

Remediation-related monitoring of heavy metal concentration of contaminated Technosol using hyperspectral measurements.

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Study Site

Introduction

Hyperspectral measurements combined with heavy metal (HM) estimation models at former sewage farms in Ragow, Berlin, provides a first study on Technosols with highly inhomogeneous soils and a high variability in HM content to improve and control existing remediation methods on HM contaminated Technosols.

Conclusion

Method

Results

Model Construction

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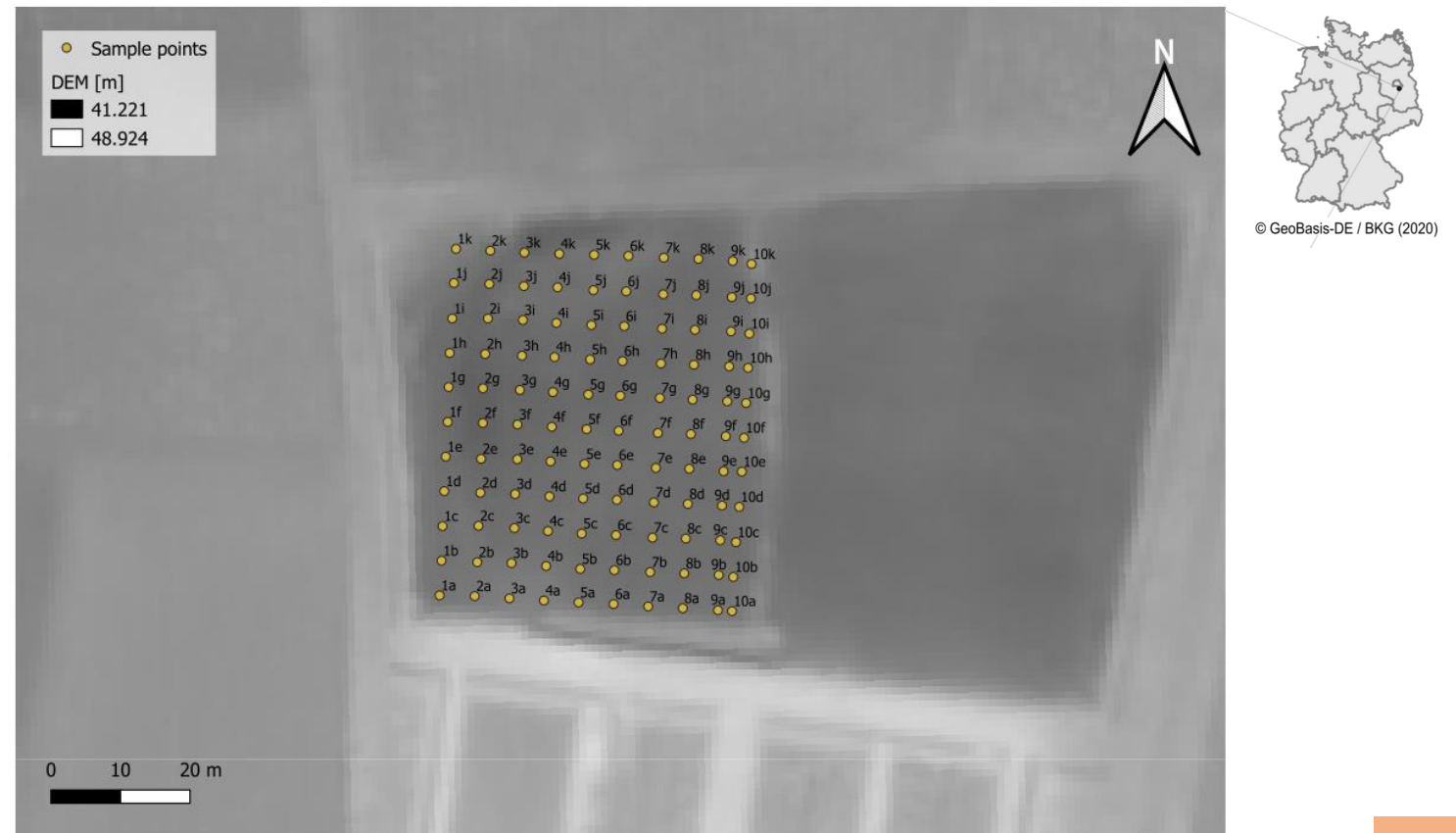


Study Site

Potentially contaminated sites e.g. former sewage farms are characterized by long-term irrigation, resulting in Technosols with HM contamination, organic pollutant and partially thick sewage sludge layer.

Soil Sampling

Such highly mixed material are found at former sedimentation basins. Here, the soil sampling took place in a 5x5m grid at the depth of 15 – 20cm.



Spatial distribution of the sample locations in Germany, Berlin. The underlying map display the sedimentation basins.

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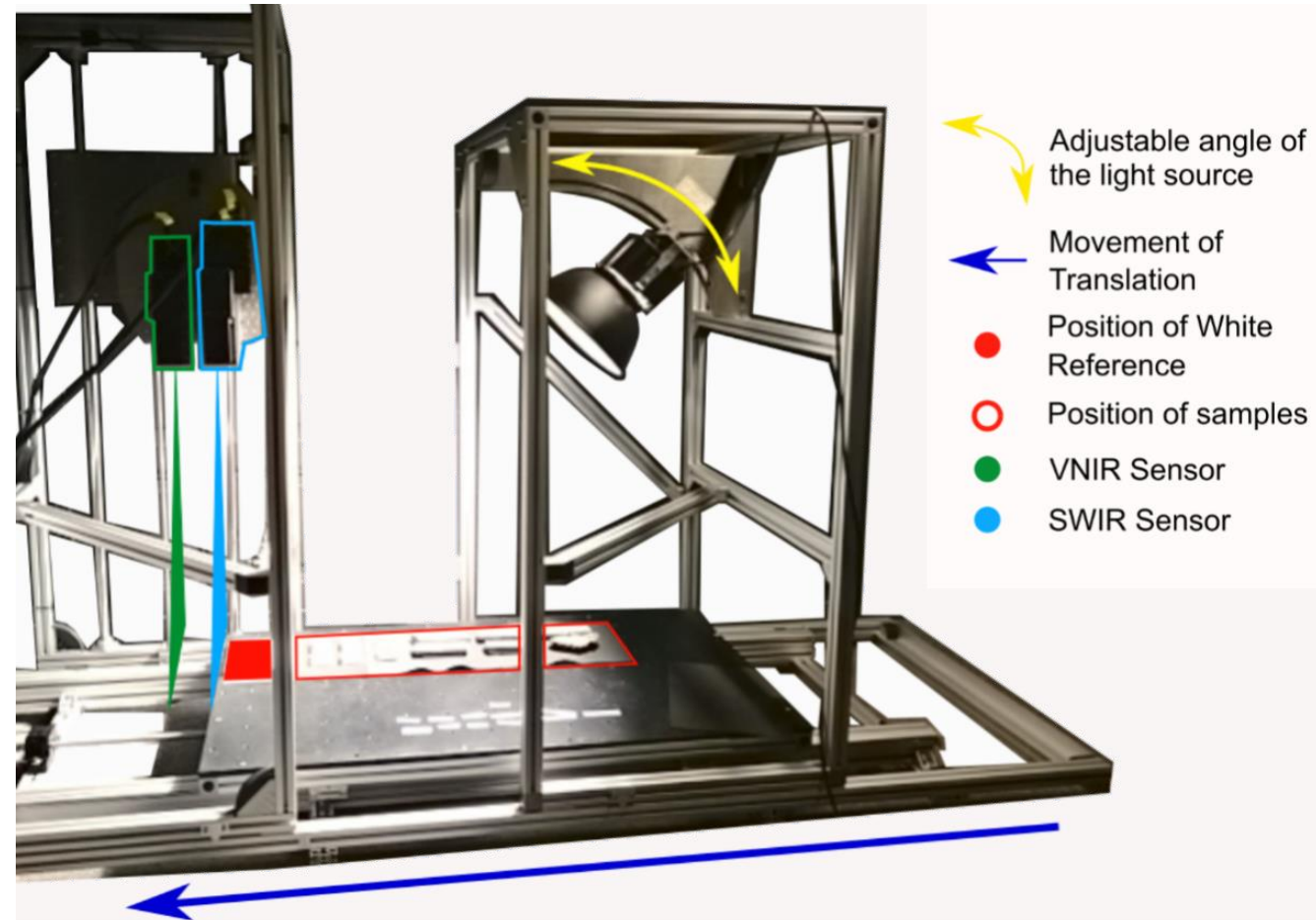
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Method

- Laboratory measurements -

Hyperspectral Imagery in the laboratory is conducted with oven-dried and sieved (< 2mm) soil samples. The HySpex system, combining a VNIR (400-1000 nm) and a SWIR (1000-2500 nm) line-scan detector is used to create first a spectral library.



HySpex System under laboratory measurements, modified after Körting, 2019.

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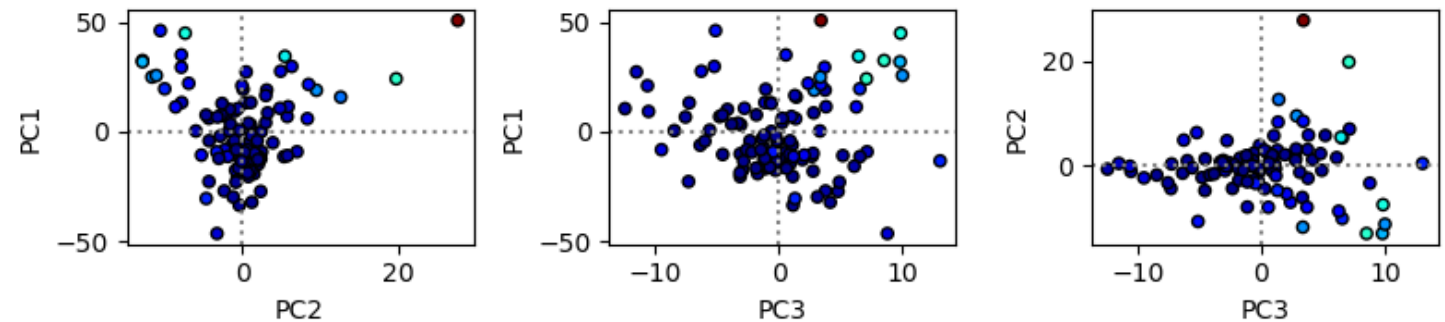


Method

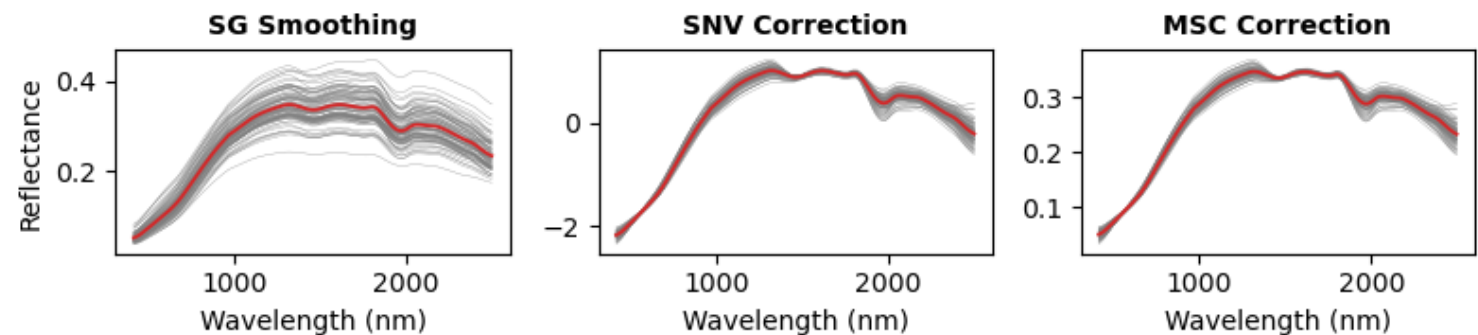
- Spectral pre-processing -

1. Savitzky-Golay (SG) Smoothing
2. Outlier detection using **Principle Component Analysis (PCA)** and the **Mahalanobis distance**

3. Applying: First derivative (FD), Standard normal variate (SNV), spectra normalization by the mean (NME) and multiplicative scatter correction (MSC) to remove baseline drifts, linear trends, multiple scattering effects (Gholizadeh et al., 2015)



Output Mahalanobis Distance Analysis.



Displaying different spectral pre-processing steps.

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Model construction

Establishing a relationship between soil spectra and soil HM concentration with Partial Least Squares Regression (PLSR) and Random Forest Regression (RFR) in a 10-fold cross validation approach.

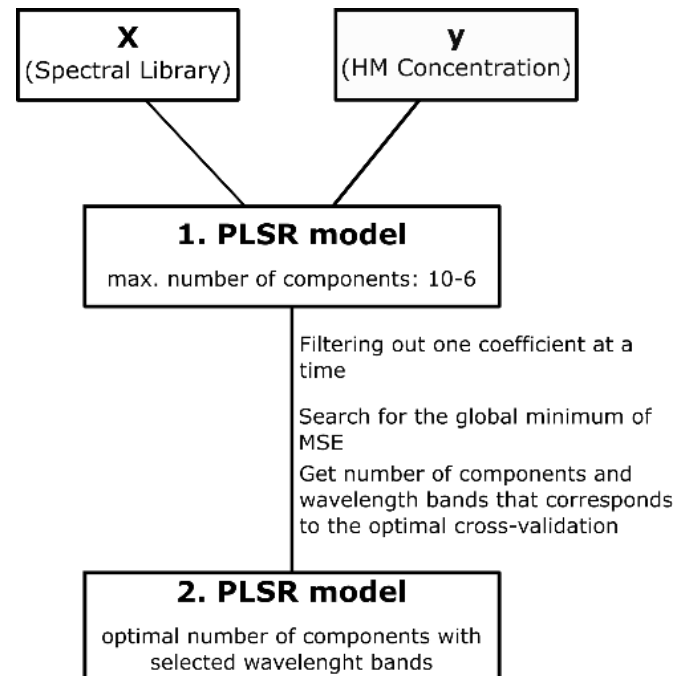
Parameter PLSR:

- Latent variable: max. 6

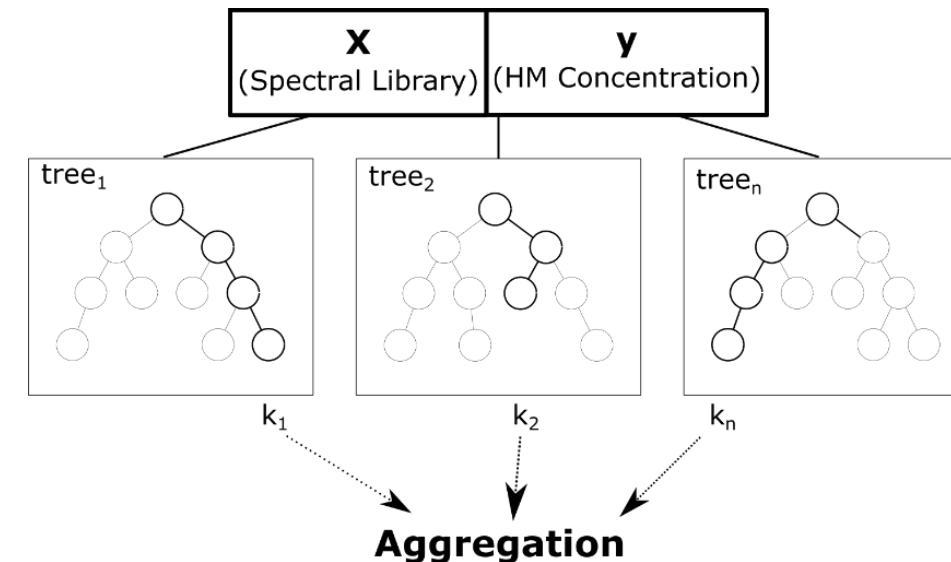
Hyper-parameter RFR:

- Number of trees: 100 – 1000 in steps of 10
- Maximum depth of the tree: 3, 7, 50, 80, 90, 100
- Number of root node (nodes): 3-6

PLSR model schema



RFR model schema



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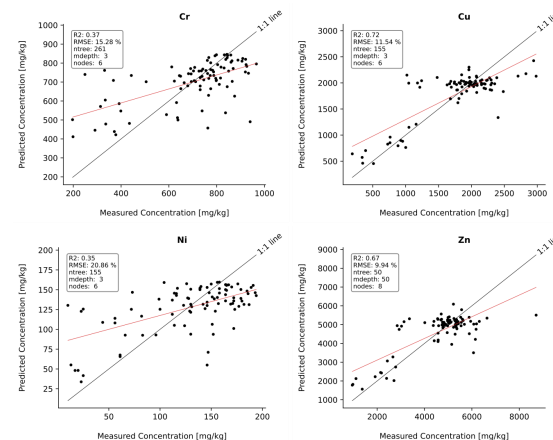
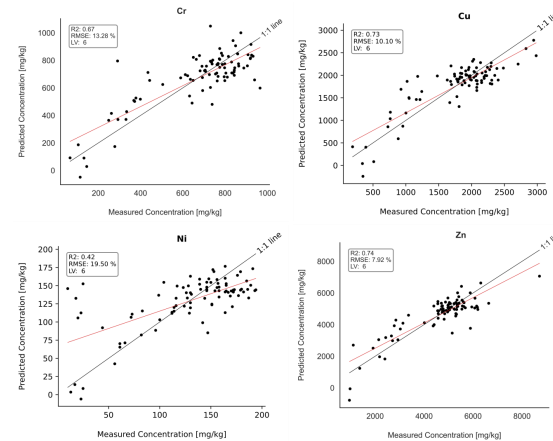


Results

PLSR and RFR performance compared through the cross-validation coefficient of determination (R²) and the root-mean-square error (RMSE) → describing goodness of model fitting

Conclusion

- Low to moderate PLSR performance
- Highly inhomogeneous soil samples have stronger impact on RFR performance



	Cr	Cu	Ni	Zn
R² (RMSE %)	0.67 (13.3)	0.73 (10.1)	0.42 (19.5)	0.74 (7.9)
Latent Variables	6	6	6	6
Discarded WB	219	171	203	106
Pre-processing	SNV	SNV	/	FD & SNV

	Cr	Cu	Ni	Zn
R² (RMSE %)	0.37 (15.3)	0.72 (11.5)	0.35 (20.9)	0.67 (9.9)
ntree	261	155	155	50
mDepth	3	3	3	50
nodes	6	6	6	8
Pre-processing	MSC	FD & MSC	FD	FD & SNV

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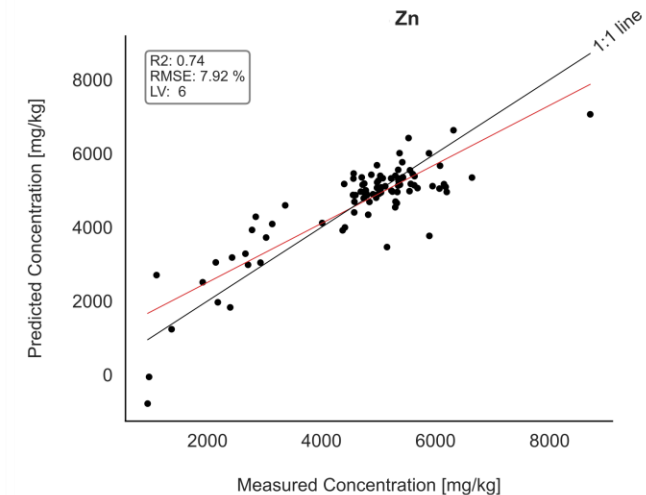
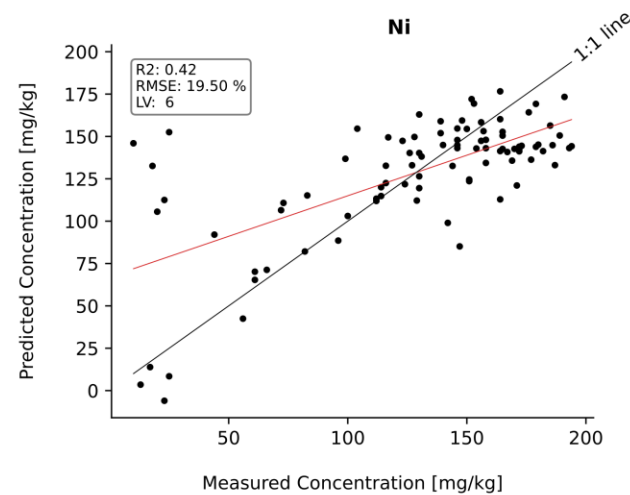
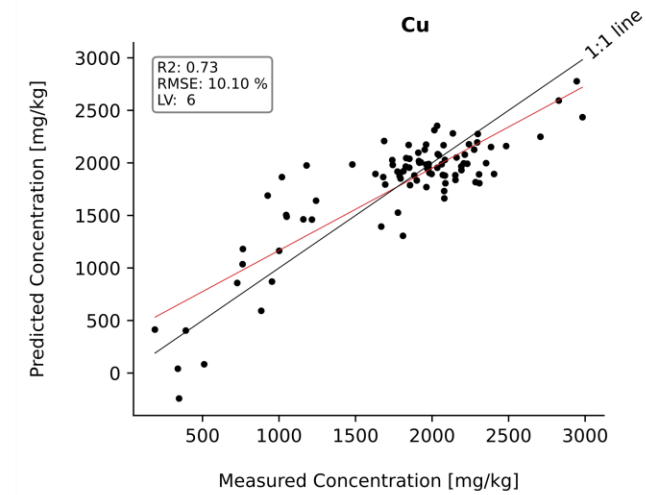
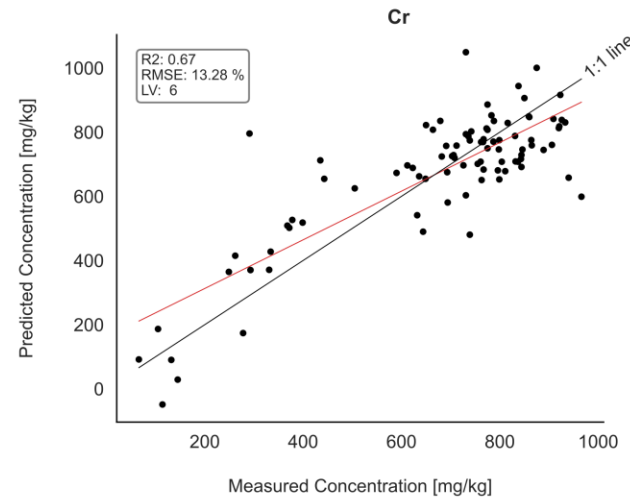
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Results

PLSR scatter plots



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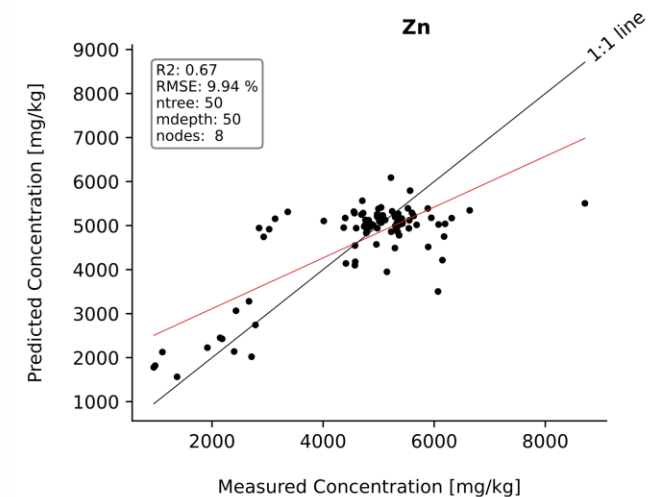
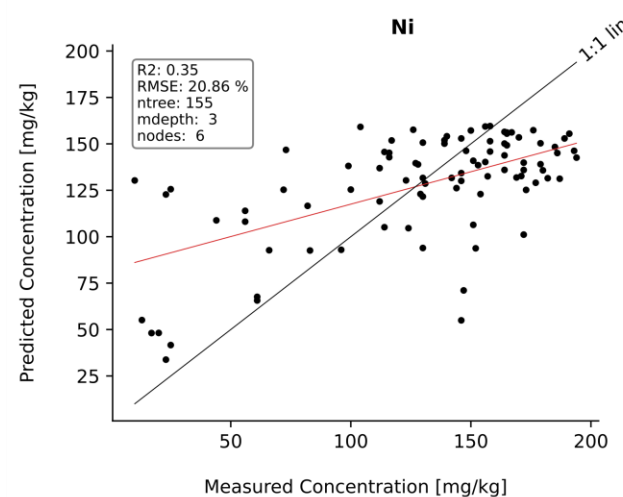
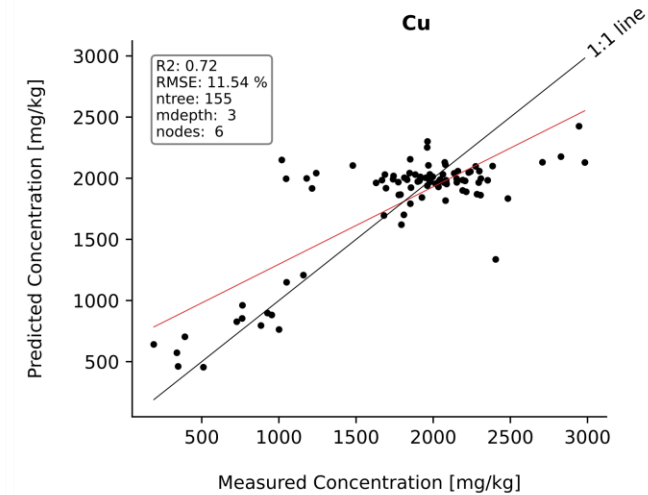
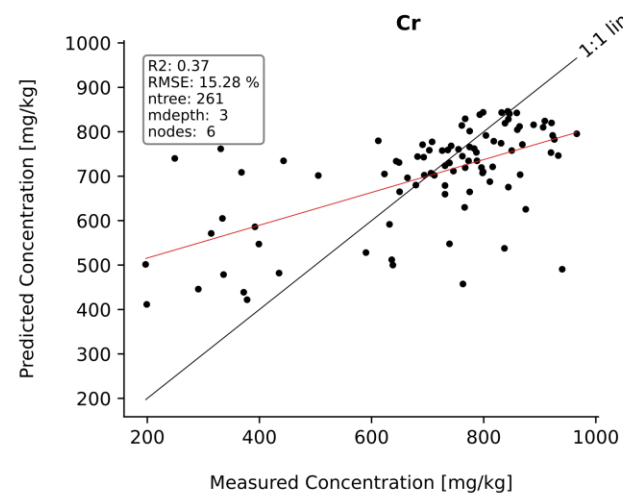
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Results

RFR scatter plots



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