NIR & Wood workshop, Italy

Bernhard Tapken M.Sc.

Georg August University Göttingen

Department Wood Biology and Wood Products

Supervisor: Prof. Dr. Carsten Mai

"Estimating the WPG of modified wood with Near Infrared and Raman spectroscopy."

Problem

- Chemical modified wood is getting more and more available
  - Acetylation and furfurylation are on market
  - In research state
    - (DMDHEU)
    - Phenol
    - Melamine

  1. Process control is necessary
     - Controlling the Weight Percent Gain of product
     - Controlling the chemical consumption

  2. Available modified wood has to be distinguished
     - e.g. waste management, etc.

State of Art

- Furfurylation

    - Eikenes, M., Flæte, P., Haartveit, E., Lande, S.;

      Prediction of Weight Percent Gain (WPG) of furfurylated wood bei FT-NIR spectroscopy; IRG; 2004

    - Venas, T., Rinnan, A.;

      Determination of weight percent gain in solid wood modified with in situ cured furfuryl alcohol by near-infrared reflectance spectroscopy; Chemometrics and intelligent laboratory systems; 2008

    - Lande, S., van Riel, S., Høibø, O., Schneider, M.;

      Development of chemometric models based on near infrared spectroscopy and thermogravimetric analysis for predicting the treatment level of furfurylated Scots pine; Wood Science and Technology; 2010

- Acetylation

    - Stefke, B., Windeisen, E., Schwanninger, M., Hinterstoisser, B.;

      Determination of the Weight Percentage Gain and of the Acetyl Group Content of Acetylated Wood by Means of Different Infrared Spectroscopic Methods; Analytic Chemistry; 2008

    - Celen, I., Harper, D., Labbe, N.;

      A multivariate approach to the acetylated poplar wood samples by near infrared spectroscopy; Holzforschung; 2008

    - Schwanninger, M., Stefke, B., Hinterstoisser, B;

      Qualitative and quantitative assessment of acetylated wood using infrared spectroscopic methods and multivariate data analysis; Spectroscopy europe; 2011

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

Targeted wood modifications

- Furfurylation
- Acetylation
- Phenol
- DMDHEU
- Melamine

- The idea is to compare NIR and Raman spectroscopy
- At the moment the Raman spectr. is pending

Used technology

- NIR equipment from Laser Laboratory Göttingen:
    - Spectrometer Polytech System 1750
        - Range: 845 – 1.645nm
        - Solution: 2nm
        - Measuring time: 2s
        - Accumulation: 10

    - Reflection sonde with diffuse reflection

    - Analysis software: Unscrambler X

NIR equipment at the Laser Laboratory e.V. Göttingen

Set up

- Wood species: Pine (*Pinus sylvestris*) & Beech (*Fagus sylvatica*)
- Samples: – 30x30x6mm
    - 10 WPG steps (4,10, …,52, 58) & unmodified samples
    - 8 radial & 8 tangential samples per step

- NIR-measurements
    - Both surfaces of each sample
    - Conditioned state (20°C, 65% RH)
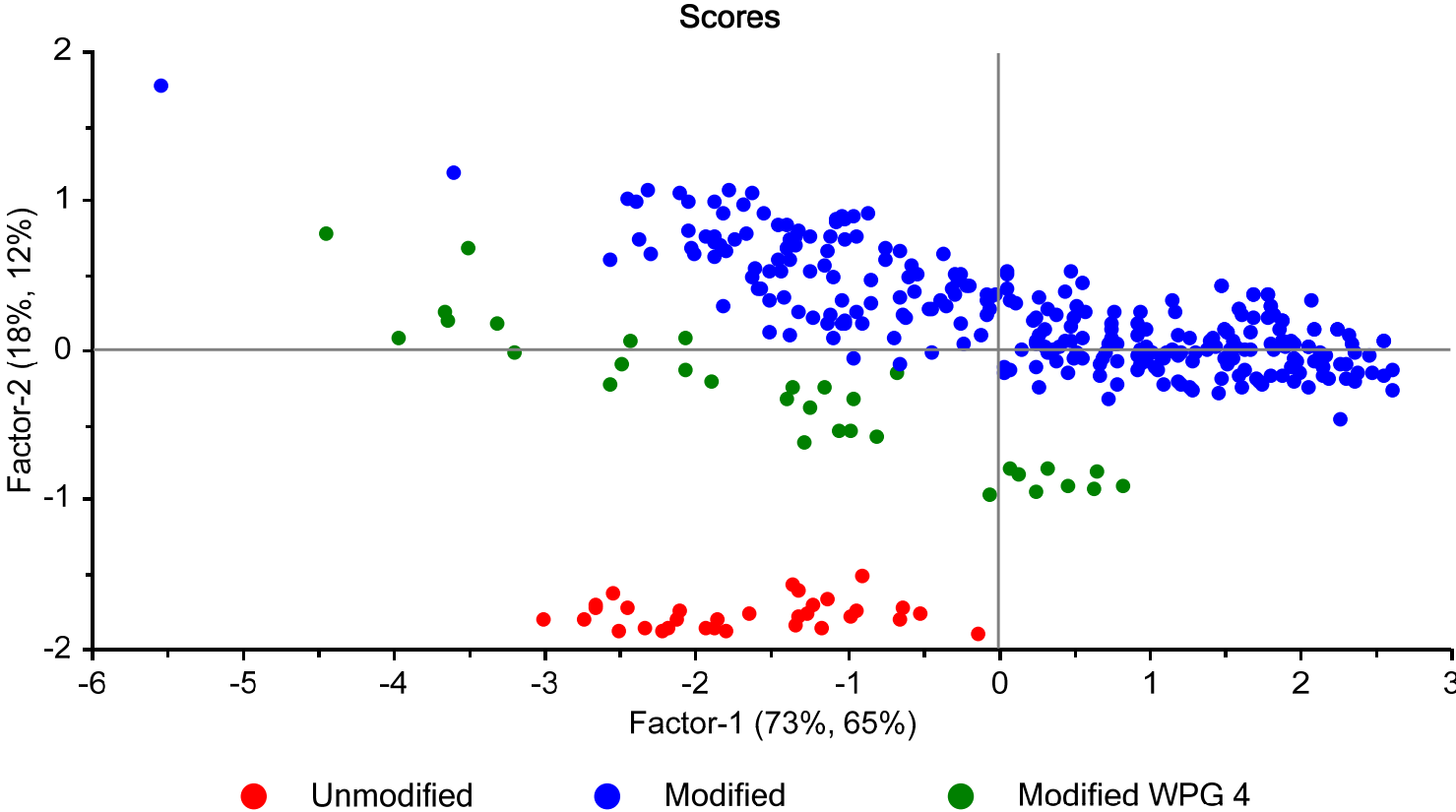   - Oven dried (103°C/24h)

Pine modified with furfurylalcohol

Analysis

- The raw data is transformed with Standard Normal Variate (SNV)
- A Partial Least Squares Regression (PLS) is performed

- The main target is to use a calibration and a validation set
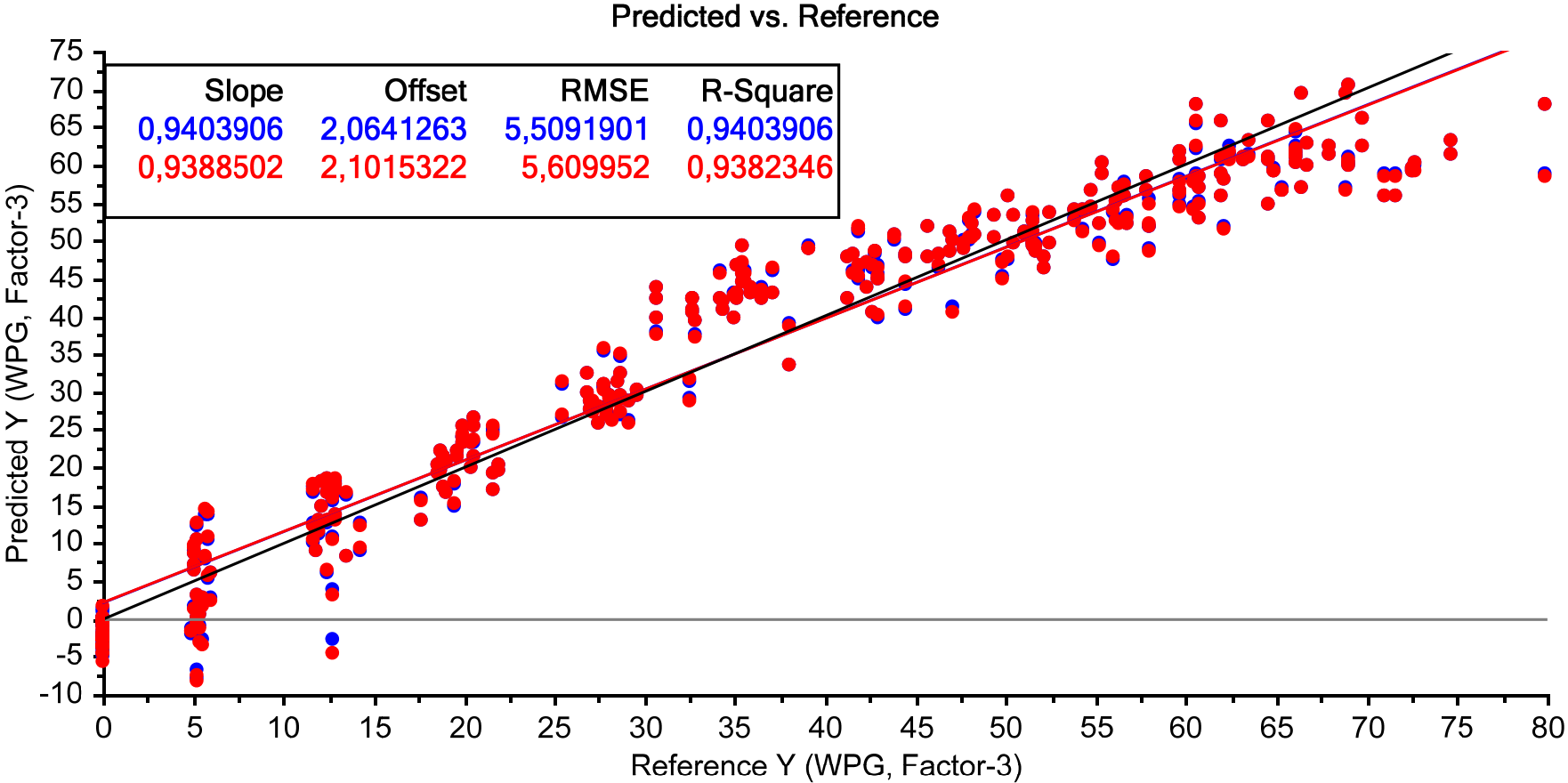- For first impression a cross validation is used

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN
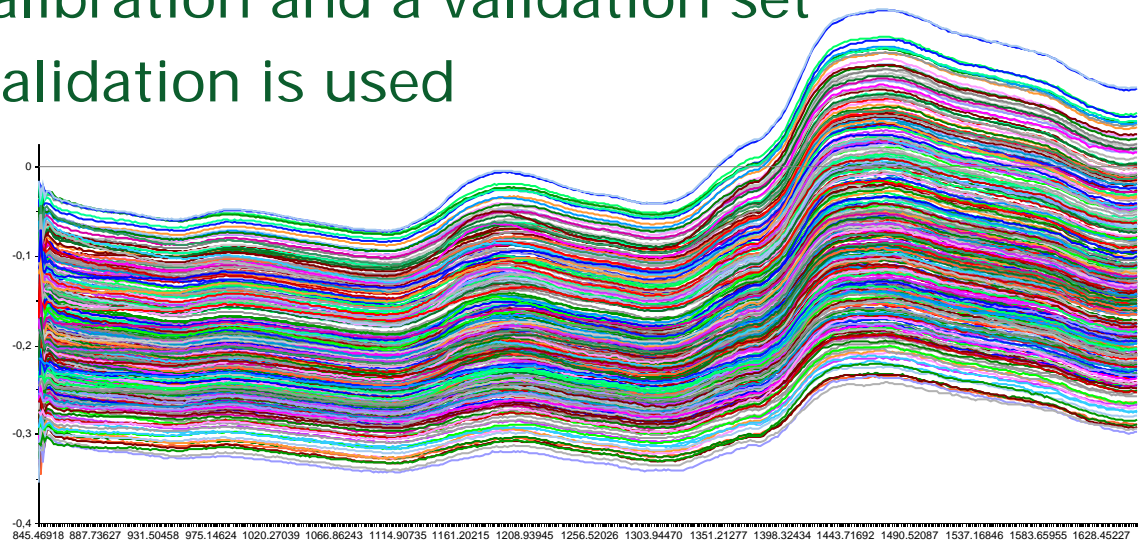
Phenol modification – Beech

PLS scoreplot for phenol modified and oven dried beech wood.

Phenol modification – Beech

Predicted vs. Reference

	Slope	Offset	RMSE	R-Square
	0,9403906	2,0641263	5,5091901	0,9403906
	0,9388502	2,1015322	5,609952	0,9382346

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

Phenol modification – Beech

Predicted vs. Reference

	Slope	Offset	RMSE	R-Square
	0,9281915	3,0108247	4,941596	0,9281915
	0,9244887	3,1699739	5,0815969	0,9246665

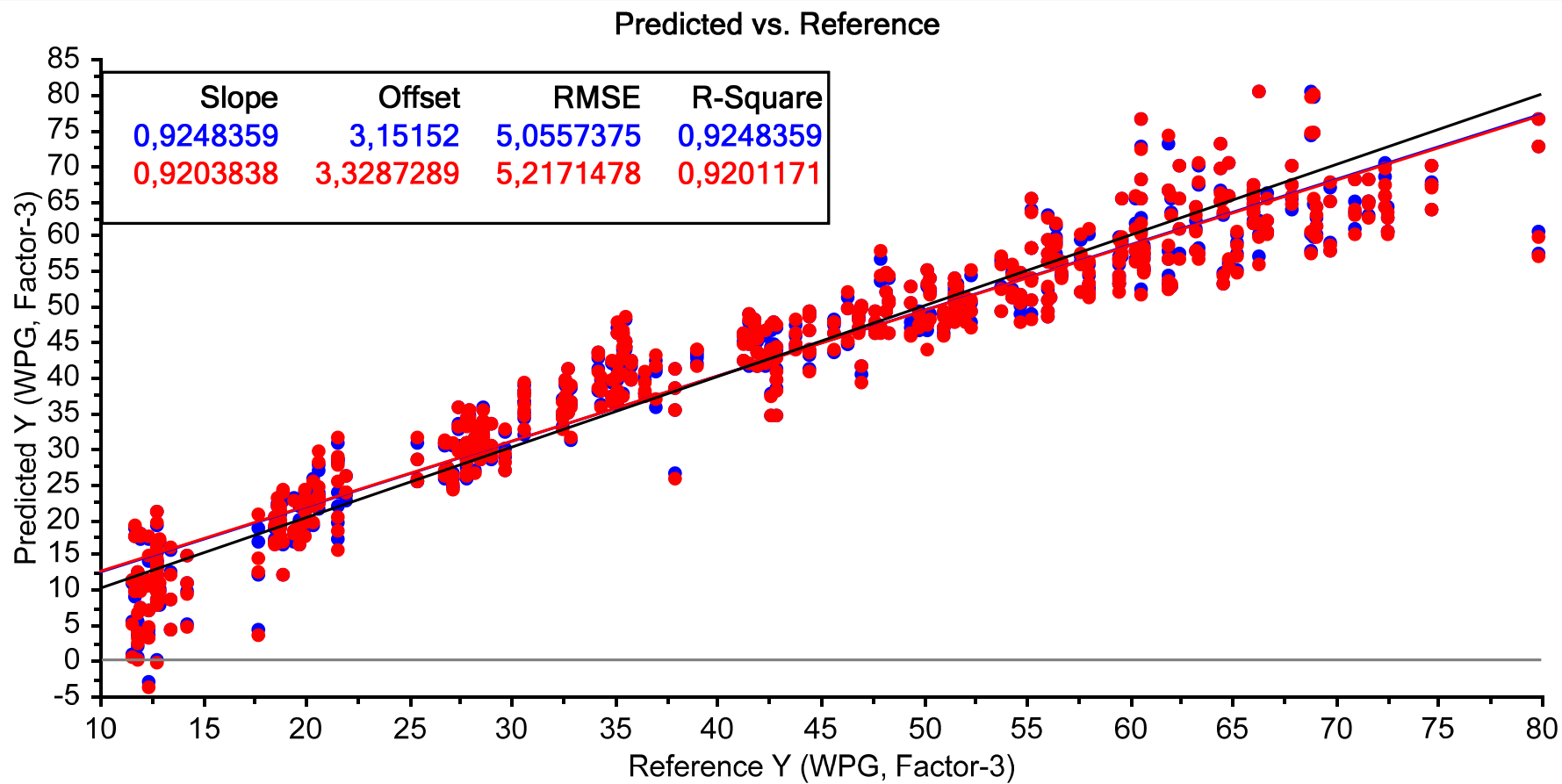Predicted Y (WPG, Factor-3)

Reference Y (WPG, Factor-3)
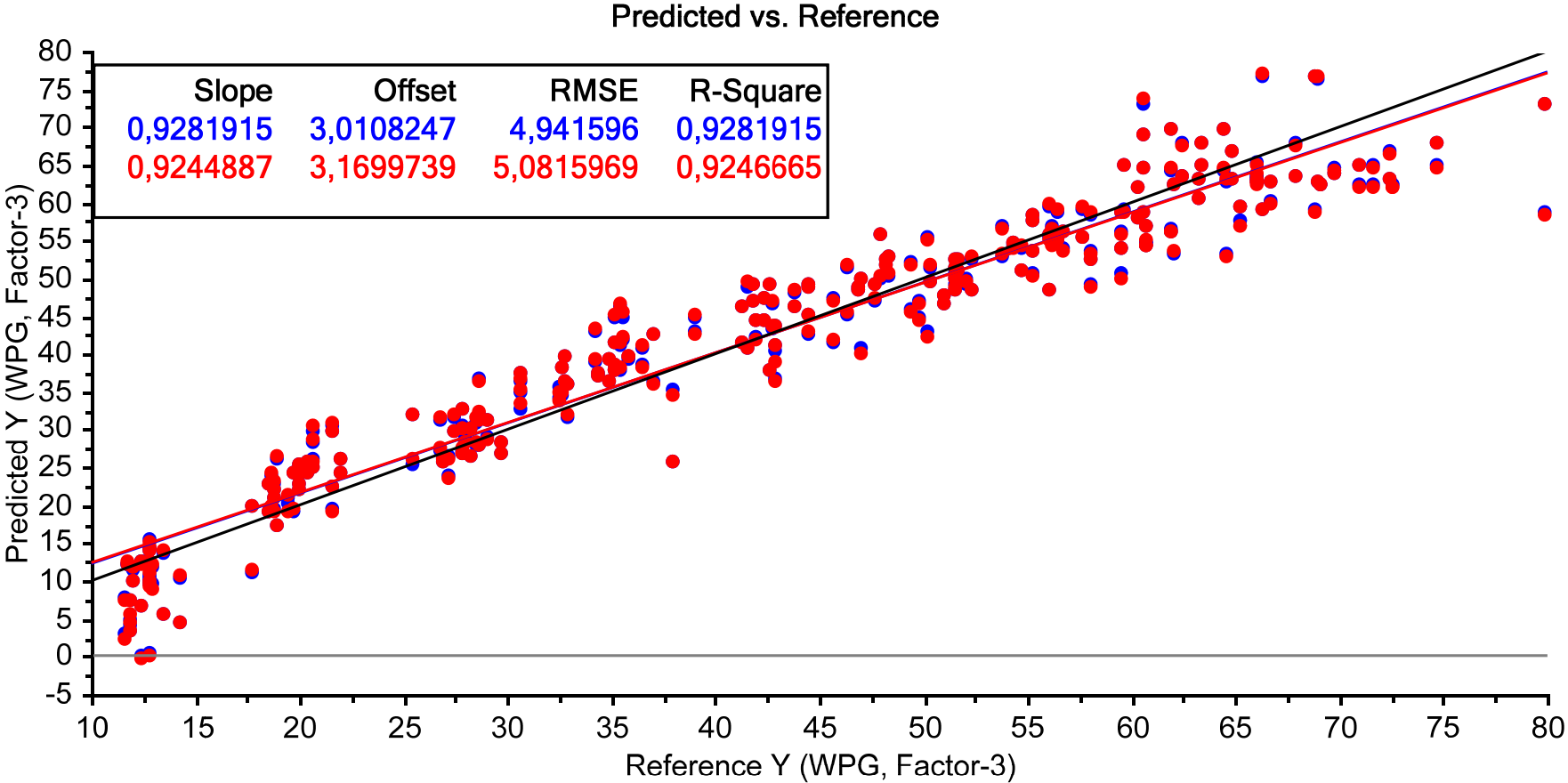
Phenol modification – Beech
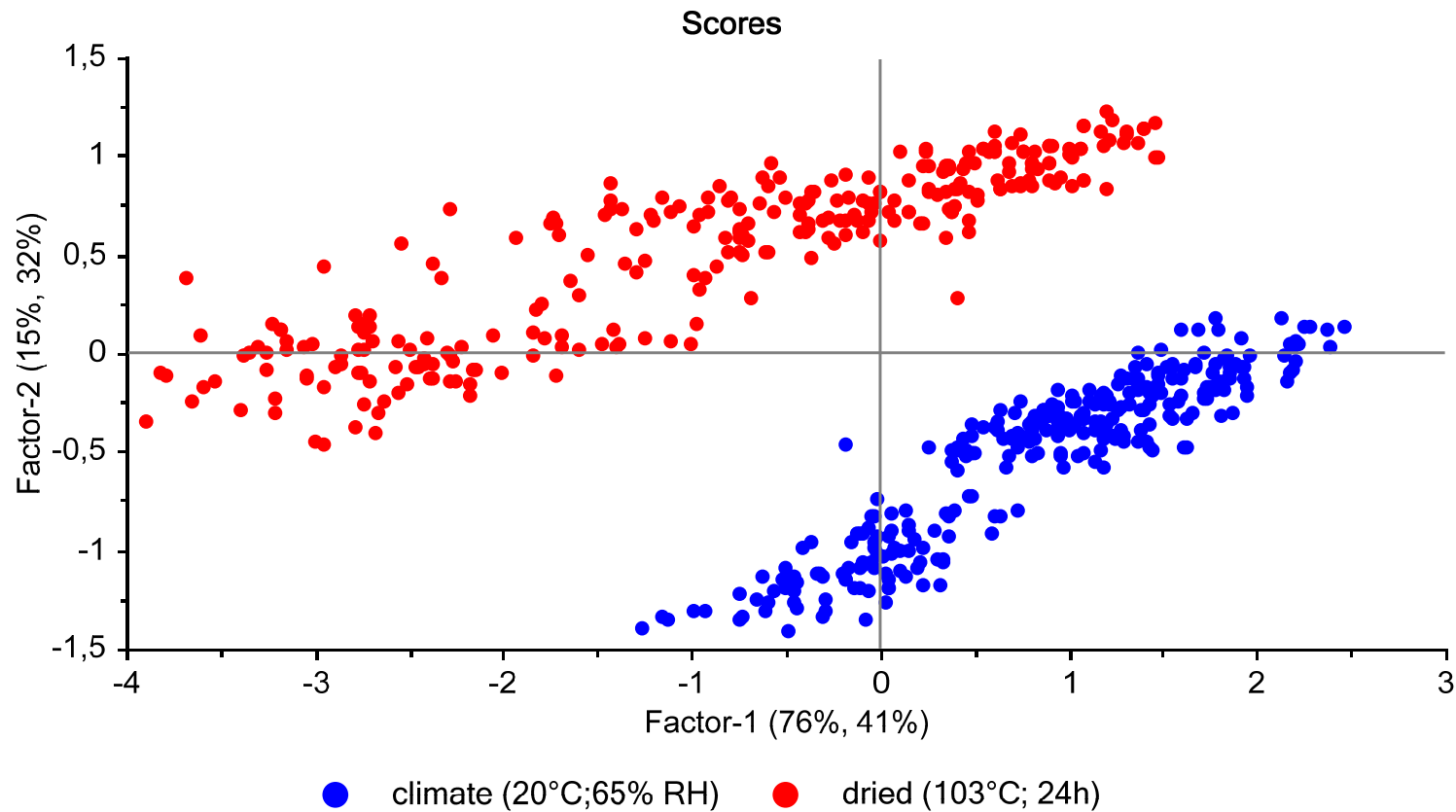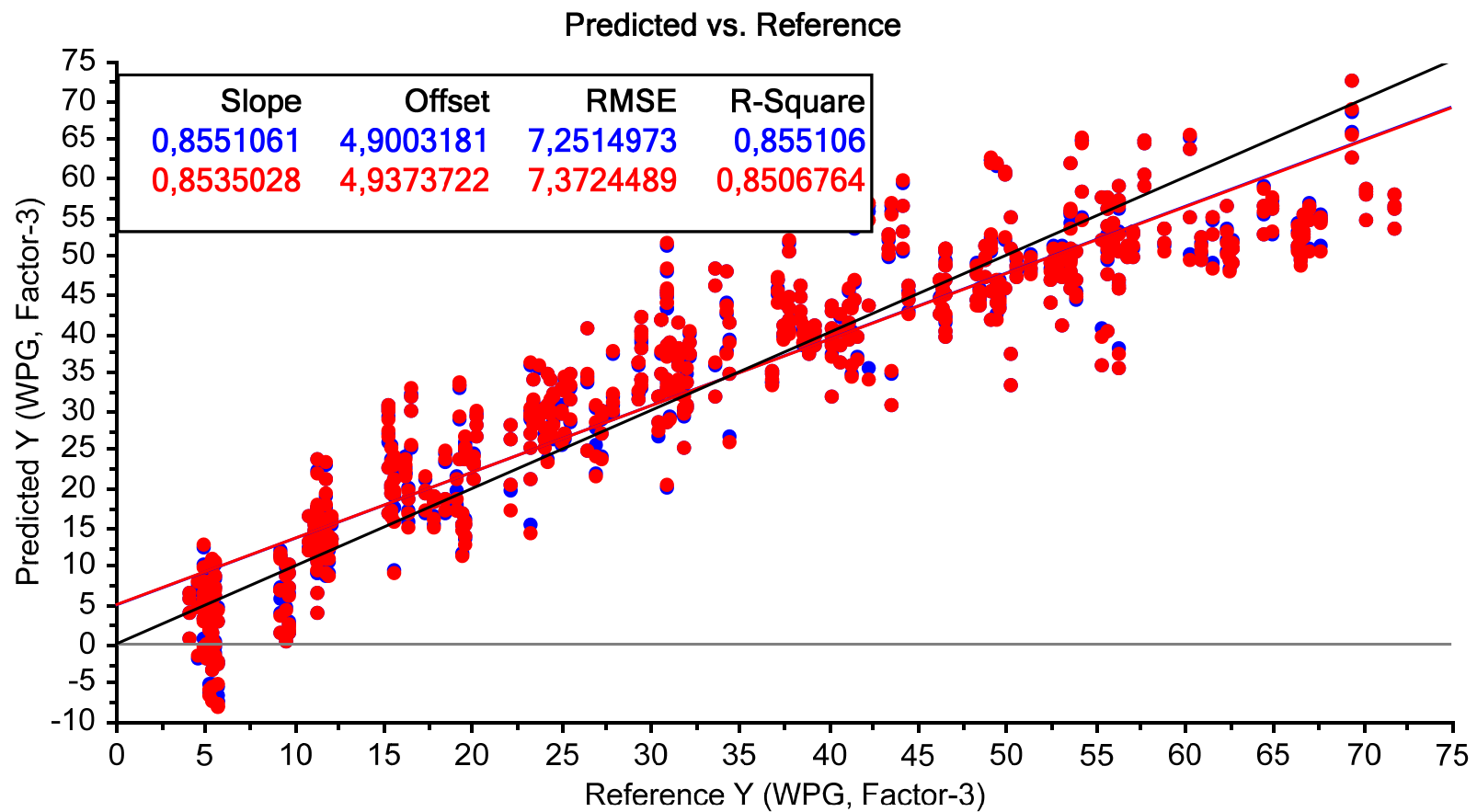

PLS scoreplot for phenol modified beech wood (climated and oven dried samples).

Phenol modification – Beech

Predicted vs. Reference

	Slope	Offset	RMSE	R-Square
	0,9248359	3,15152	5,0557375	0,9248359
	0,9203838	3,3287289	5,2171478	0,9201171

Predicted Y (WPG, Factor-3)

Reference Y (WPG, Factor-3)

Phenol modification – Pine

Predicted vs. Reference

Slope	Offset	RMSE	R-Square
0,8551061	4,9003181	7,2514973	0,855106
0,8535028	4,9373722	7,3724489	0,8506764

Predicted Y (WPG, Factor-3) vs. Reference Y (WPG, Factor-3)

DMDHEU modification – Beech

Predicted vs. Reference

	Slope	Offset	RMSE	R-Square
	0,9194914	2,1019475	5,305686	0,9194913
	0,9133886	2,2776814	5,7035198	0,9078365

Predicted Y (WPG, Factor-7)
Reference Y (WPG, Factor-7)

DMDHEU modification – Pine

Predicted vs. Reference

	Slope	Offset	RMSE	R-Square
	0,7981882	4,2743168	6,8149719	0,7981883
	0,7947145	4,3390045	7,0094328	0,7868299

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

Questions

- Can I use the spectra of both surfaces of one specimen in the cross validation?

- Is there a difference if I use the WPG (%) or the mass of chemical (g) for the PLS?

Thank you for your attention.