Q & A

Paolo Berzaghi

Q: is any reason to upgrade from WinISI II v. 1.50 to WinISI v. 1.60?

- ????????
- Don't have 1.6;
- Used once during WInISI training, didn't see differences in the calibration, Center, Select;
- Does Foss has something to add?

Tough questions

- What is Paolo's procedure for taking all of the data he receives from the NIRSC to make a calibration?
- what [illegible] calibration that [illegible] samples selected that [illegible]

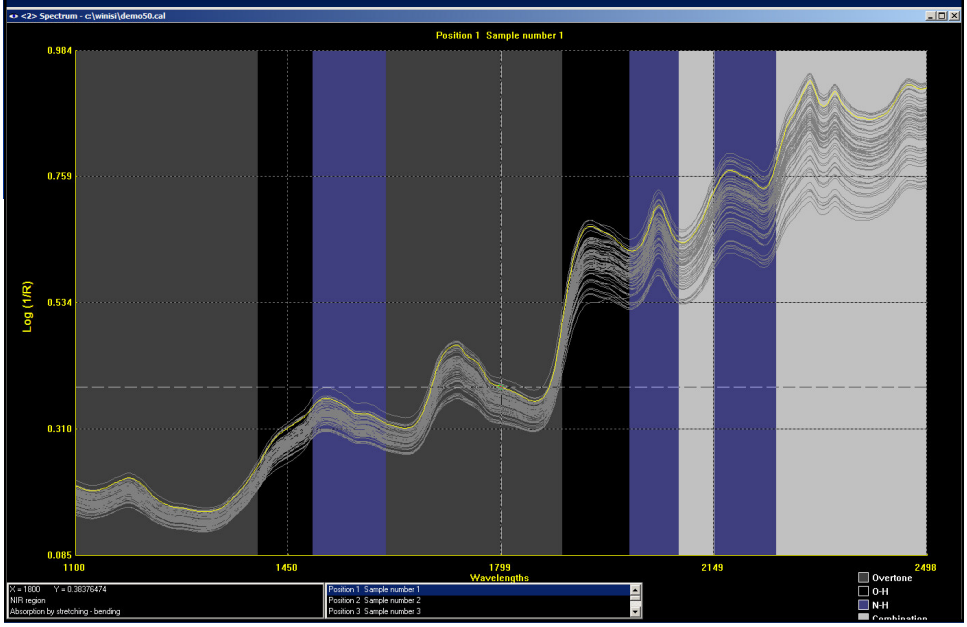
Top Secret..!!!

Tough questions

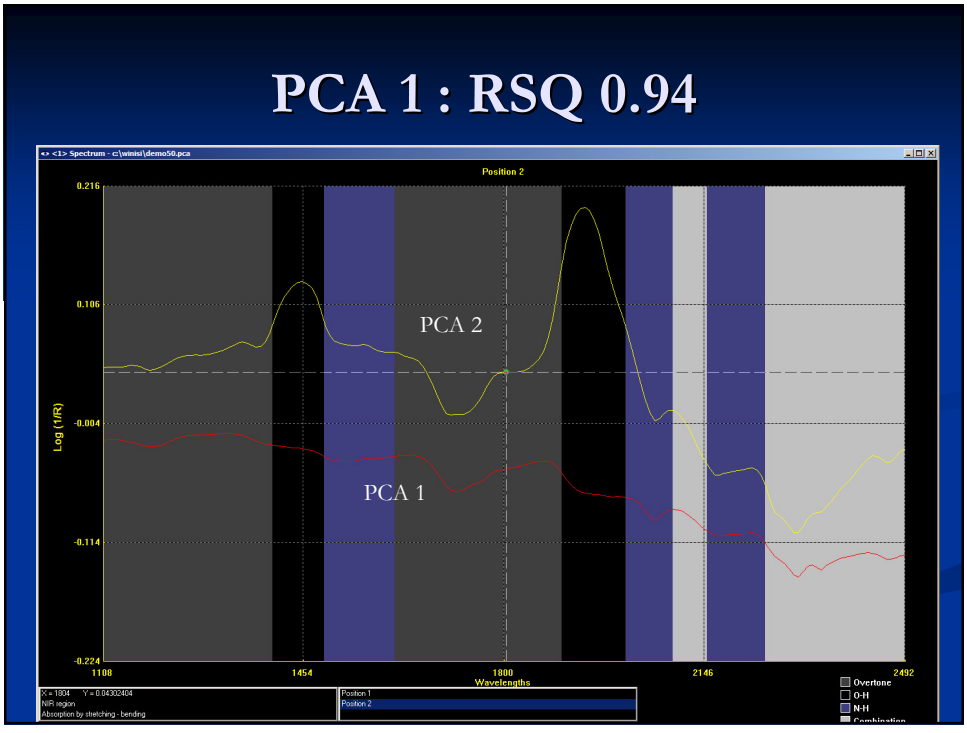
Q: What is Paolo's procedure for taking all of the data he receives from the NIRSC to select samples andmake a calibration?

A: In the past it was PCA only. In the past years we had more specific projects (NDFD, starch) I've had to switch to PLS1 to be more effective. PCA vs. PLS1????

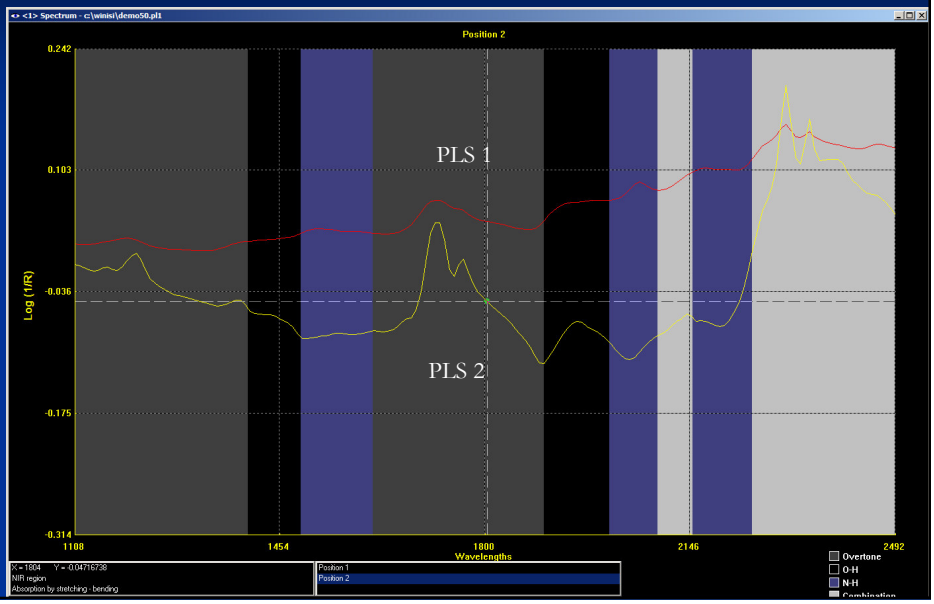
Demo.cal (5000)



PCA 1 : RSQ 0.94



PLS 1 : RSQ 0.64



PCA vs PLS

- PCA – it models the shape of spectra regardless of sample composition
- PLS1 – it models the shapes of spectra which are RELEVANT to sample composition;
- The PLS1 allow us to select those samples that are more important to develop calibration for a specific constituent

Steps to get a good calibration

- Get the right samples!!!!!!
- High quality spectra and high quality chemistry;
- It is cheaper to get good quality spectra than chemistry ---- Take duplicates and average them.
- Prepare a good validation file to fine tune the calibration.

Easy question?

Q: What is a validation set and how do you use a validation set?

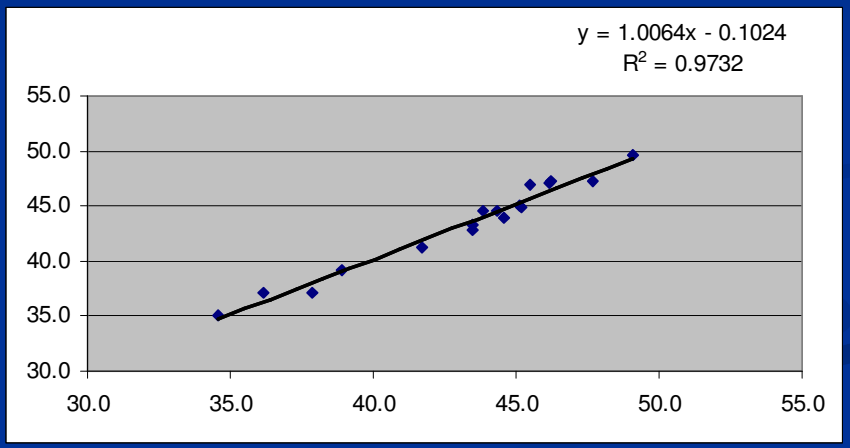
A: a validation set is like a navigation system, without it you may get lost, if you are lucky or you studied the maps (Shenk's notes) you will get were you want to be.

Easy question?

- A validation is a data set of spectra and chemistry not used in calibration. The values predicted based on the spectra are compared to its chemistry defining the accuracy of the calibration.
- Validation samples have to be representative of population variability
- A random validation set may "randomly" give you the wrong answer

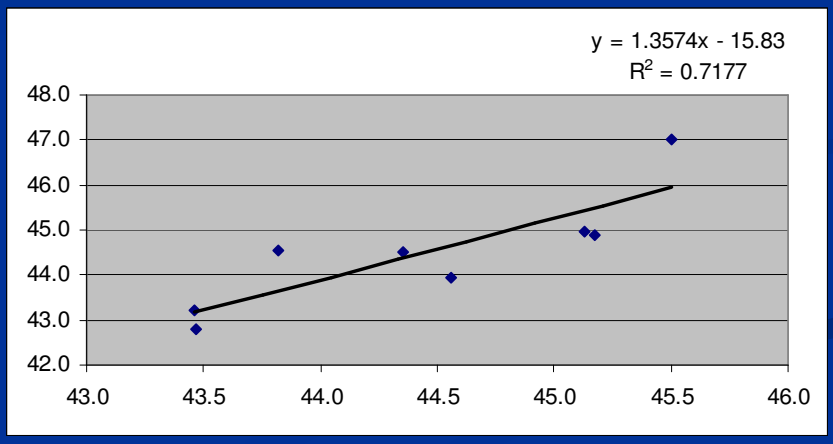
Validation set

Bias=-0.17; SEP=0.68



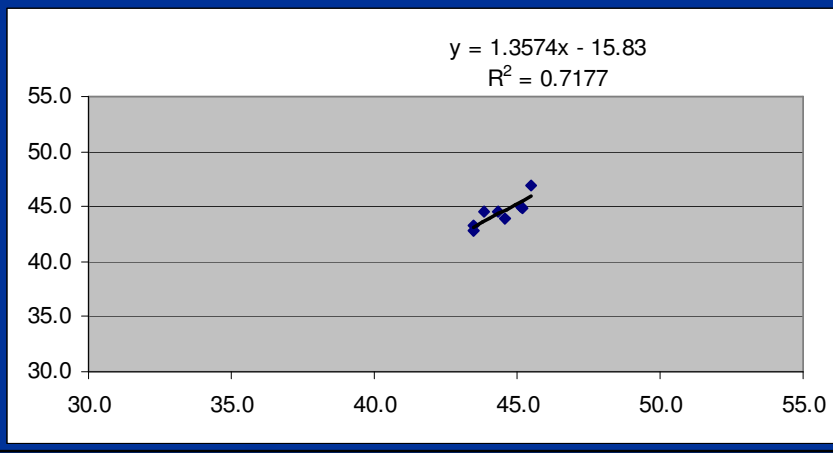
Validation set

Bias=-0.17; SEP=0.47



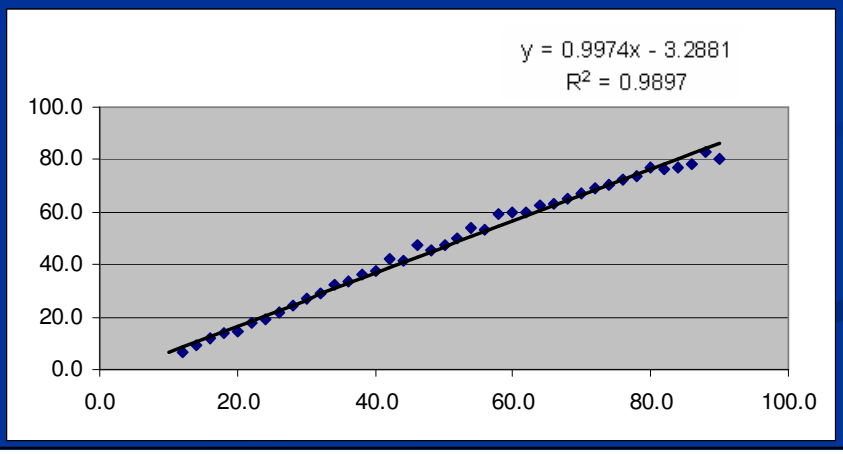
Validation set

Bias=-0.17; SEP=0.47



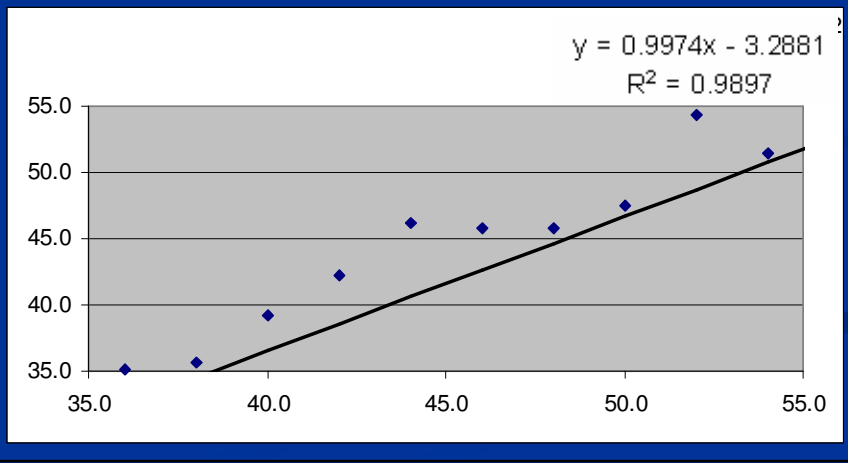
Validation set

Bias=-3.07; SEP=3.87

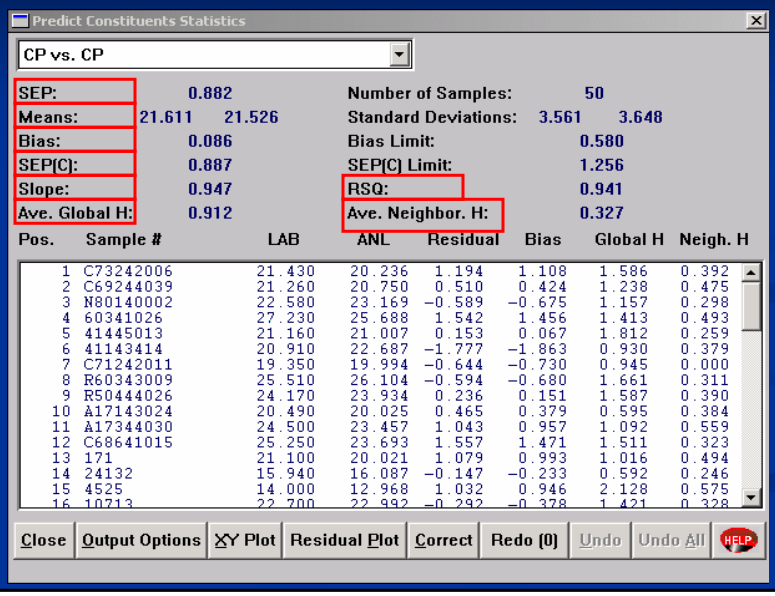


Validation set

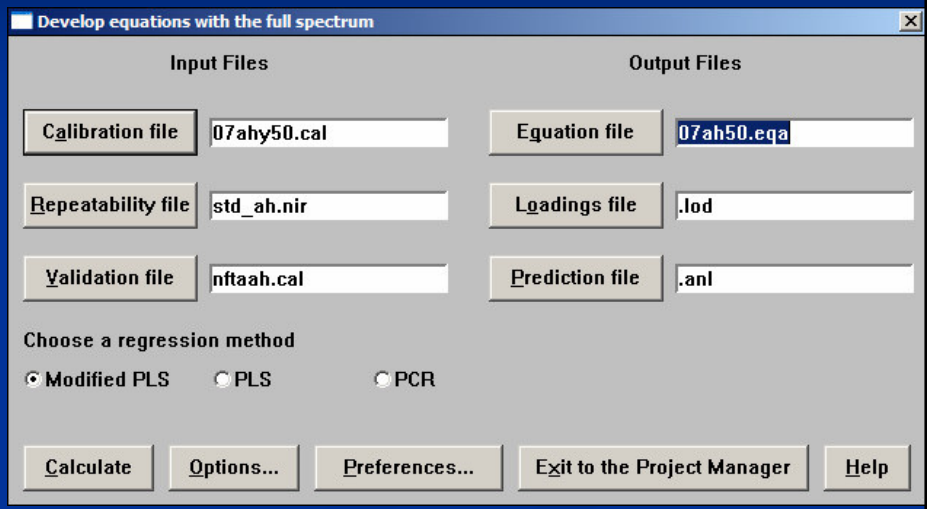
Bias=-3.07; SEP=3.87



Monitor results



Validation file



Validation file

Modified PLS Regression Statistics

Input File	calah.cal		REP File	None	
Validation File	valah.cal		Equation File	None	
Math Treatment	1, 4, 4, 1		Number of variables	173	
Scatter Corrected	SNV and Detrend		Downweight outliers	No	
Constituent	PROTEIN		Number of samples	620	
Mean	20.756	Range	7.82 - 27.52	Standard deviation	2.990

	SEC	R^2	F	SECV	1-VR
1	1.816	0.631	1060.20	1.832	0.628
2	1.098	0.865	1073.90	1.139	0.856
3	1.060	0.874	45.85	1.102	0.865
4	0.951	0.899	150.80	1.007	0.888
5	0.876	0.914	109.82	0.936	0.903
6	0.842	0.921	51.85	0.906	0.909
7	0.758	0.936	145.35	0.842	0.921
8	0.700	0.945	105.99	0.795	0.930
9	0.665	0.951	67.10	0.773	0.934
10	0.639	0.954	51.79	0.732	0.941
11	0.614	0.958	51.88	0.711	0.944
12	0.593	0.961	44.54	0.697	0.946
13	0.577	0.963	34.53	0.693	0.947

Validation file

- Validation file is one of the most important file you must have;
- It MUST have the best quality data you can have because based on that data:
  - We define accuracy
  - We fine tune calibrations

Repeatability file

Q: Is there a repeatability file created using NIRSC instruments that is available to NIRSC labs for calibration purposes? If there is, who would I have to contact to get it?

A: Contact Paolo!!

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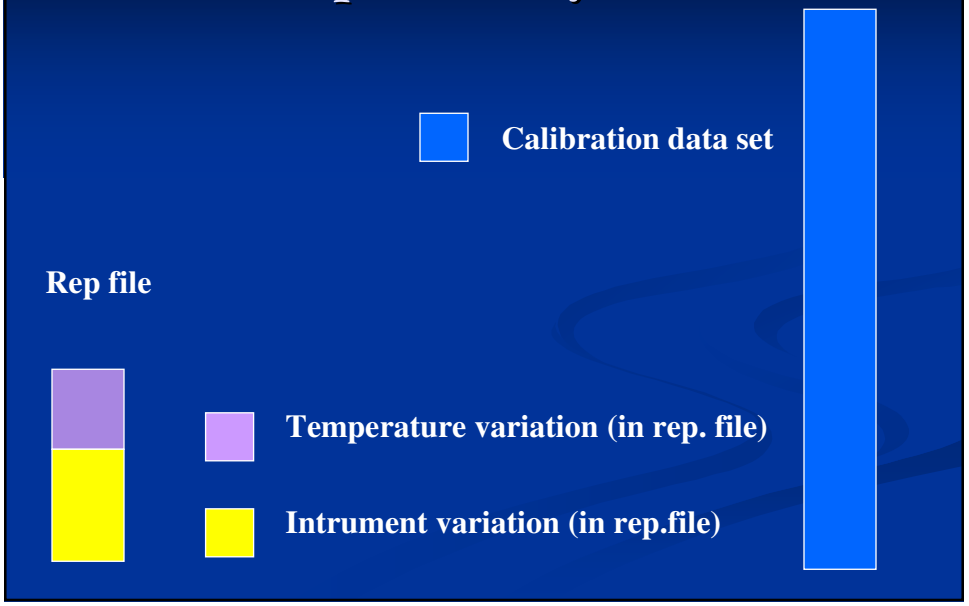
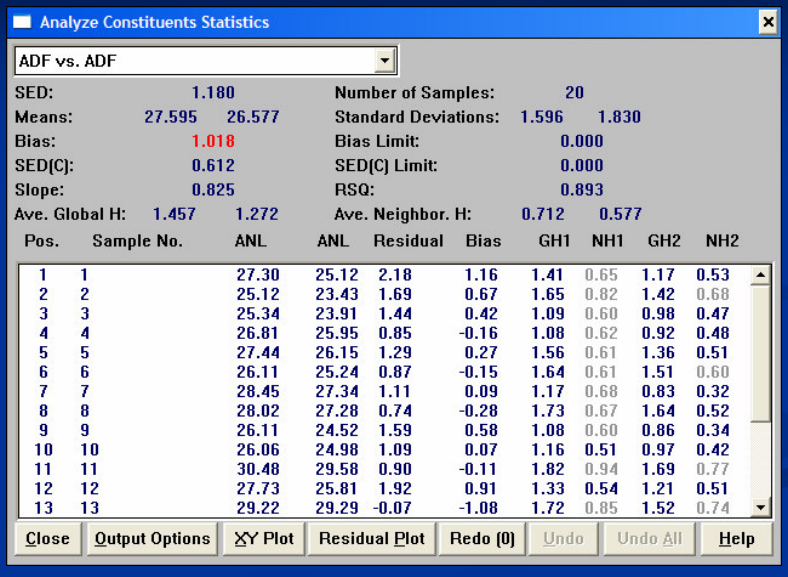
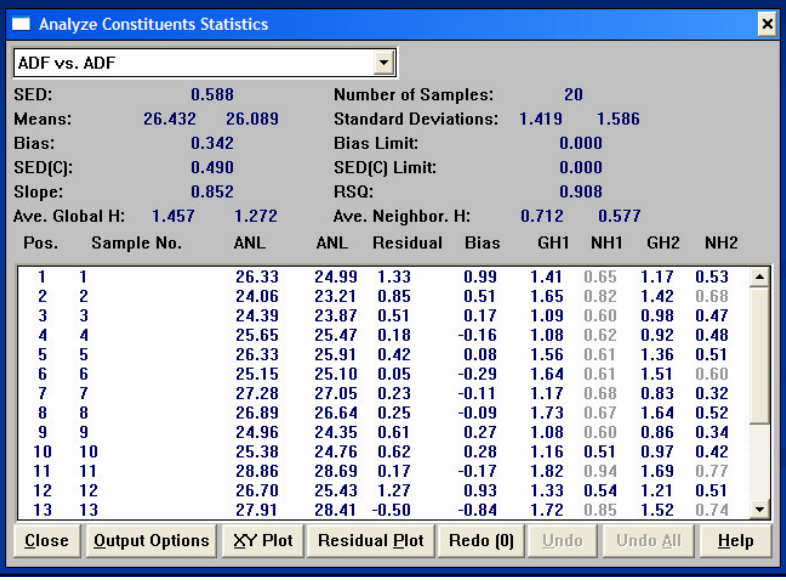
Repeatability file



NO rep



With REp targeting particle size



Repeatability file

- Rep file have to target specific factors for a lab or a network like the NIRC;
- For NIRC we need REP file to increase robustness for particle size, temperature and instrument alignment;
- For your own eqa in your own lab you probably need a rep file targeting different factors

Repeatability file

- Rep file target specific factors for a lab or a network like the NIRC;
- For NIRC we need REP file to increase robustness for particle size, temperature and instrument alignment;
- For your own eqa in your own lab you probably need a rep file targeting different factors;
- Use sample selection and rep file to increase robustness of eqa