Overview of the best PLSR-results for metal content prediction

	Cu	Pb	Zn	Cd	Ni	Cr	K
R^2_{cv}	0.65	0.76	0.69	0.77	0.64	0.71	0.51
$RMSE_{cv}$	14.79	11.24	53.81	0.51	3.55	23.36	291.59
RPD_{cv}	1.53	1.95	1.80	2.11	1.71	1.66	1.42
input spectra	1st	1st	1st	1st	1st	1st	CR
n of components	2	2	1	1	1	1	3

- 50 % of the input data (n =21) were used for model **calibration**
- 50 % of the input data (n = 21) were used for model **validation**
- PLSR-model run with a maximum number of 20 components, including **leave-one-out cross-validation**
- **Akaike Information Criteria** was implemented to select the best model result

R^2 = coefficient of determination

RMSE = Root Mean Square Error (in mg kg^{-1})

RPD = Ratio of *Prediction Deviation*

CV = Cross Validation

1st = 1st derivative reflectance spectra

CR = Continuum removed reflectance spectra