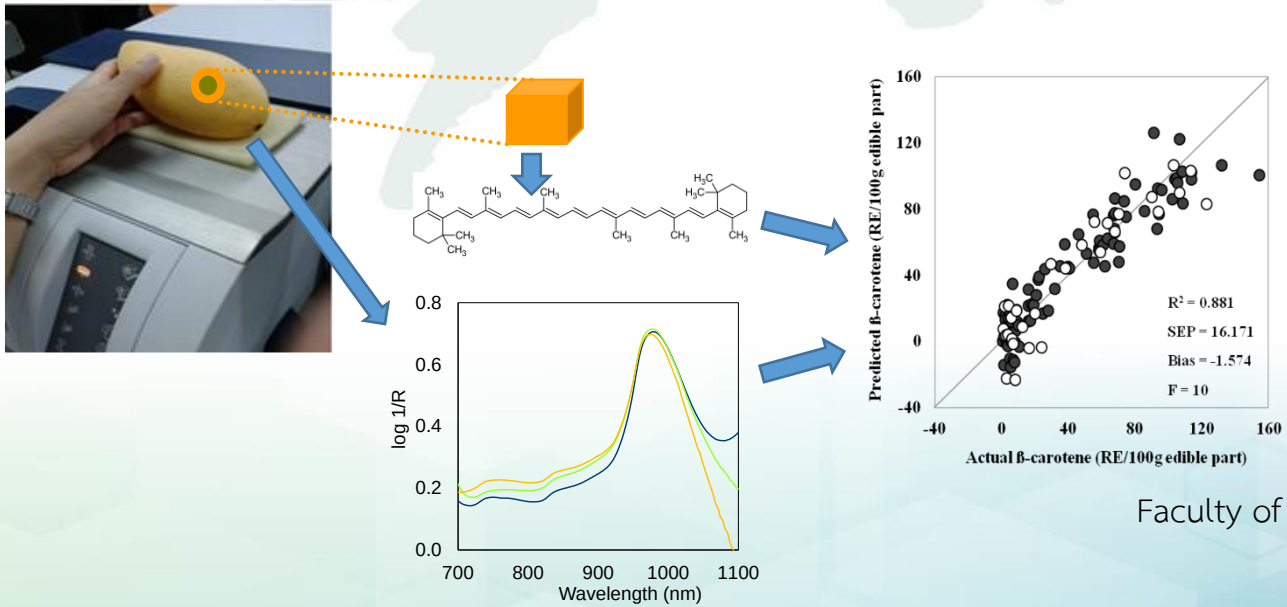
Demonstration 4_ 28 April 2023

Analysis of bioactive compounds in fresh and dried food products using non-destructive method

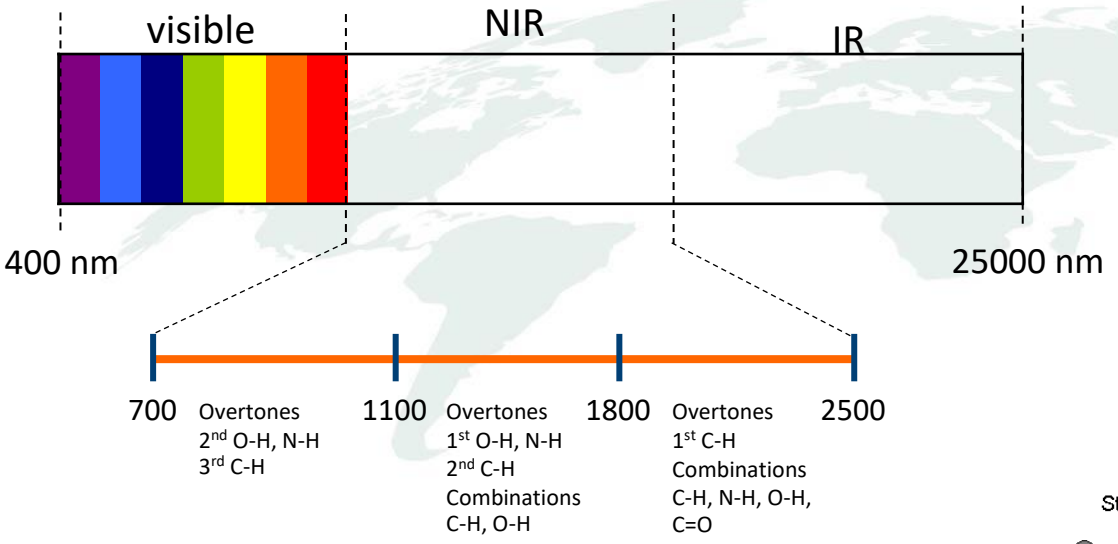


Dr.PARIKA RUNGPICHAYAPICHET
Dr.KHWANJAI KLINJONGKOL
Department of Food Technology
Faculty of Engineering and Industrial Technology
Silpakorn University, Nakhon Pathom
Thailand

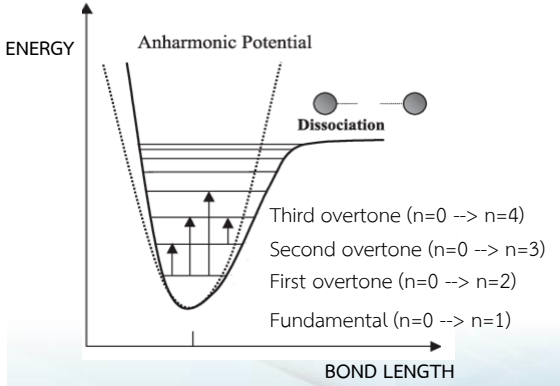
Principle of Near infrared spectroscopy (NIR)

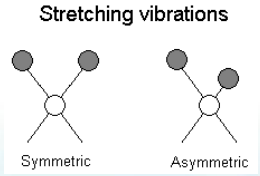
Wavelength : 700 - 2500 nm

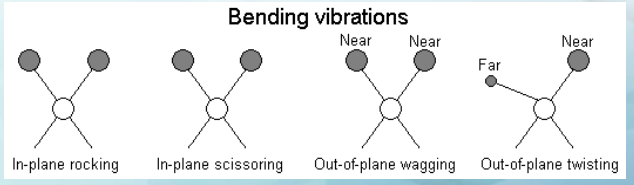
Frequency: 12500 – 4000 cm^{-1}



Only organic compounds that contains functional group C-H, O-H, N-H, O=H can absorb NIR energy



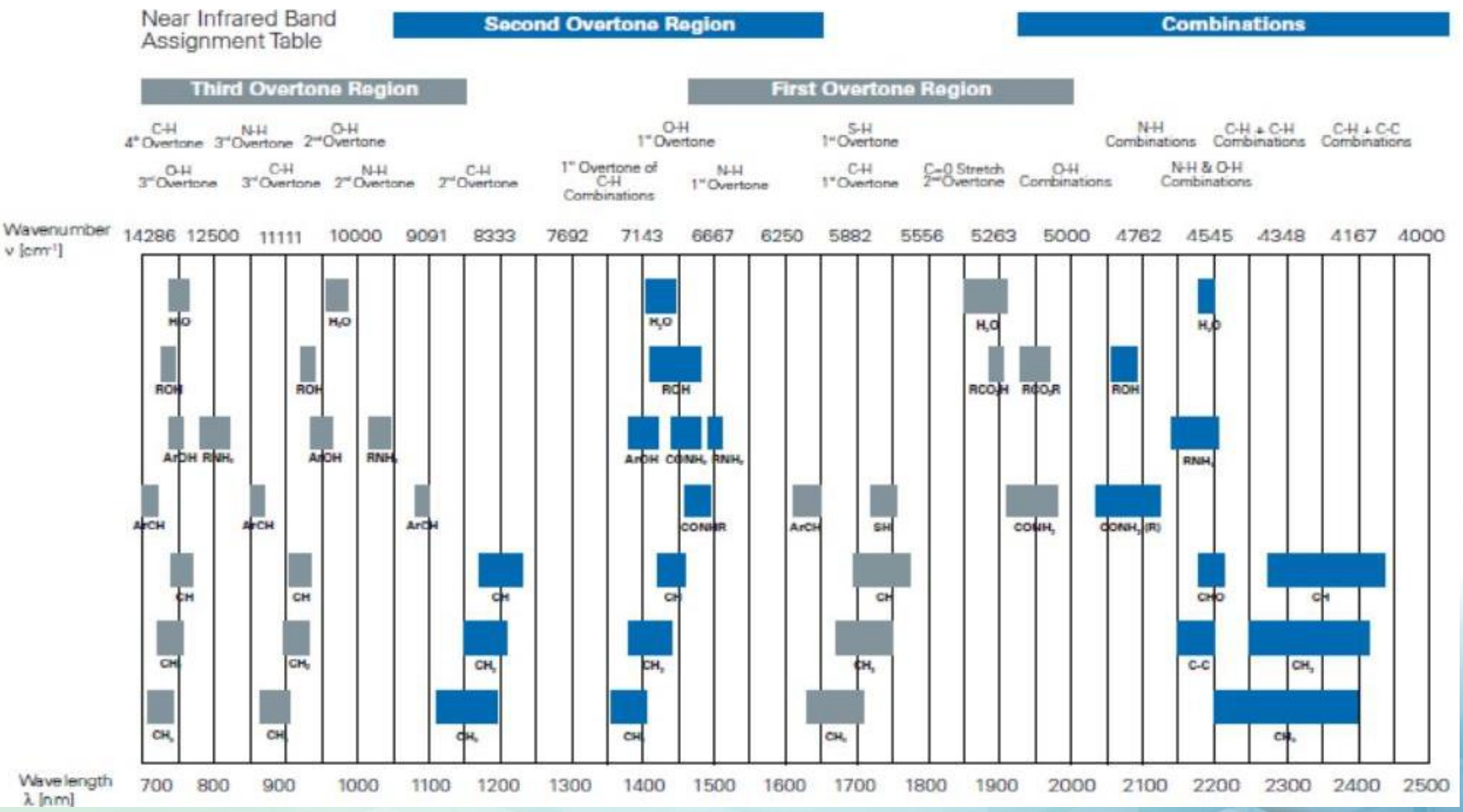




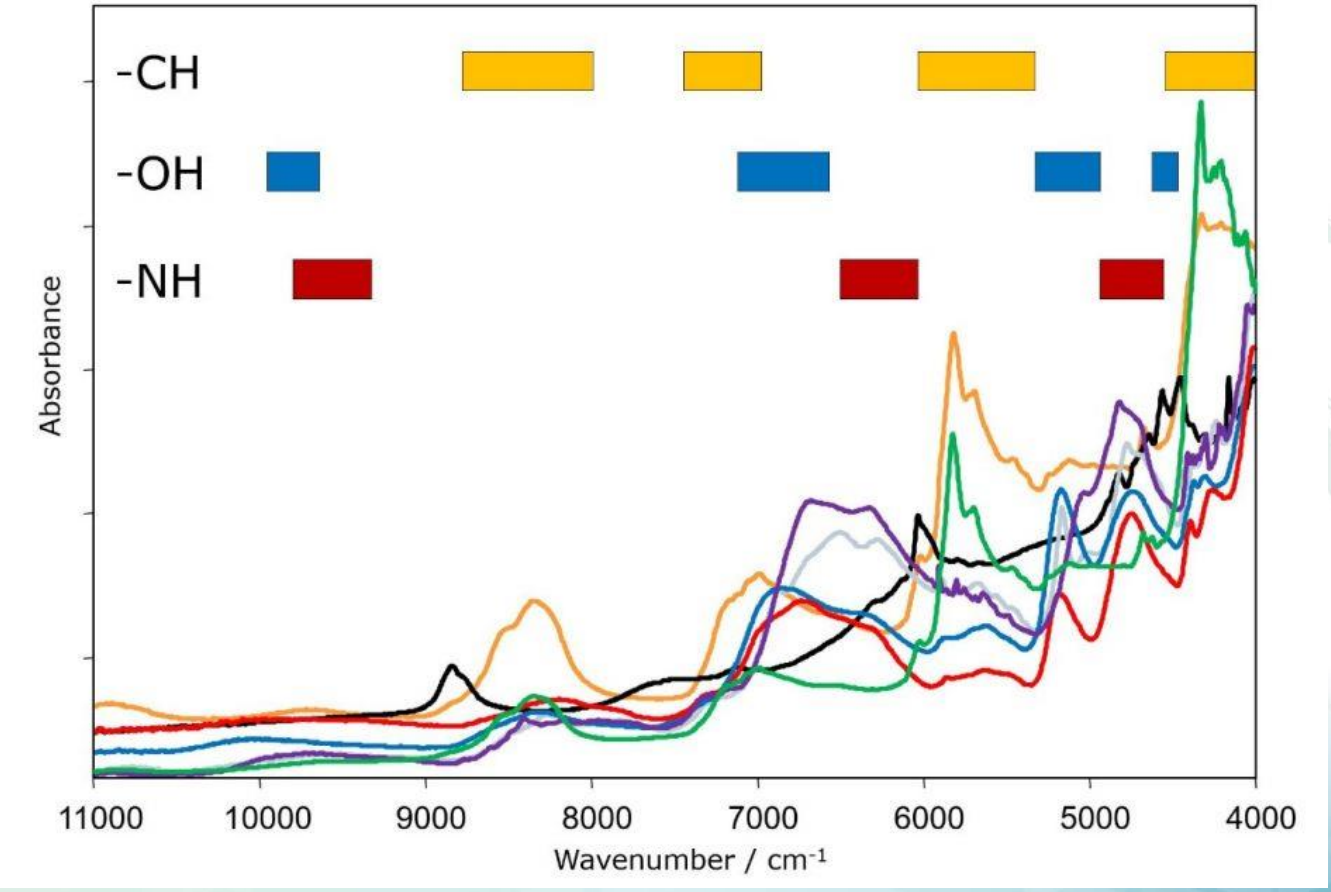
Molecules absorb the energy from the light at NIR region

Molecular bonding is vibrated causes electron transition

Chemical assignments of some observed near infrared absorption bands



Principle of Near infrared spectroscopy (NIR)



NIR spectra

Principle of Near infrared spectroscopy (NIR)

NIR light at 700-2500 nm is absorb by substances

↓

Bonding of functional groups is vibrated (stretching & bending)

↓

Electron transition at overtone & combination and show as broad band spectrum

Reference data →

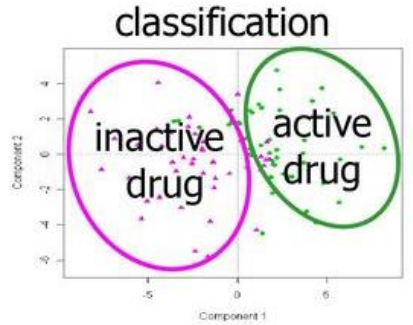
↓

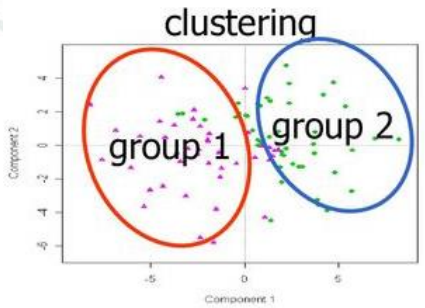
Chemometrics & Calibration development

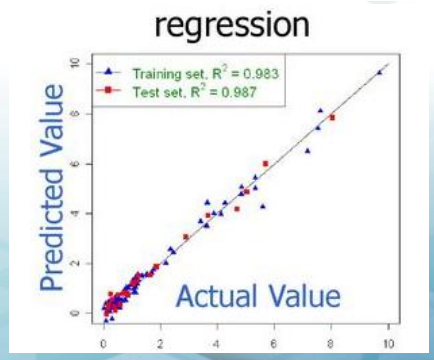
↓

Qualitative analysis (Identification)

Quantitative analysis (Quantification)

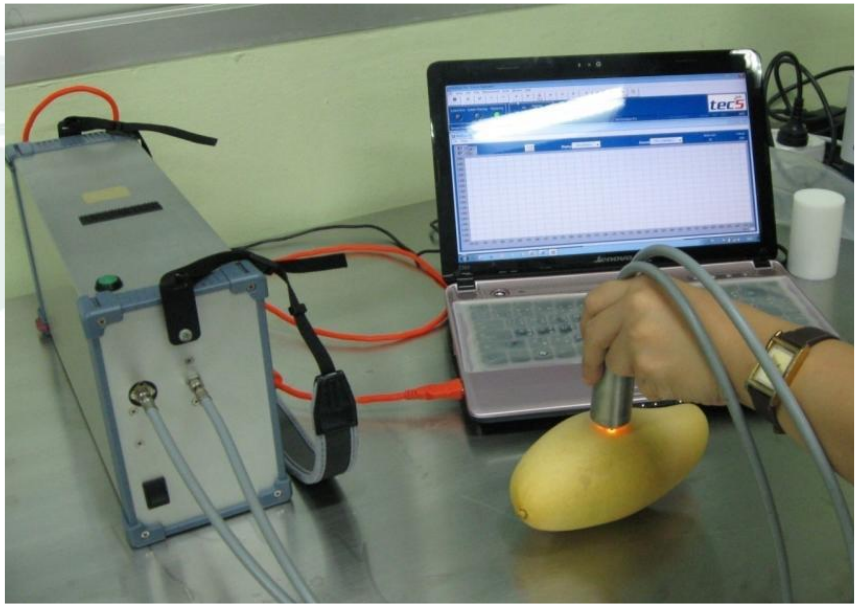






How to measure the spectra using NIR spectrophotometer

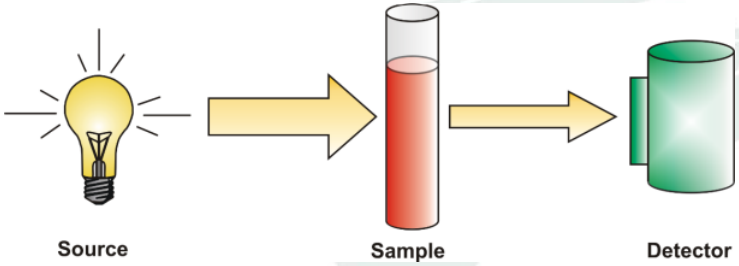
Multipurpose analyzer (MPA), Bruker optic



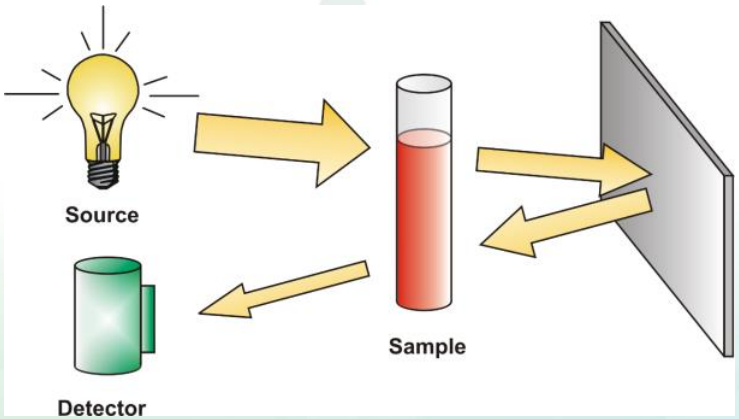
Portable vis/NIR photo-diode array spectrometer (HandySpec Field 1000), tec5 AG

How to measure the spectra using NIR spectrophotometer

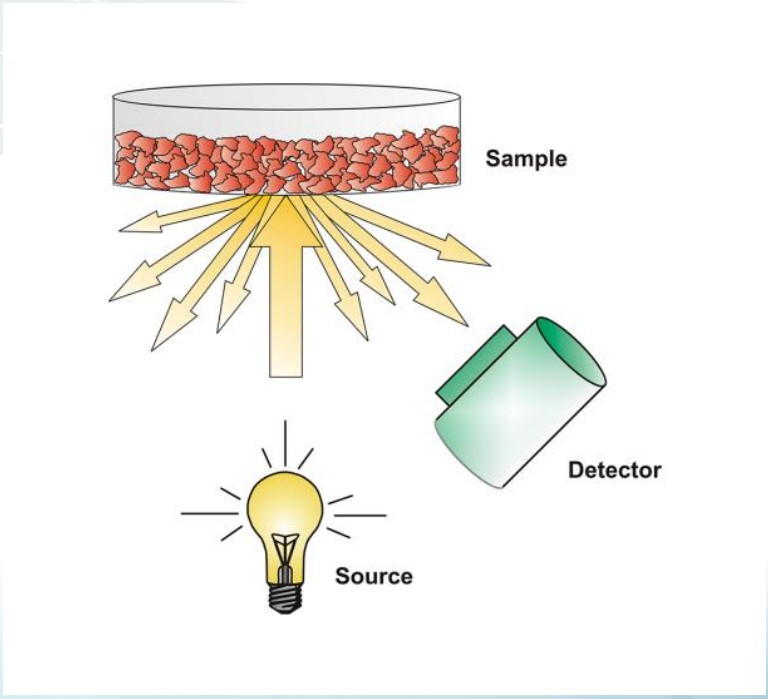
1. Select the mode of measurement



Transmittance mode



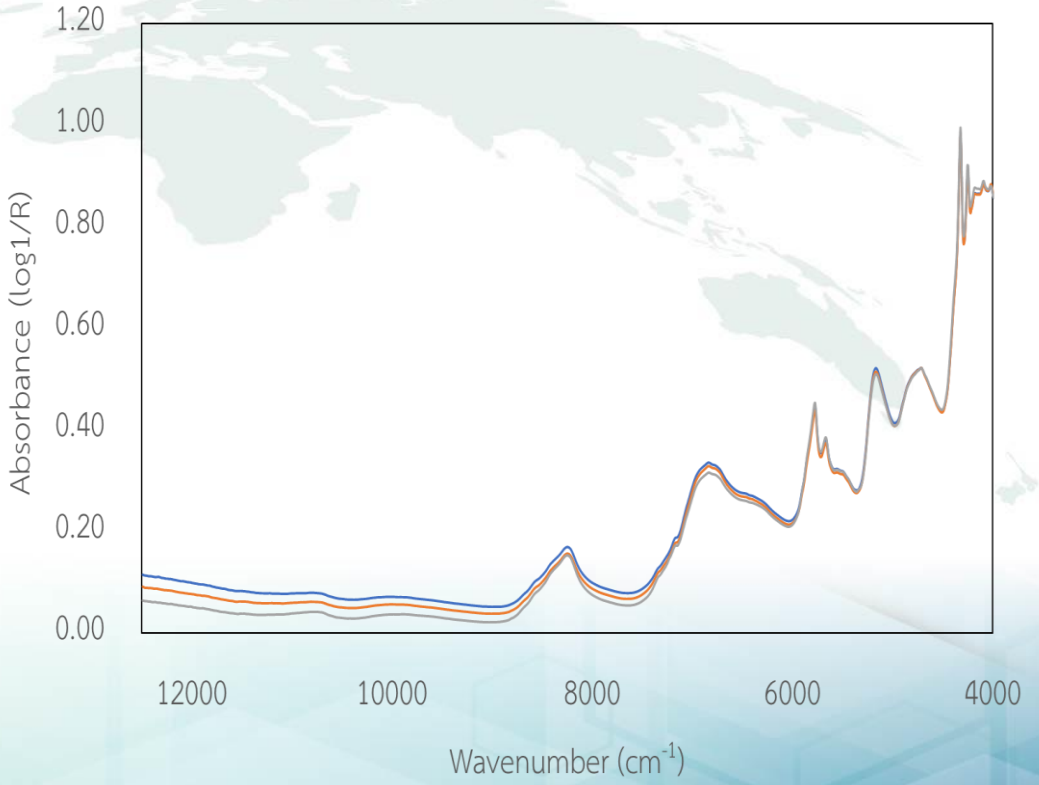
Transflectance mode



Reflectance mode

How to measure the spectra using NIR spectrophotometer

2. Setting the measurement parameter
   - Resolution
   - Scan time
3. Spectral acquisition



NIR spectra

NIR data analysis : Spectral pretreating techniques

NIR analysis procedure

Samples

NIR measurement

NIR spectra

Spectral pretreatments

Chemical analysis

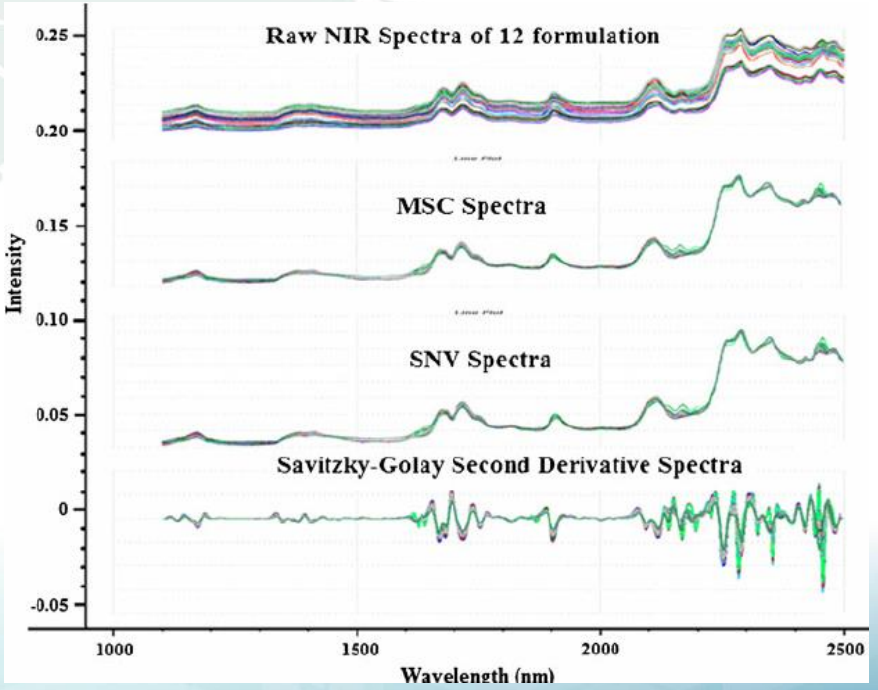
Reference data

Chemometrics & Calibration development

Identification

Quantification

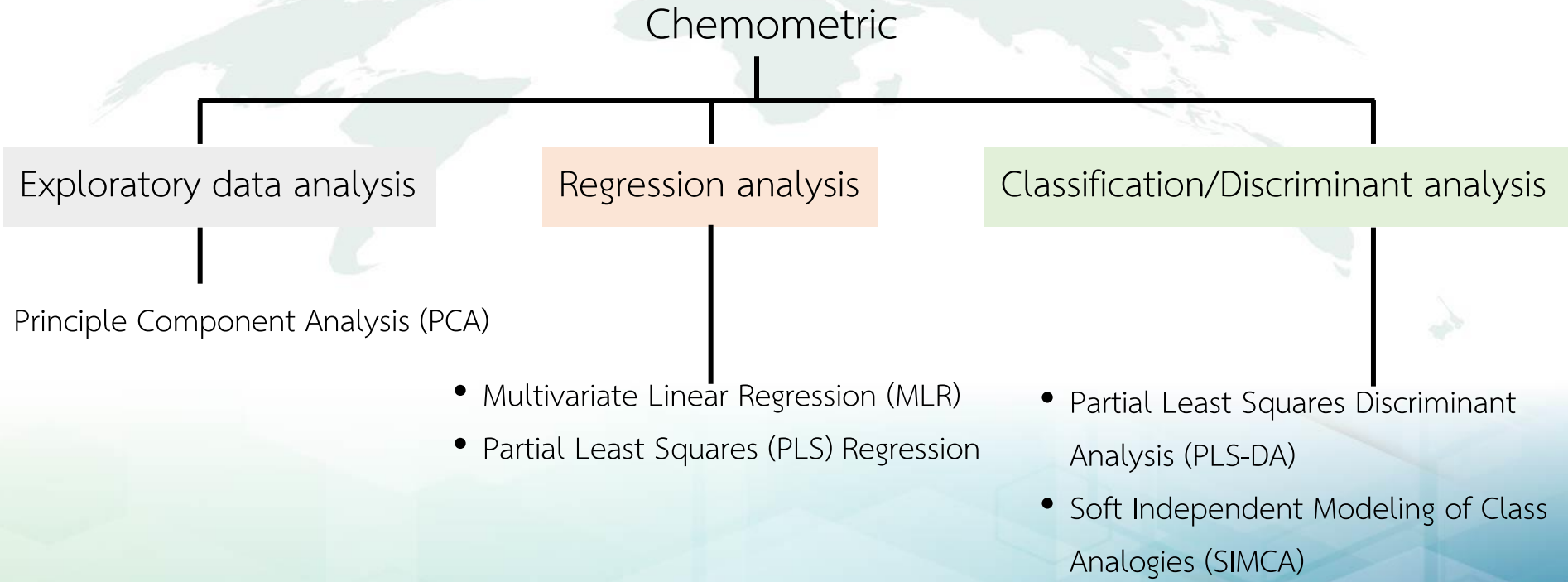
Spectral pretreating techniques



Source : Awotwe-Otoo et al. (2012)

NIR data analysis : Chemometric

Chemometric – Multivariate mathematic and statistic techniques that assist to find the relationship between spectral data and reference data



NIR data analysis : Calibration development

NIR spectral data and reference data are divided into

- Calibration set (Prediction model)
  - Collected data must represent of the population
  - Reference data must cover the range of sample chemical data (highest & lowest value)
  - Use the standard method for reference analysis to obtain the accurate and precise results
- Validation set (Test set)
  - Another set of data use to validate the accuracy of prediction model

NIR data analysis : Calibration performance

Statistic parameters

- Coefficient of determination (R^2)
- Standard error of calibration (SEC)
- Standard error of prediction (SEP)
- Bias
- Ratio of standard error of Performance to standard Deviation (RPD)

NIR data analysis

Coefficient of Determination (R^2)

- Describes how well the data points fit the statistical model (the line of regression)
- Values range from 0 to 1

Value of R^2	Interpretation
0 to 0.25	Not usable in NIRs calibration
0.26 – 0.49	Poor calibration, research the reasons
0.50 – 0.64	Rough screening
0.66 – 0.81	Screening and approximate calibration
0.83 – 0.90	Usable with caution for most applications, including research
0.92 – 0.96	Usable in most applications, including quality assurance
> 0.98	Usable in any application

Source: Williams (2007)

NIR data analysis

Standard error of calibration (SEC)

- Variability in the difference between predicted values and reference values when the equation is developed from the calibration data set

Standard error of prediction (SEP)

- Variability in the difference between predicted values and reference values when the equation is developed from the validation data set

Bias

- The average difference between the NIR-predicted value and the actual value

NIR data analysis

Ratio of standard error of Performance to standard Deviation (RPD)

- The ratio of standard deviation of validation set to SEP
- Indicate the precision behavior of the prediction in comparison with the average composition of all the samples

RPD	Interpretation
< 1.5	Not usable in NIRs calibration
1.5 – 2.0	Possibility of differentiating the variability of the data
2.0 – 3.0	Good predicting performance
> 3.0	Excellent predicting performance

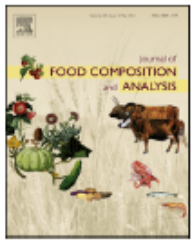
Source: Saeys *et al.* (2005)

Journal of Food Composition and Analysis 38 (2015) 32–41

Contents lists available at ScienceDirect

Journal of Food Composition and Analysis

journal homepage: www.elsevier.com/locate/jfca



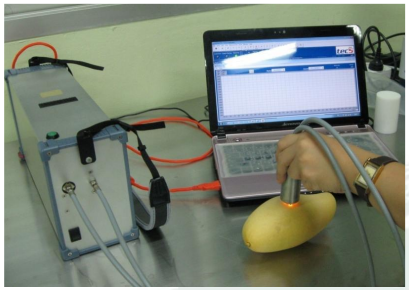
Original Research Article

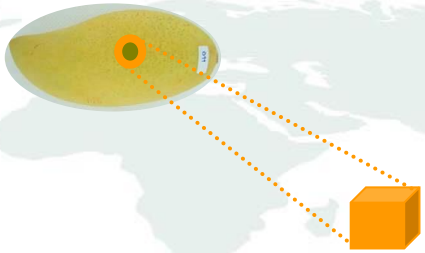
Non-destructive determination of β-carotene content in mango by near-infrared spectroscopy compared with colorimetric measurements

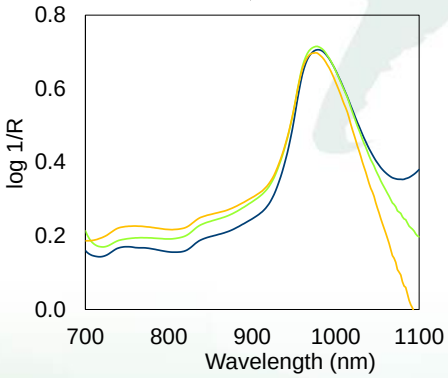
Parika Rungpichayapichet [a], Busarakorn Mahayothee [b,*], Pramote Khuwijitjaru [b], Marcus Nagle [a], Joachim Müller [a]

[a] Universität Hohenheim (440e), Institute of Agricultural Engineering, Tropics and Subtropics Group, Stuttgart 70599, Germany
[b] Silpakorn University, Faculty of Engineering and Industrial Technology, Department of Food Technology, Nakhon Pathom 73000, Thailand

Use of NIRS to predict the quality of mango







Destructive quality measurement

- Peel and flesh color
- β-carotene content

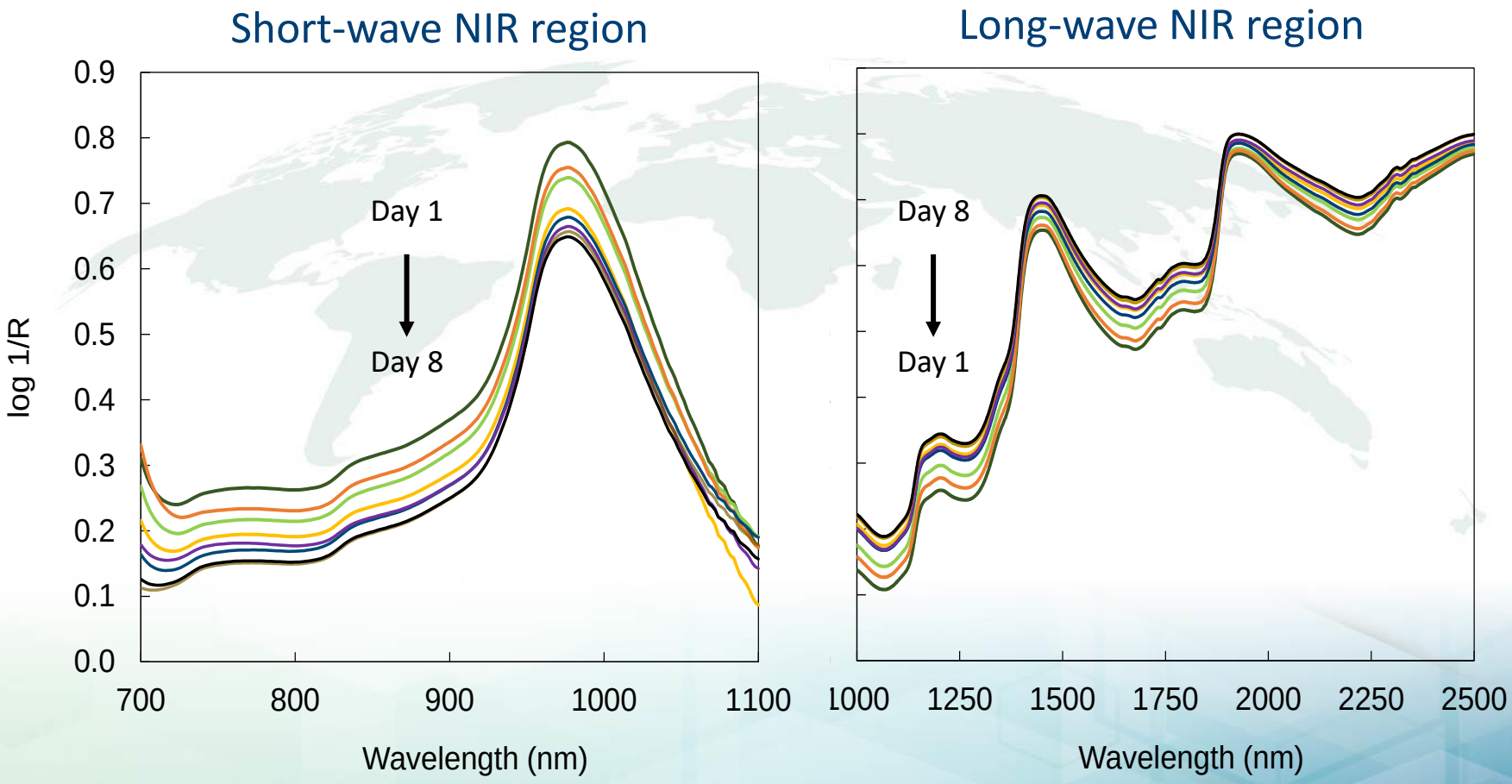
Preprocessing spectral data

Calibration model development using chemometrics (i.e., PLS, MLR)

Validation and prediction model

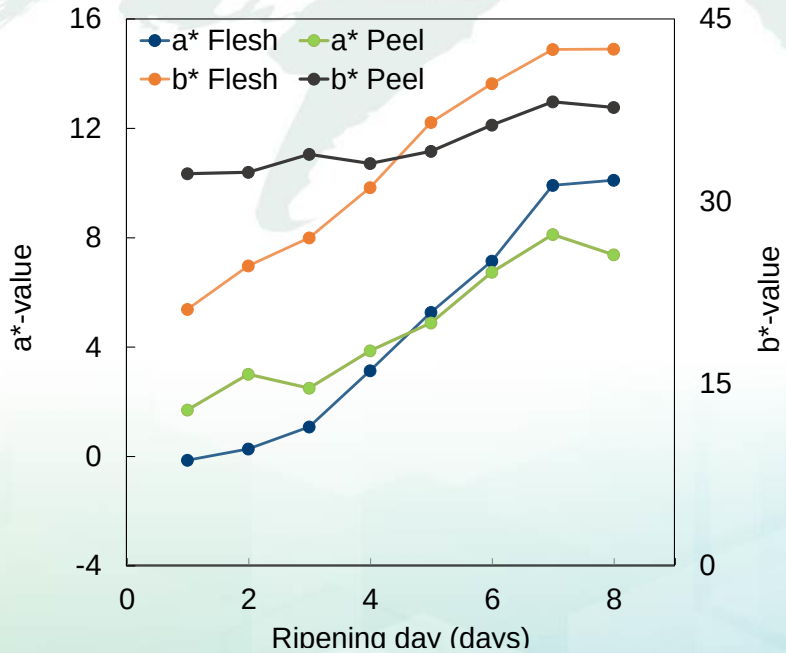
PLS: Partial least square regression
MLR: Multiple linear regression

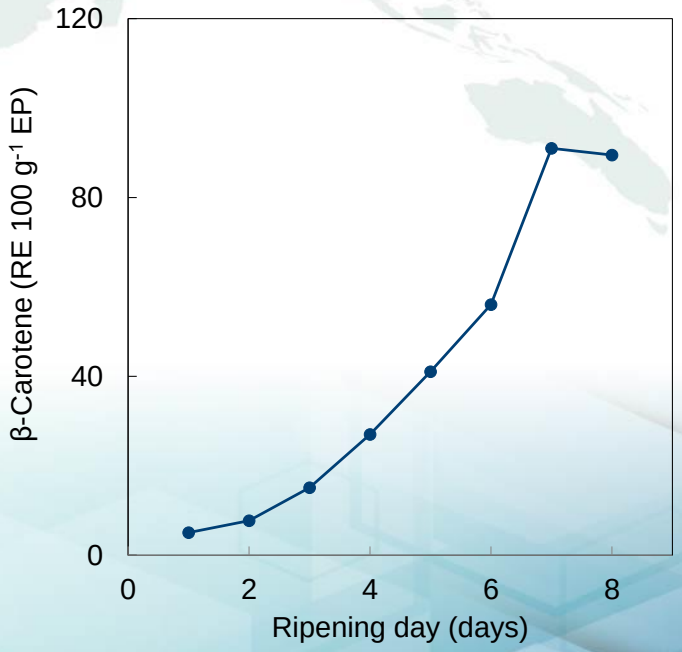
Average raw NIR spectral of mango in different wavelength regions



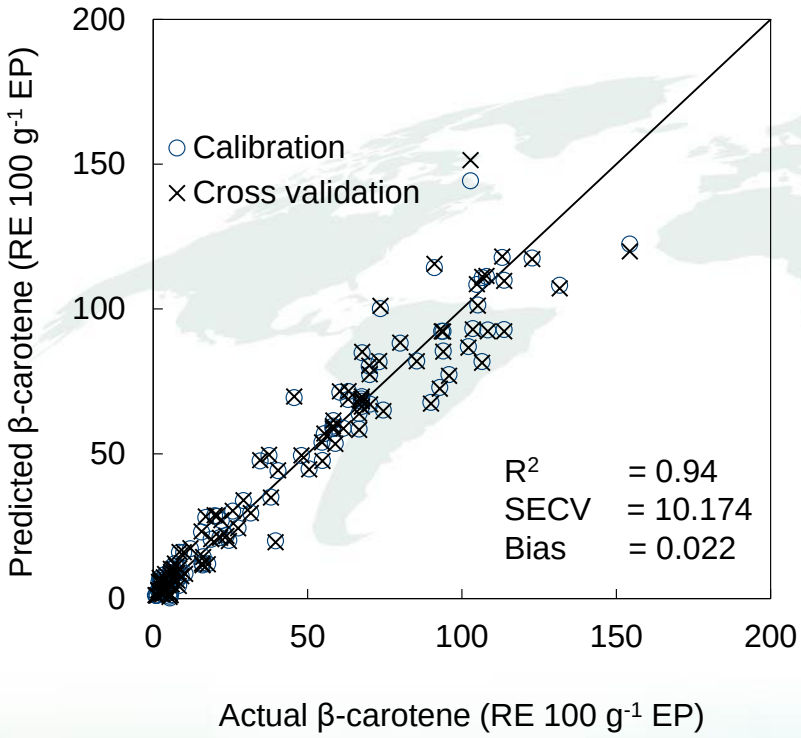
Pearson correlation (r) between β-carotene and color parameters

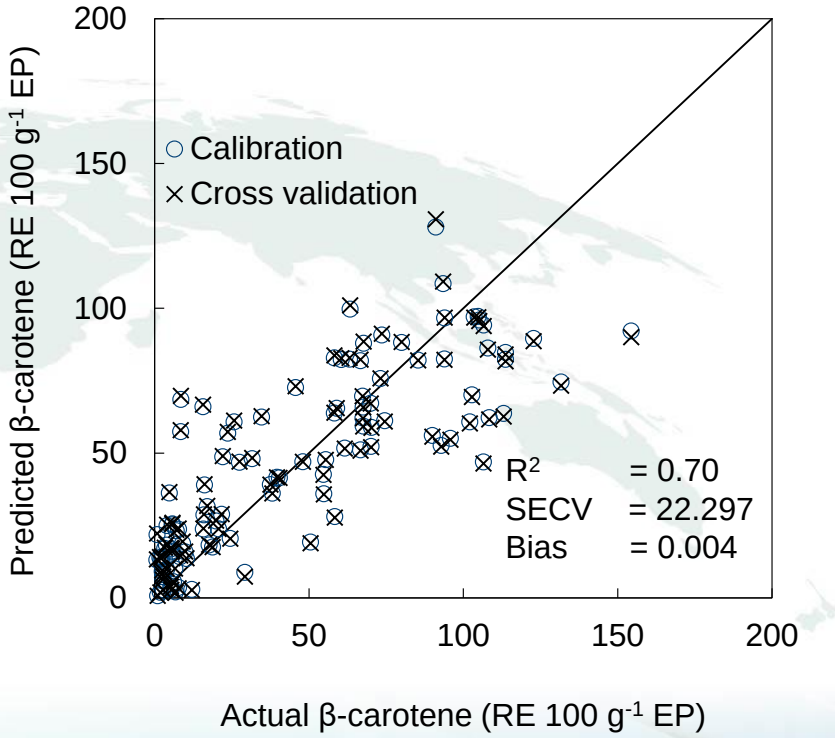
	L*	a*	b*	h°	C
Peel	-0.638	0.743	0.701	-0.691	0.730
Flesh	-0.909	0.959	0.859	-0.934	0.872





MLR calibration from flesh and peel color





Flesh: $[\beta_{carot}] = 212.75 + 39.733C^* - 39.703b^* - 2.293h^\circ$

Peel: $[\beta_{carot}] = 376 + 5.254a^* - 5.116L^*$

PLS regression results of β-carotene prediction: Short-wave region

Spectral preprocessing method	F	RPD	Calibration (n=71)		Validation (n=24)		
			R_C^2	SEC*	R_V^2	SEP*	Bias*
Untreated	9	2.42	0.83	15.296	0.83	15.639	0.325
Savitzky-Golay smoothing (SG)	10	2.39	0.85	14.404	0.83	15.813	-0.854
Savitzky-Golay second derivative (SG´´)	8	2.39	0.82	15.791	0.82	15.818	-3.315
Standard normal variate (SNV)	10	2.14	0.87	13.038	0.78	17.681	-0.339
Multiplicative scatter correction (MSC)	9	2.13	0.97	13.048	0.78	17.740	-0.235
SNV and SG	10	2.42	0.79	16.915	0.82	15.644	-4.476
SNV and SG´´	7	2.36	0.83	15.227	0.82	16.041	-1.702
MSC and SG	9	2.42	0.78	17.076	0.81	15.625	-4.782
MSC and SG´´	7	2.32	0.83	15.198	0.81	16.300	-2.999

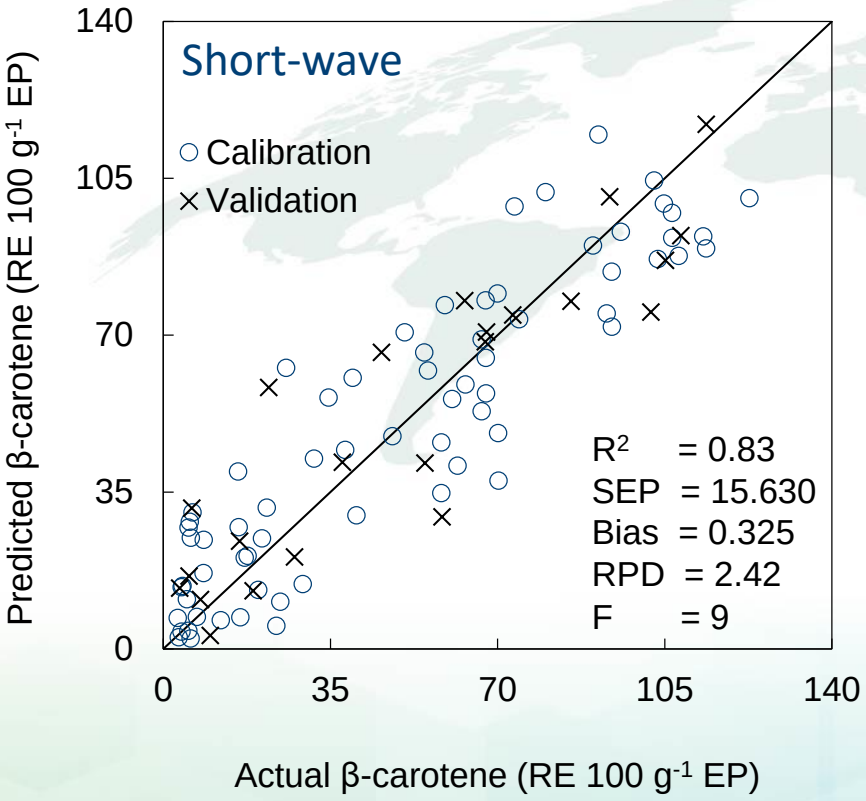
R_C^2: Coefficient of determination, R_V^2: Coefficient of prediction,
SEC: standard error of calibration, *SEP*: standard error of prediction,
F: number of factor, n: number of samples
RPD: the ratio of prediction to deviation
* Unit: RE $100g^{-1}$ EP

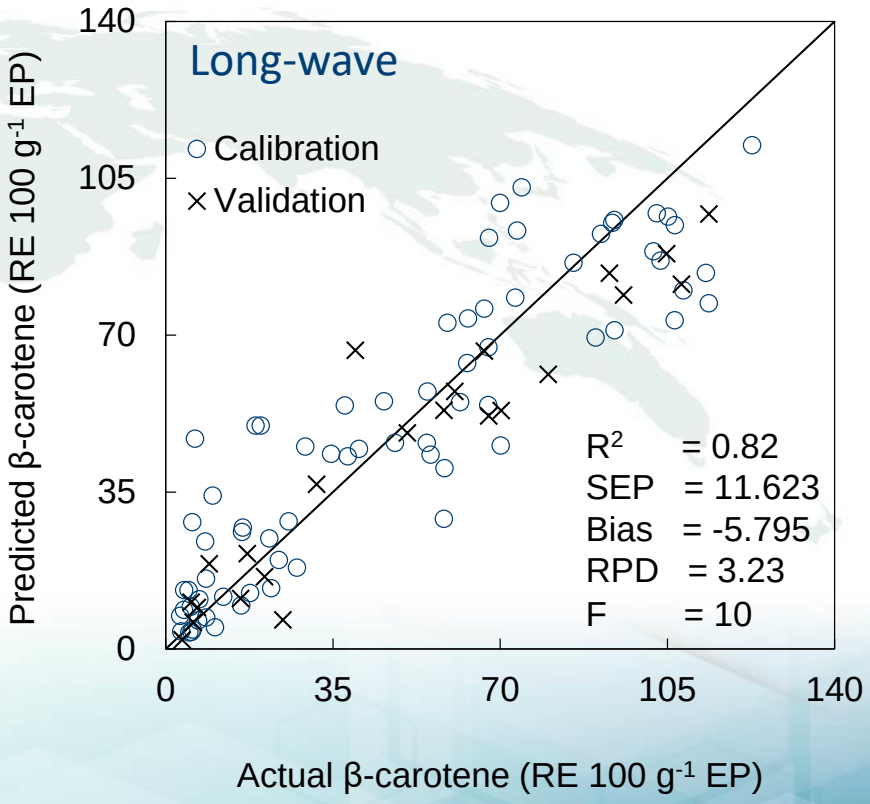
PLS regression results of β-carotene prediction: Long-wave region

Spectral preprocessing method	F	RPD	Calibration (n=75)		Validation (n=25)		
			R_C^2	SEC*	R_V^2	SEP*	Bias*
Untreated	8	2.57	0.69	20.807	0.84	14.606	-2.705
Savitzky-Golay smoothing (SG)	8	2.56	0.68	21.170	0.84	14.672	-2.743
Savitzky-Golay second derivative (SG´´)	4	1.84	0.76	18.146	0.69	20.388	-4.238
Standard normal variate (SNV)	10	3.23	0.82	15.668	0.88	11.642	-5.795
Multiplicative scatter correction (MSC)	10	3.06	0.82	15.753	0.87	12.291	-5.035
SNV and SG	10	3.19	0.80	16.719	0.88	11.778	-5.249
SNV and SG´´	4	1.86	0.79	17.162	0.69	20.173	-5.112
MSC and SG	10	3.01	0.80	16.822	0.88	12.470	-4.340
MSC and SG´´	4	1.87	0.79	17.151	0.69	20.150	-5.109

R_C^2: Coefficient of determination, R_V^2: Coefficient of prediction,
SEC: standard error of calibration, *SEP*: standard error of prediction,
F: number of factor used in calibration, n: number of samples
RPD: the ratio of prediction to deviation
* Unit: RE $100g^{-1}$ EP

Scatter plot of PLS model for β-carotene prediction





Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
Volume 240, 15 October 2020, 118576

Quality assessment of instant green tea using portable NIR spectrometer

Yemei Sun, Yujie Wang, Jing Huang, Guangxin Ren, Jingming Ning, Weiwei Deng, Luqing Li, Zhengzhu Zhang

Using NIR to determine catechin and caffeine contents in instant green tea