Using NIRS to determine sample differences: range, homogeneity,..

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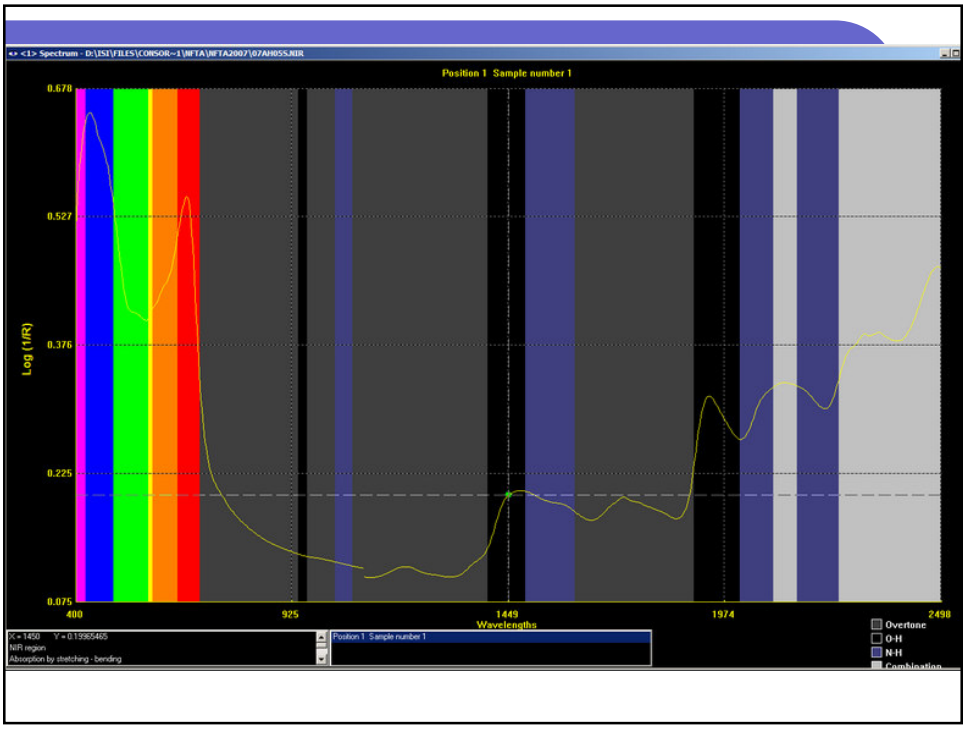
Factors that affect spectra

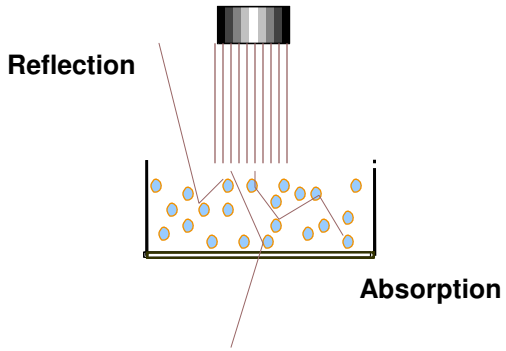
- *Sample prep: drying, grinding;*
- *Chemical composition;*
- Lab environment (Temp. and humidity);
- *Cups/cuvette sampling and packing;*
- Instruments within manufactures;
- Instruments between manufactures;
- …….

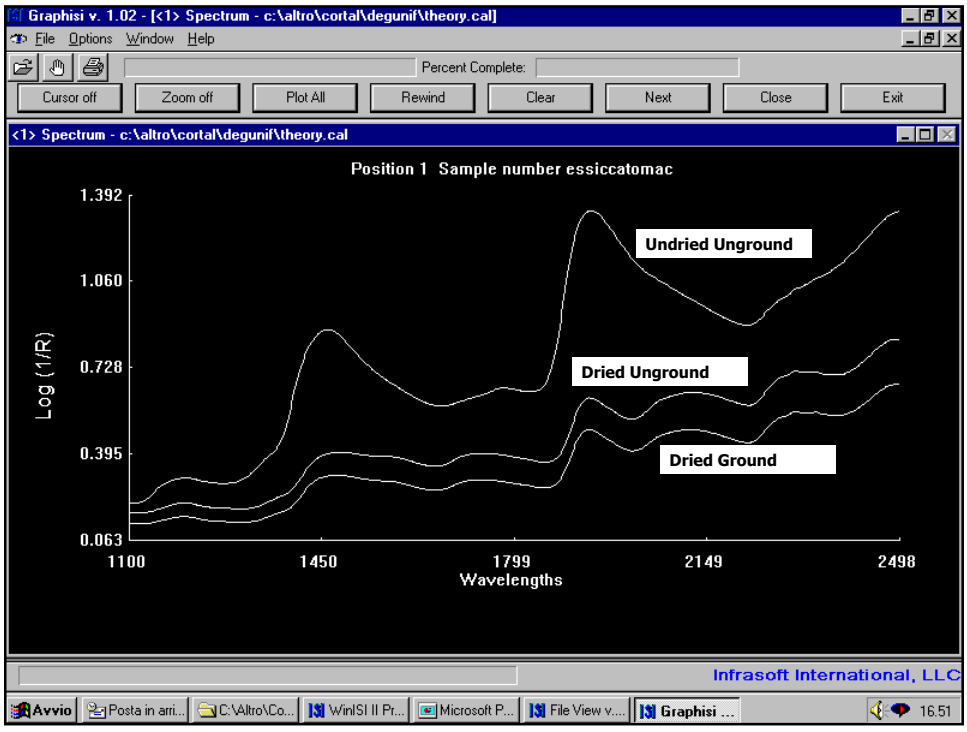
Factors that affect spectra

- *Sample prep: drying, grinding;*
  - Drying will affect chemical composition like residual moisture and fiber content;
  - Particle size will affect the amount of light absorbed;



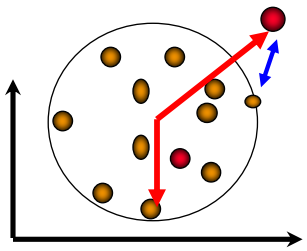
Light - Matter interaction





H values

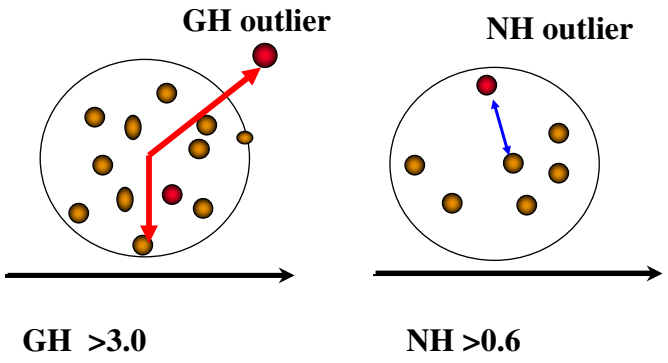
- Scores are used to calculate H values.



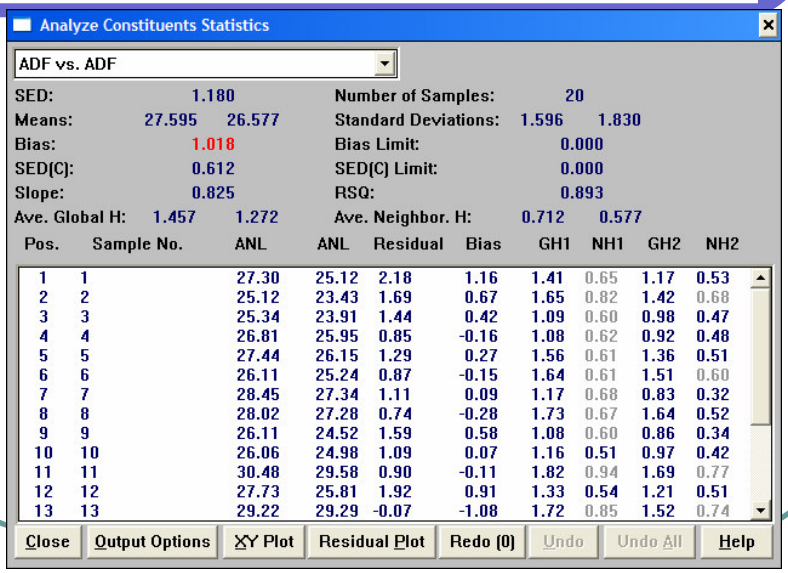
Global H number = distance from the population average [CENTER] (maximum value=3.0)

Neighborhood H number = distance from the closest sample [select] (value=0.6)

PCA & LIB = their use



Effect of sample grinding



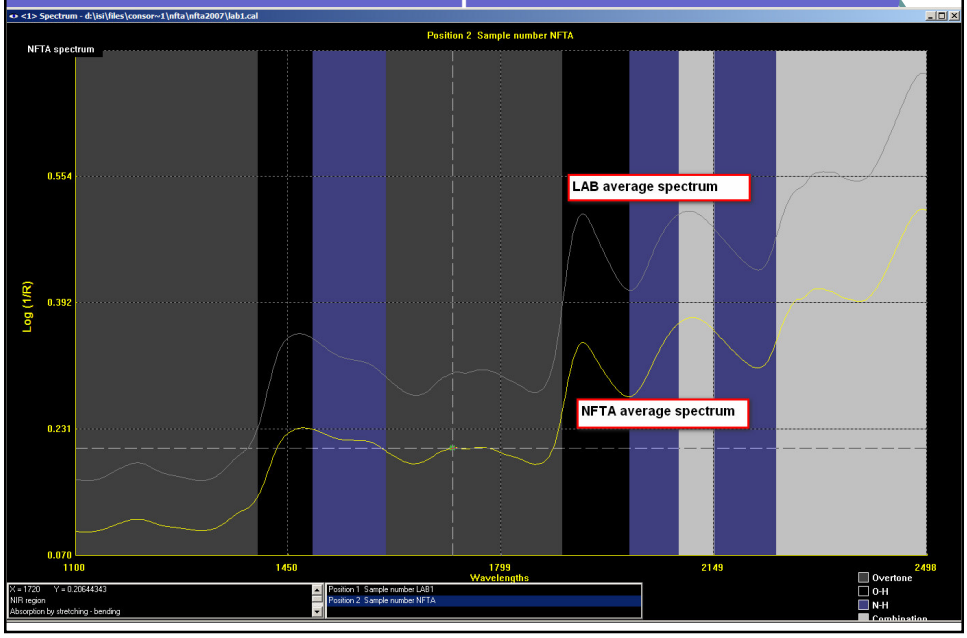
Factors that affect spectra

Real Problem:

"Using NIRSC equation I get good results for NFTA, but predictions don't match composition for my samples"

1. Your chemistry is not good!
   - Nope, we get straight A's with NFTA samples
2. Is something wrong with your sample prep?
   - Nope, we dry at 60℃ and grind at 1mm.

Factors that affect spectra



Factors that affect spectra

1. Is something wrong with your sample grinding?
   - *"Yea, I checked the grinder that is used for the NIR and the impact ring is worn almost completely smooth. "*

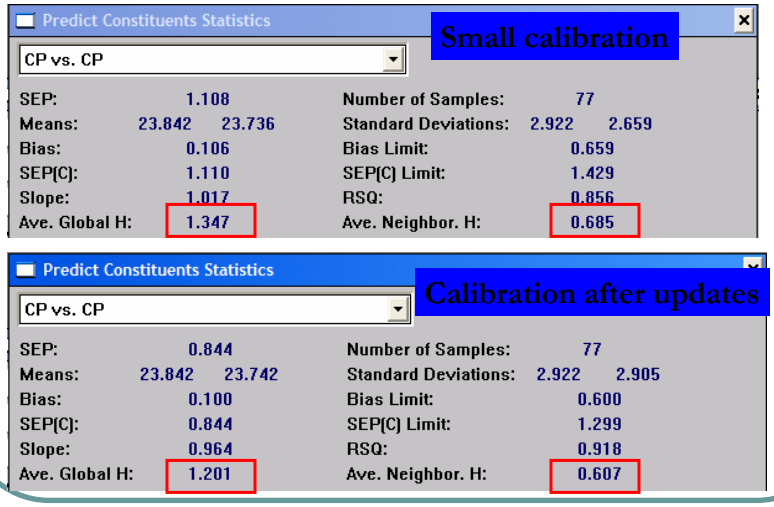
Factors that affect spectra

- *Chemical composition;*
  - Calibration are regression that needs to be built with a range of chemical composition.
  - Odd chemical composition/sample won't contribute to improve calibration;

Look for high NH and GH values.

That doesn't mean high NH and GH have odd composition

Effect of size of calibration on H values

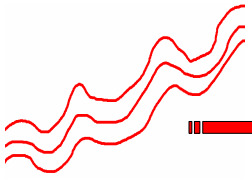


Factors that affect spectra

- *Cups/cuvette sampling and packing;*
  - *It affects repeatability of spectra → results*
  - *How to check?*
    - *Look at predictions;*
    - *Look at spectra;*

Cups/cuvette sampling and packing

Look at predictions;



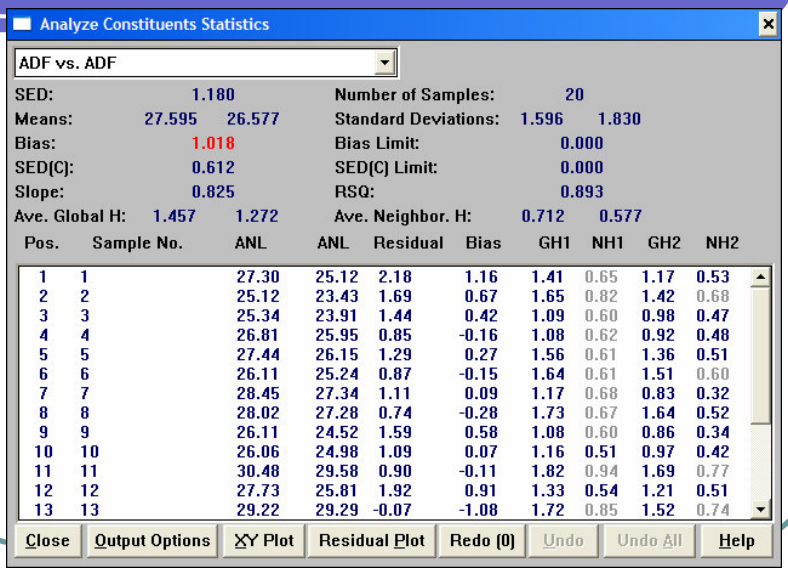
Y=b0+ b1x1+ b2x2+ ……+ bnxn

	#1	#2	#3
DM	93.9	94.2	94.2
CP	15.0	14.8	14.8
ADF	34.2	33.9	34.0
NDF	40.1	39.8	40.0

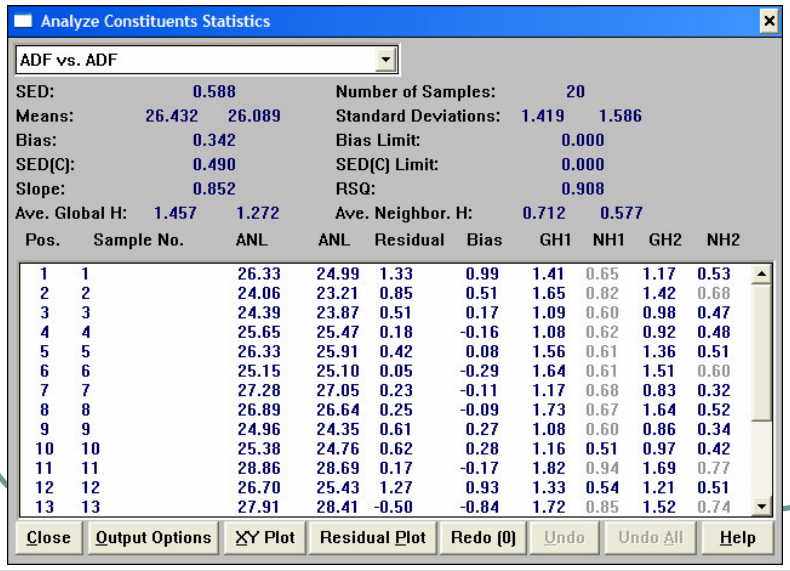
They depends on

- *the calibration equation;*
- *spectra;*

Two prep procedures – same eqa(1)

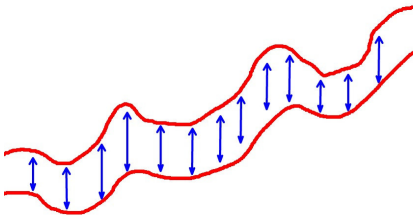


Two prep procedures – same eqa(2)



Root means square (RMS)

- Calculated like SEP (accuracy) or SED repeatability



$$RMS = \sqrt{\frac{\sum_1^n (y_{n1} - y_{n2})^2}{n}}$$

Cups/cuvette sampling and packing

- To increase accuracy run duplicates;
- Check dups with RMS;
- Rescan dups with high RMS;
- Average either spectra or prediction;

SAMPLE	MEAN
1	Only one sample in group, no RMS possible
2	3100
3	2591
4	1972
5	2028
6	5601
7	3997
8	2181
9	4217
10	1276
17	4392
..	
Overall mean:	2252

Summary

- Spectra contains all the information
  - First look at spectra, apply PCA and look at H's values or at RMS [difficult].
- Use the spectra for prediction but remember that eqa can be built for robustness and predictions may not reveal all of the problem.
- Looking at spectra and prediction give us a complete picture of what's going on.