristics of the acquisition methods such as light scattering in NIR
- ……etc

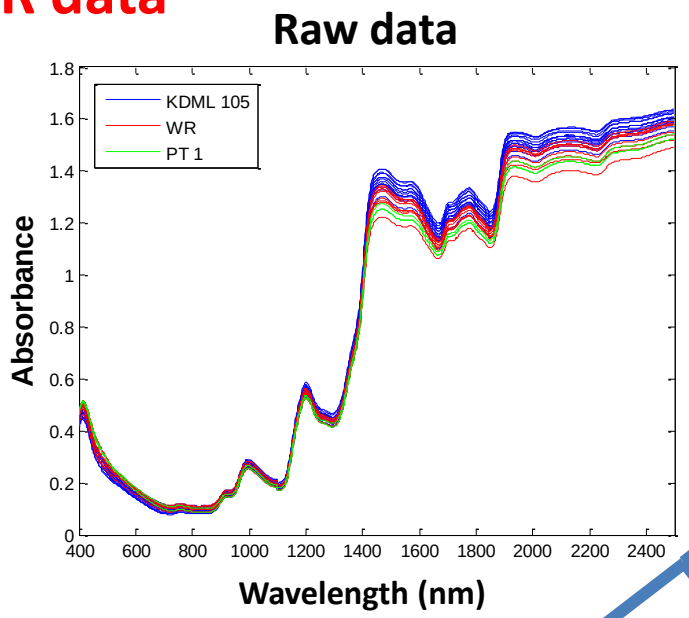
Data preprocessing

- Data pre-processing is to apply a mathematical modification to the values of a matrix prior to formal data analysis methods.
- A raw data may be shifted/rescaled along the variables/samples to place emphasis on the aspects wanted from the data analysis or to improve the interpretation of the data.
- This is to ensure that the right trends are being studied, and the analysis methods do not get confused by non-essential information.

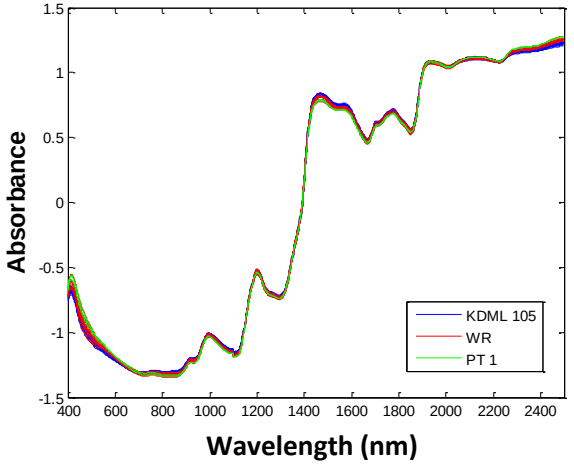
UV-Vis data


Raw data
Absorbance
Wavelength
Log scaling
Mean centring
Raw scaling
Standardization

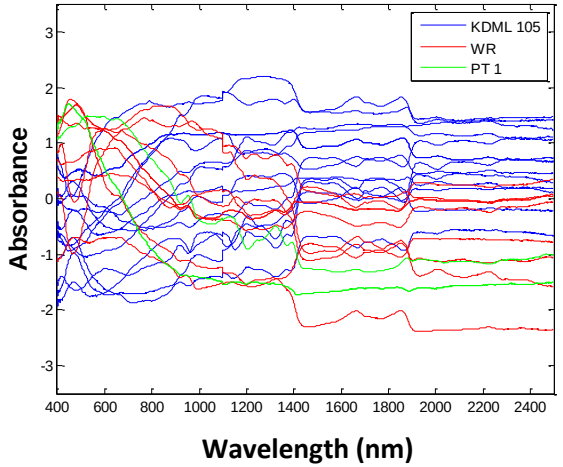
NIR data



SNV

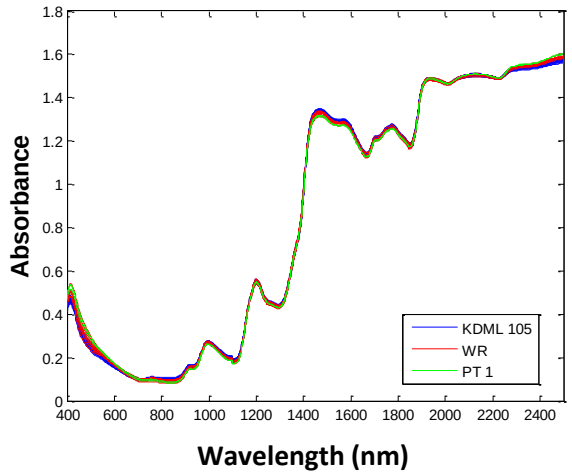


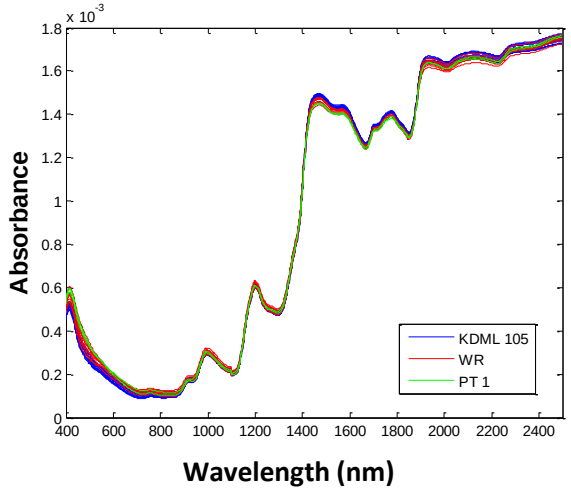
Standardization



Raw scaling

MSC



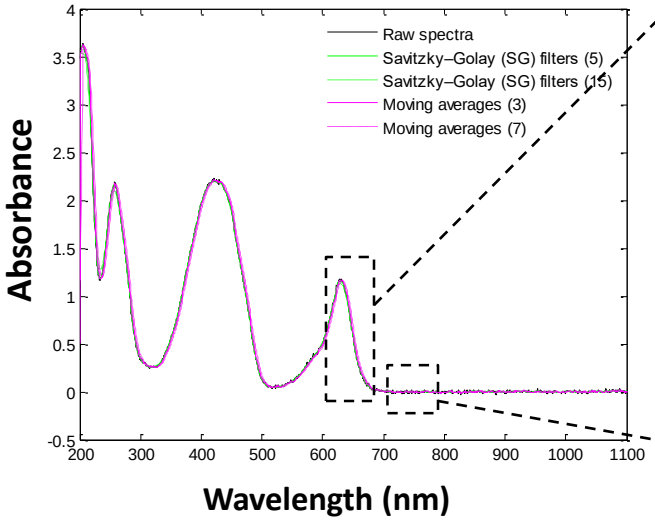


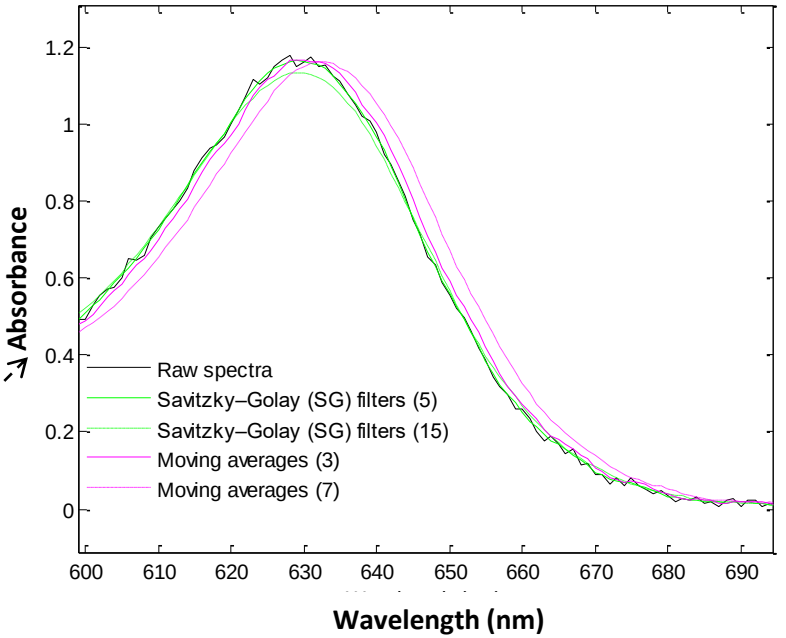
Data preprocessing

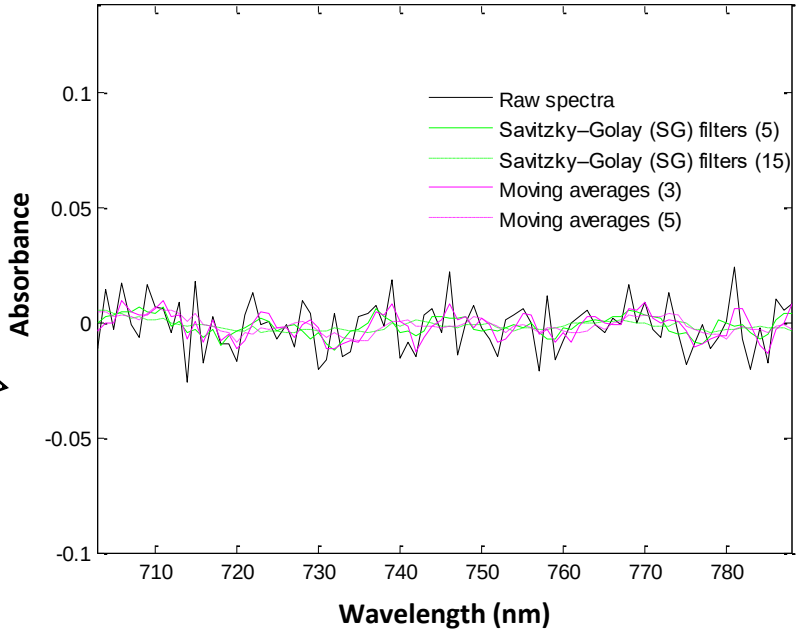
1. **Data smoothing**
   - Savitzky–Golay (SG) filters
   - Moving averages
2. **Data scaling**
   - Square root scaling
   - Log scaling
3. **Normalization**
   - Row scaling
4. **Auto scaling**
   - Mean centring
   - Standardization
5. **Others**
   - SNV
   - MSC
   - Derivatives

1. Data Smoothing

- Savitzky–Golay (SG) filters
- Moving averages



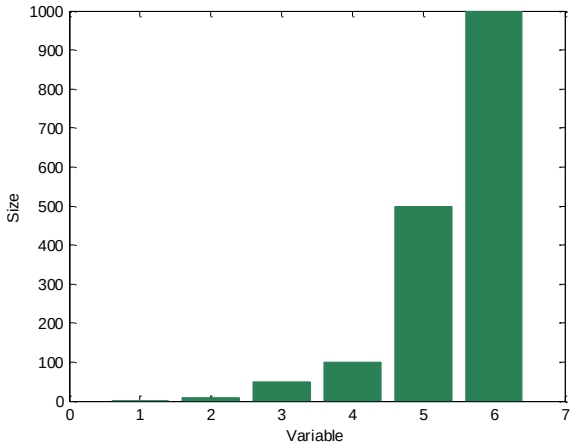




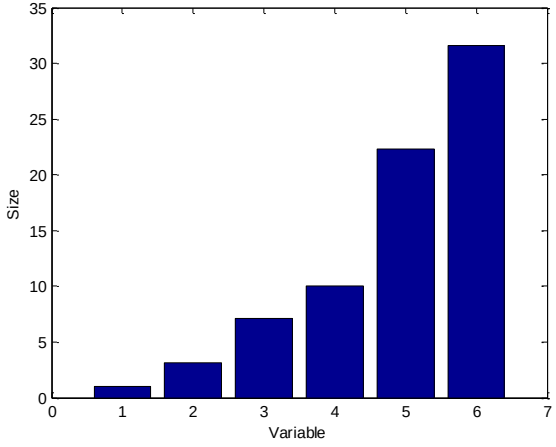
2. Data scaling

- Square root scaling $\boldsymbol{X}_{sqrt} = \sqrt{\boldsymbol{X}}$
- Log scaling $\boldsymbol{X}_{log} = \log \boldsymbol{X}$

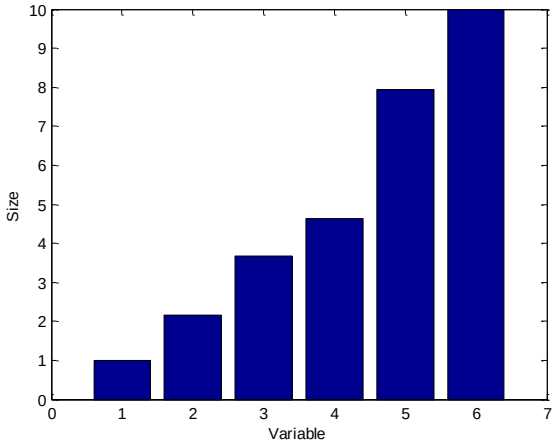
Raw data ($\boldsymbol{X}$)



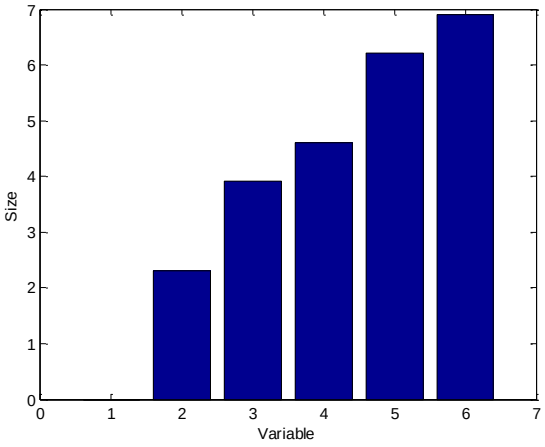
$X_{sqrt.5} = \sqrt{X}$



$X_{sqrt.33} = \sqrt[1/3]{X}$



$X_{log} = \log X$



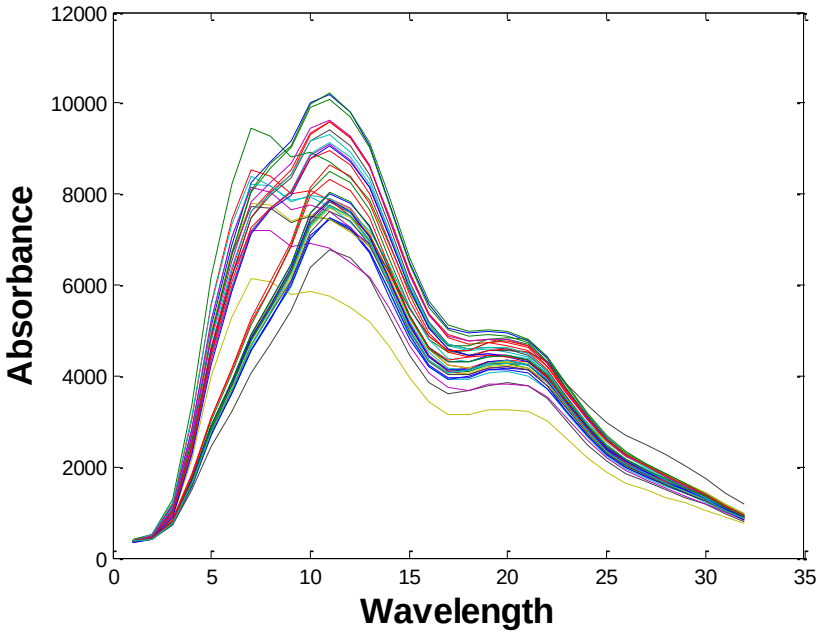
3. Normalization

– Row scaling

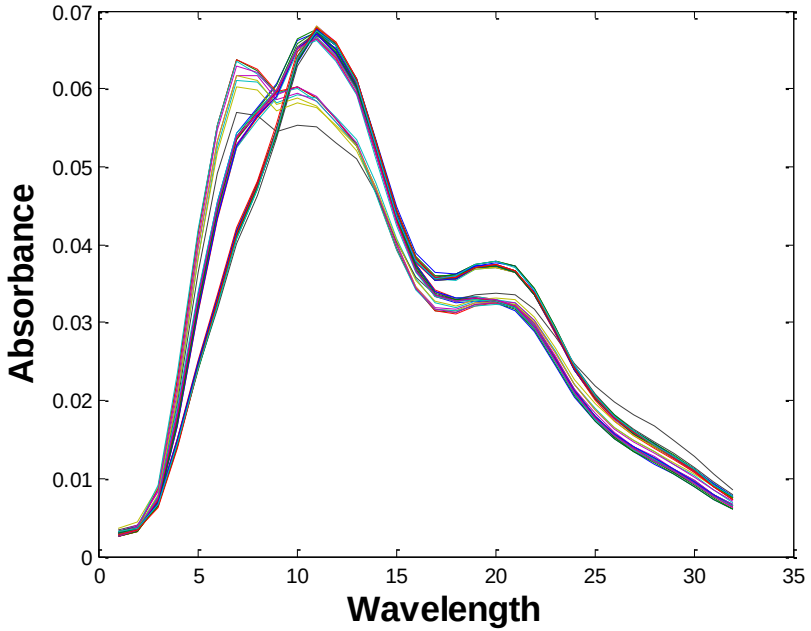
$$ {}^{rs}x_{ij} = \frac{x_{ij}}{\sum_{J=1}^{J} x_{ij}} $$

${}^{rs}x_{ij}$ = normalized value of x_{ij}

J = number of parameter



Raw data



Row scaling

4. Auto scaling

– Mean centring

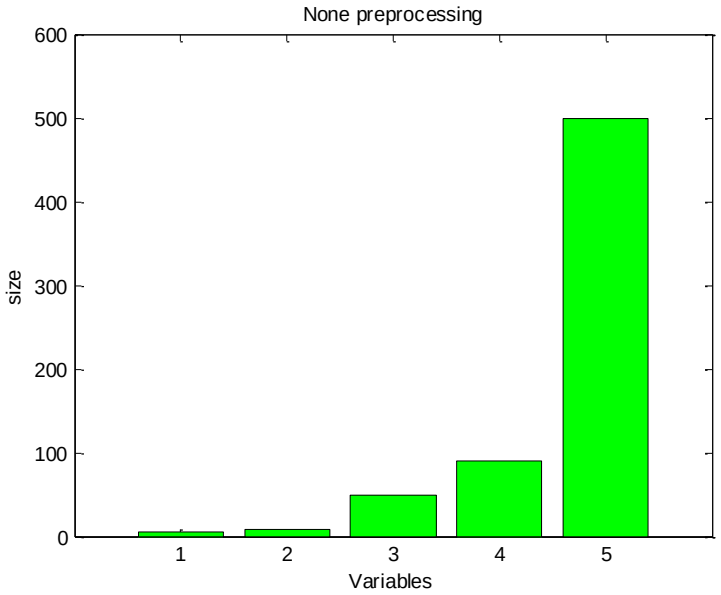
$$ {}^{cent}x_{ij} = x_{ij} - \bar{x}_j $$

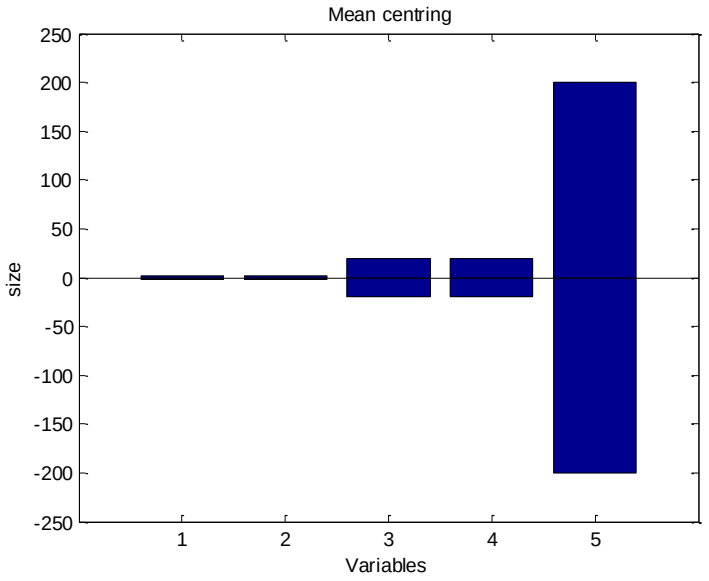
$$ \bar{x}_j = \frac{\sum_{i=1}^{I} x_{ij}}{I} $$

Raw data

1	5	10	50	100
2	6	20	60	200
3	7	30	70	300
4	8	40	80	400
5	9	50	90	500

${}^{cent}x_{ij}$= mean centring value of x_{ij} with average value of $\bar{x}_j$





4. Auto scaling

– Standardization

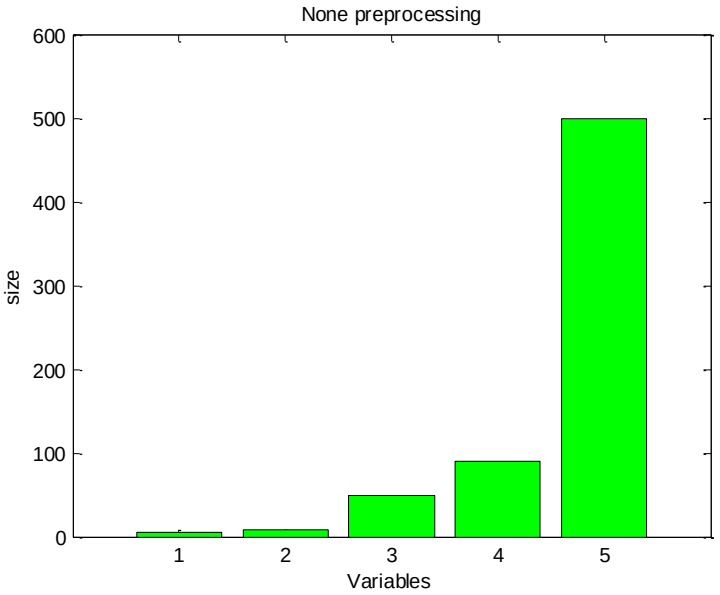
$$ {}^{std}x_{ij} = \frac{x_{ij} - \bar{x_j}}{S_j} $$

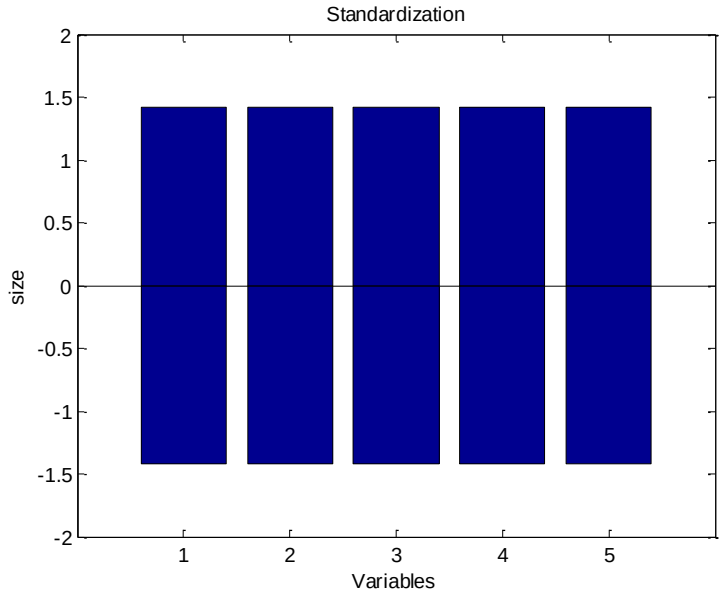
$$ S_j = \frac{\sum_{i=1}^{I} \left(x_{ij} - \bar{x_j} \right)^2}{I} $$

Raw data

1	5	10	50	100
2	6	20	60	200
3	7	30	70	300
4	8	40	80	400
5	9	50	90	500

${}^{std}x_{ij}$ = standardized element of x_{ij} using mean of $\bar{x_j}$ standard deviation of S_j





5. Others

- Standard normal variate (SNV)

$$^{SNV}A_{ij} = \frac{A_{ij} - \bar{x}_i}{SD_{ev}}$$

i = spectrum counter
j = absorbance value counter of i^{th} spectrum
$^{SNV}A_{ij}$ = corrected absorbance value
A_{ij} = measured absorbance value
$\bar{x}_i$ = mean absorbance value
SD_{ev} = standard deviation

- Multiplicative scatter-correction (MSC)

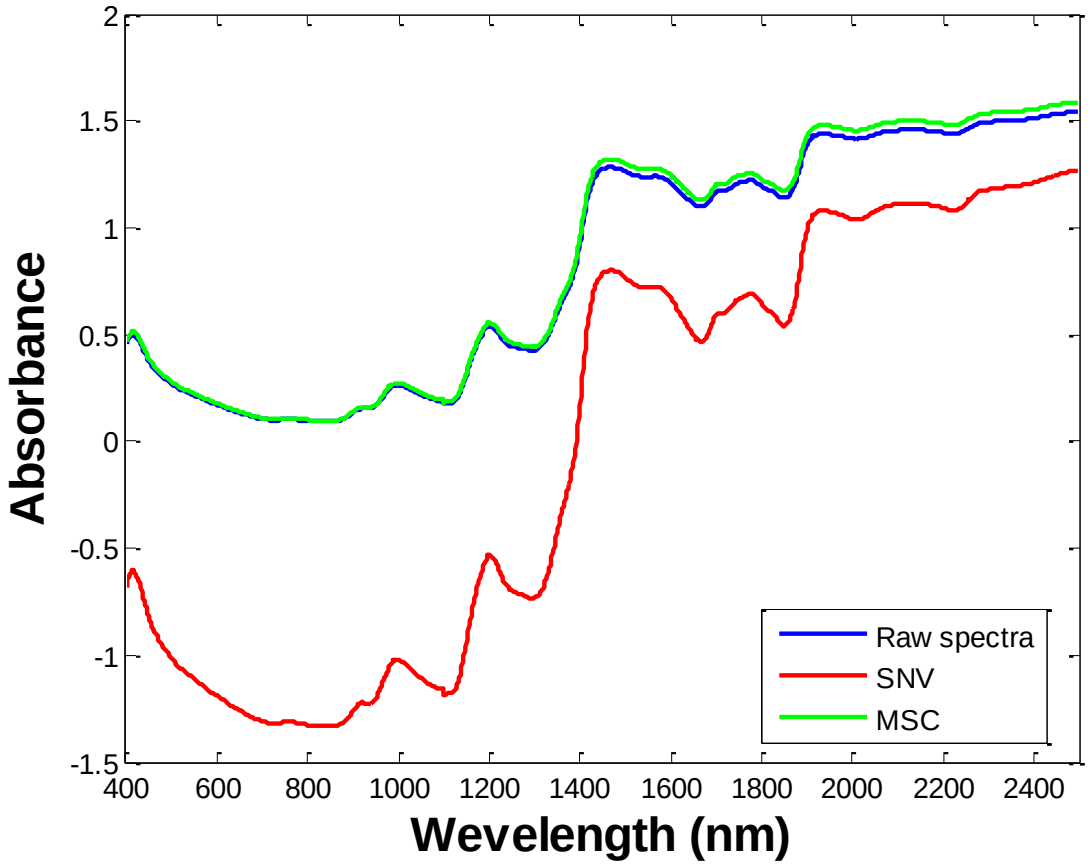
$$x_i = a + b\, y_{average} + \varepsilon$$

$$^{MSC}x_{ij} = \frac{x_{ij} - a}{b}$$

x_i = the i^{th} spectrum collection
x_{ij} = the absorbance of the i^{th} spectrum and j^{th} wavelength of the collection

For each sample, *a* and *b* are estimated by ordinary least-squares regression of spectrum x_i versus $y_{Average}$ over the available wavelengths *j*

https://www.labcognition.com/onlinehelp/en/standard_normal_variate_correction.htm
https://www.labcognition.com/onlinehelp/en/multiplicative_scatter_correction.htm

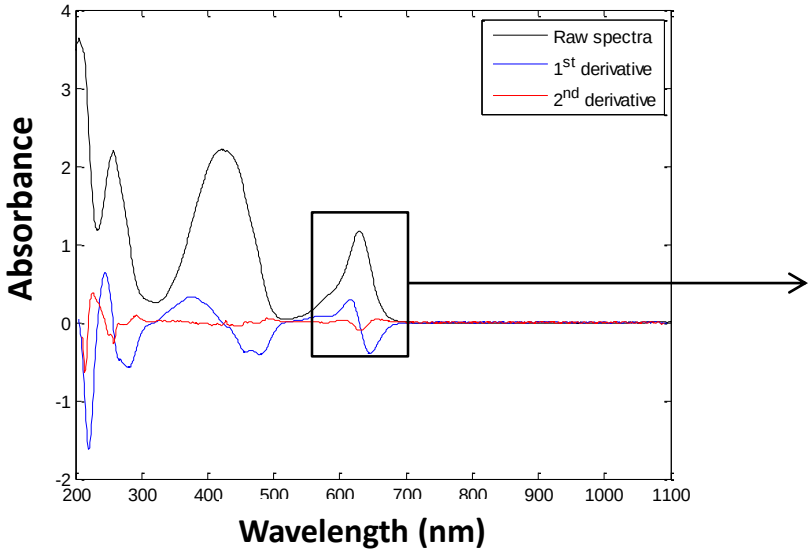

Absorbance
Wevelength (nm)
Raw spectra
SNV
MSC
2
1.5
1
0.5
0
-0.5
-1
-1.5
400
600
800
1000
1200
1400
1600
1800
2000
2200
2400

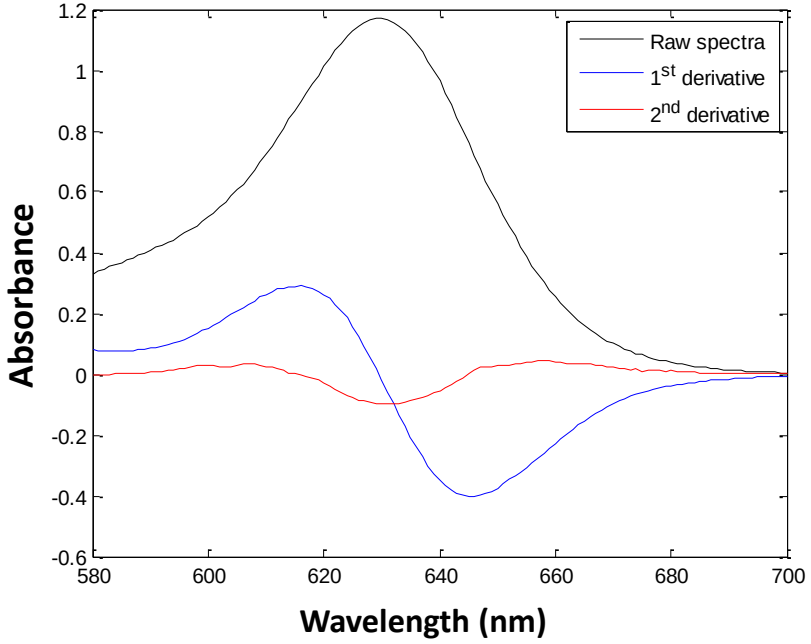
5. Others

– Derivatives

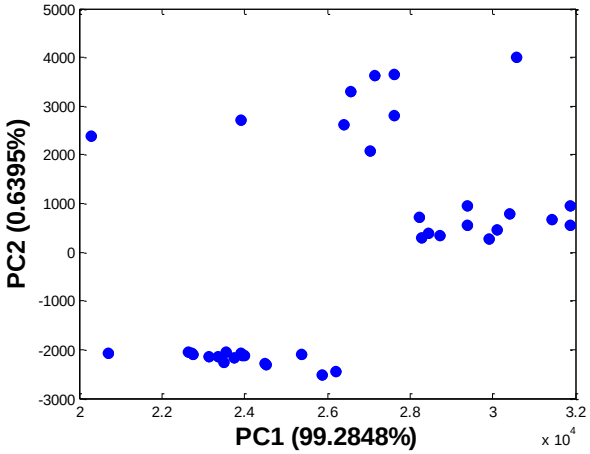
1st derivative → $dX/dY = \frac{\Delta X}{\Delta Y}$

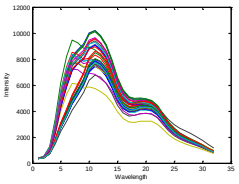
2nd derivative → $d^2X/dY^2 = \frac{\Delta^2 X}{\Delta Y^2}$

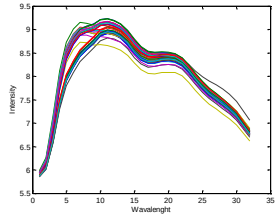


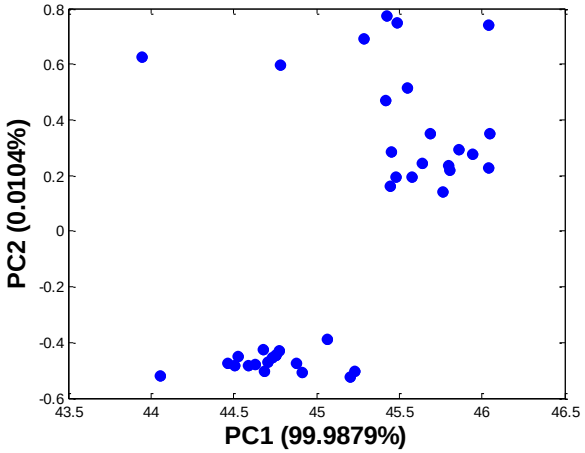


PCA score plots







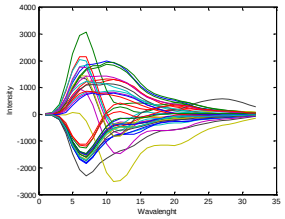


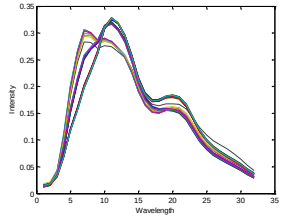
Log scaling

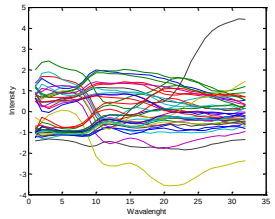
Standardization

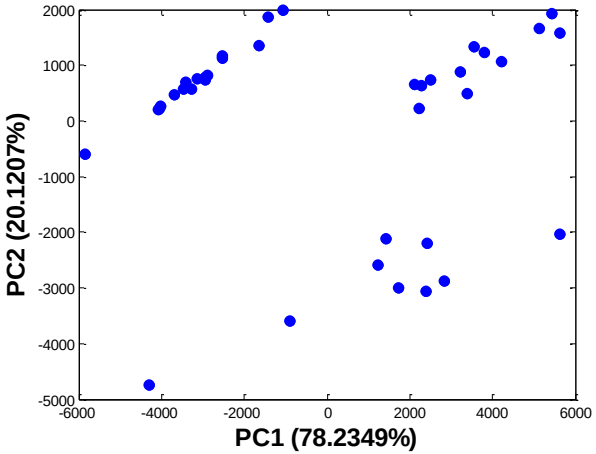
Raw scaling

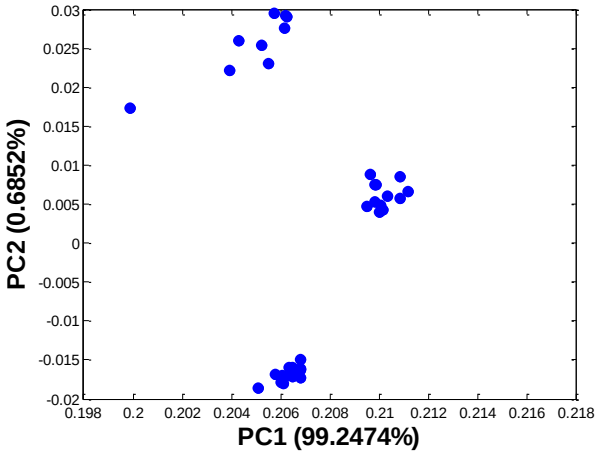
Centring

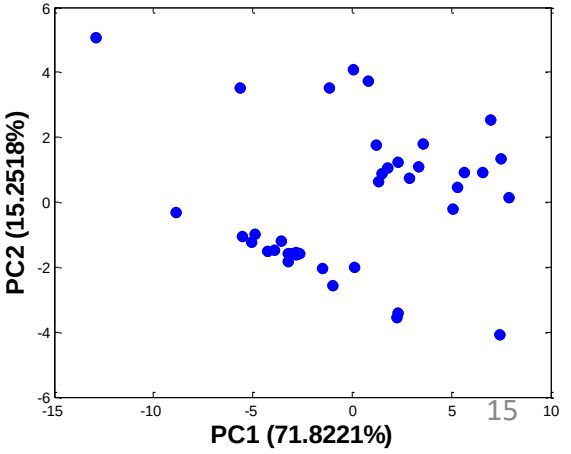




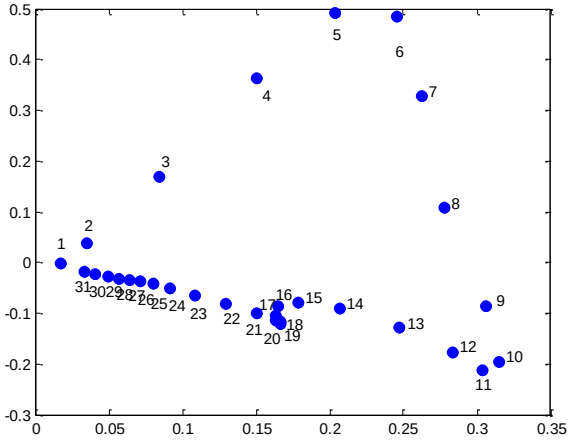


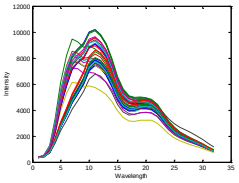


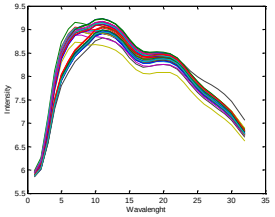


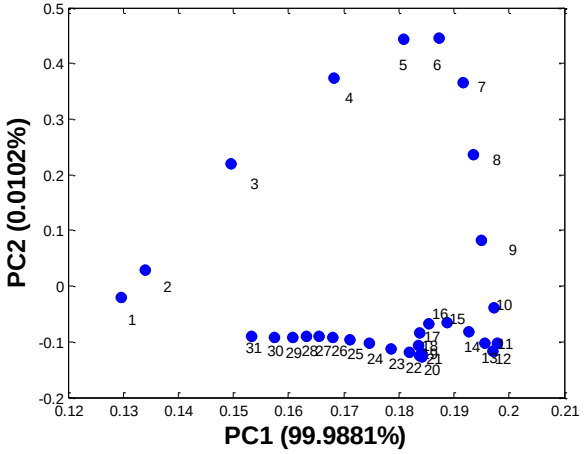


PCA loading plots







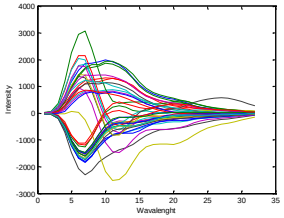


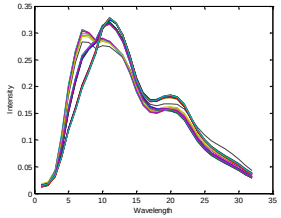
Log scaling

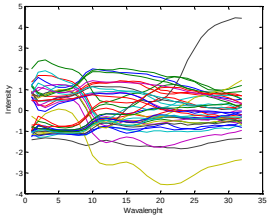
Standardization

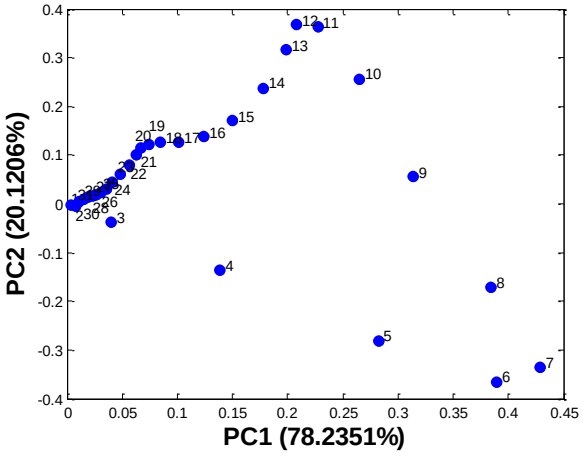
Raw scaling

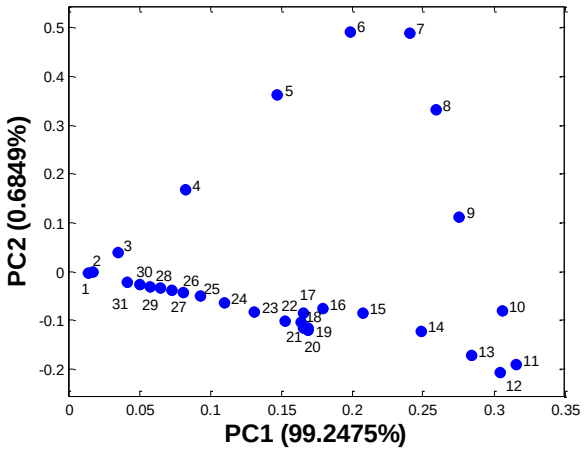
Centring

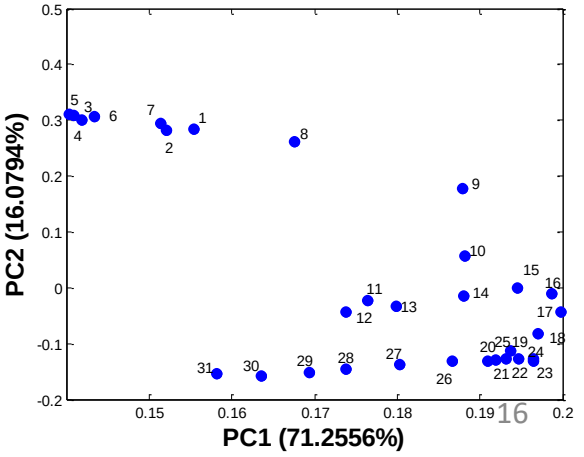




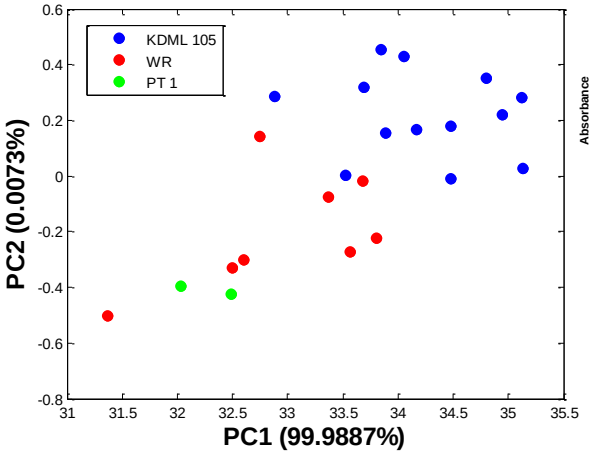


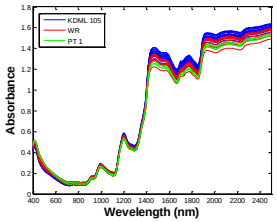




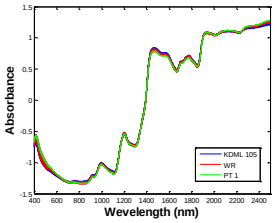


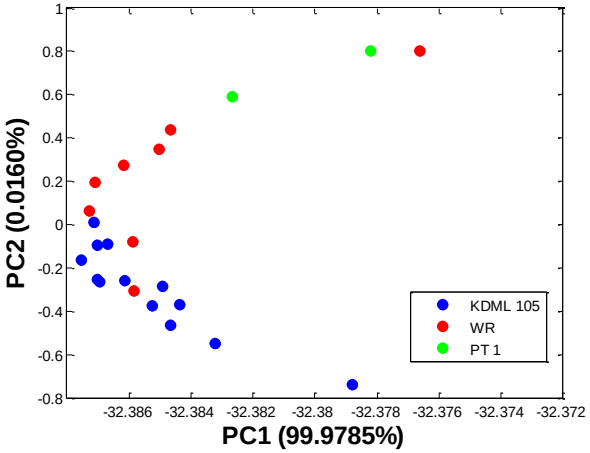
Raw data





SNV

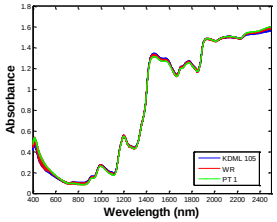


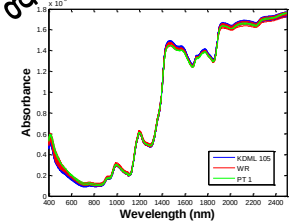


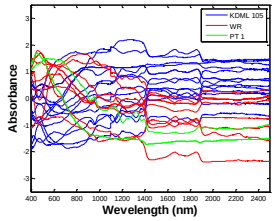
MSC

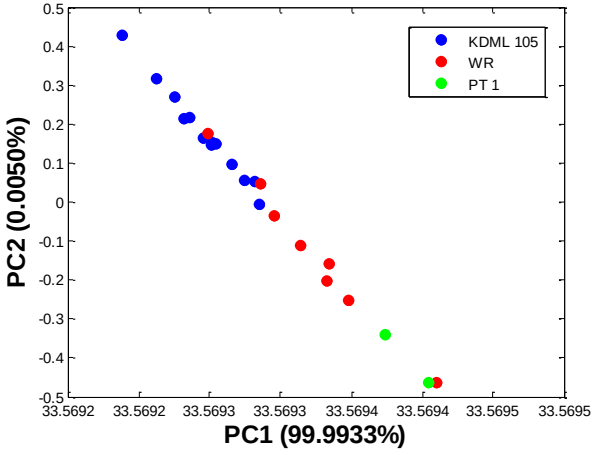
Raw scaling

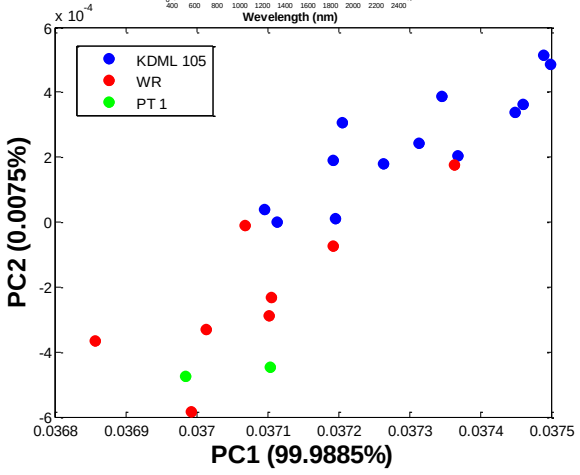
Standardization

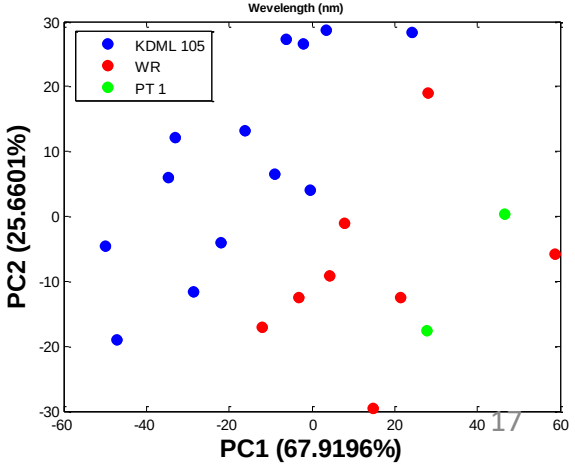




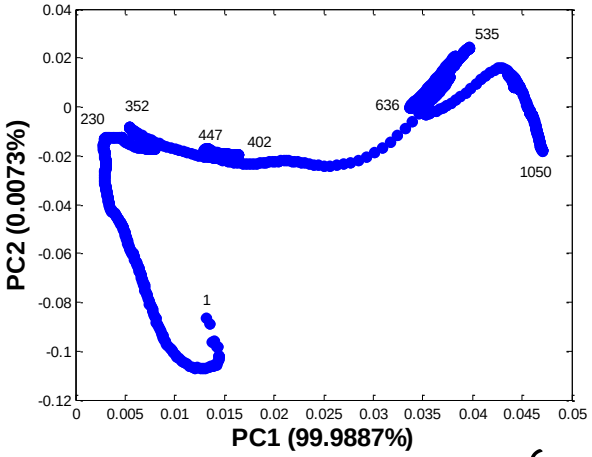


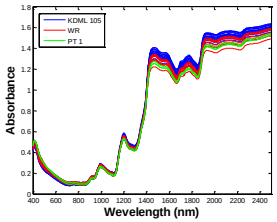


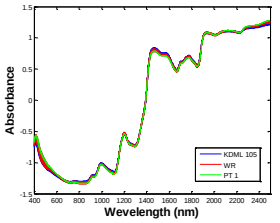




PCA loading plots







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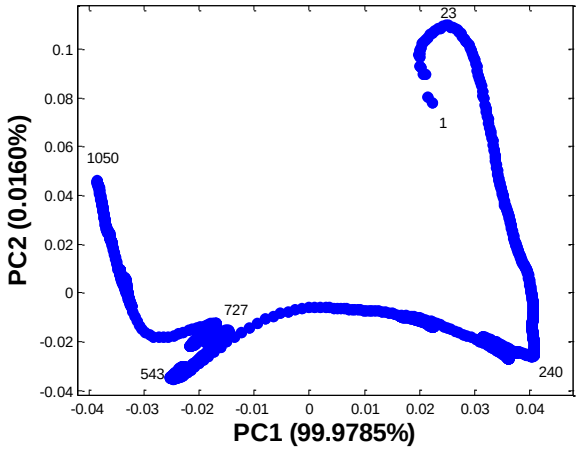

MSC

Raw scaling

Standardization