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Quantitative REE modelling using Reflectance Spectroscopy

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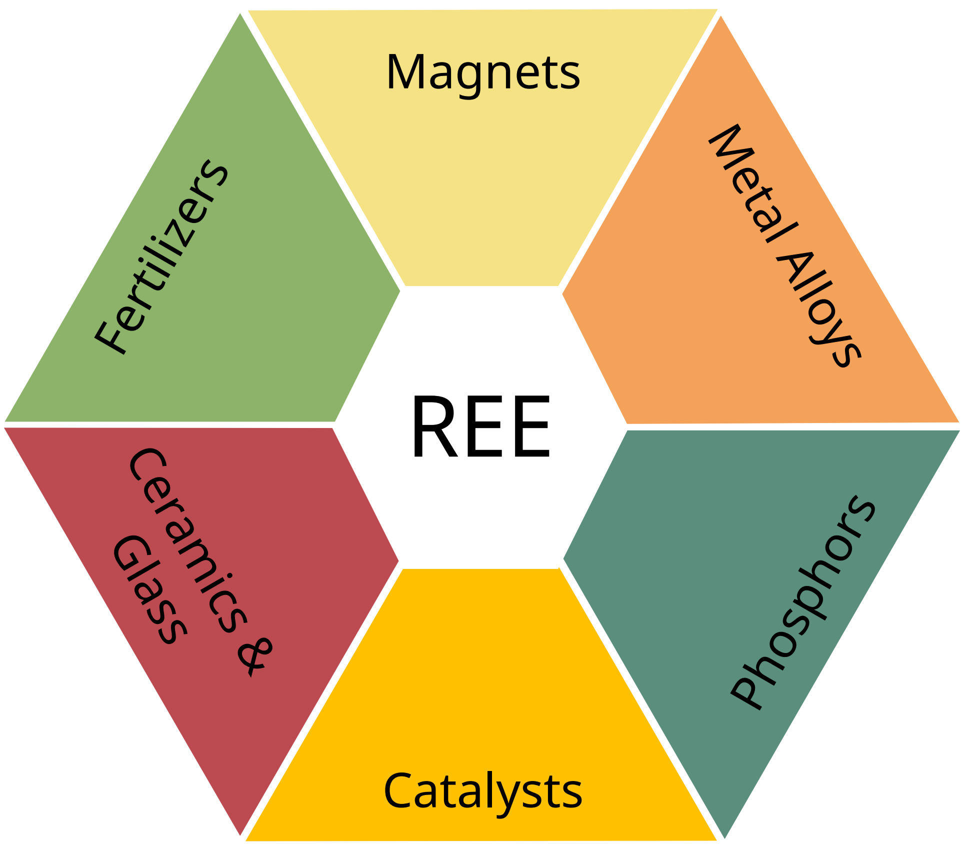
Why Rare Earth Elements?



Necessary in (green) technology

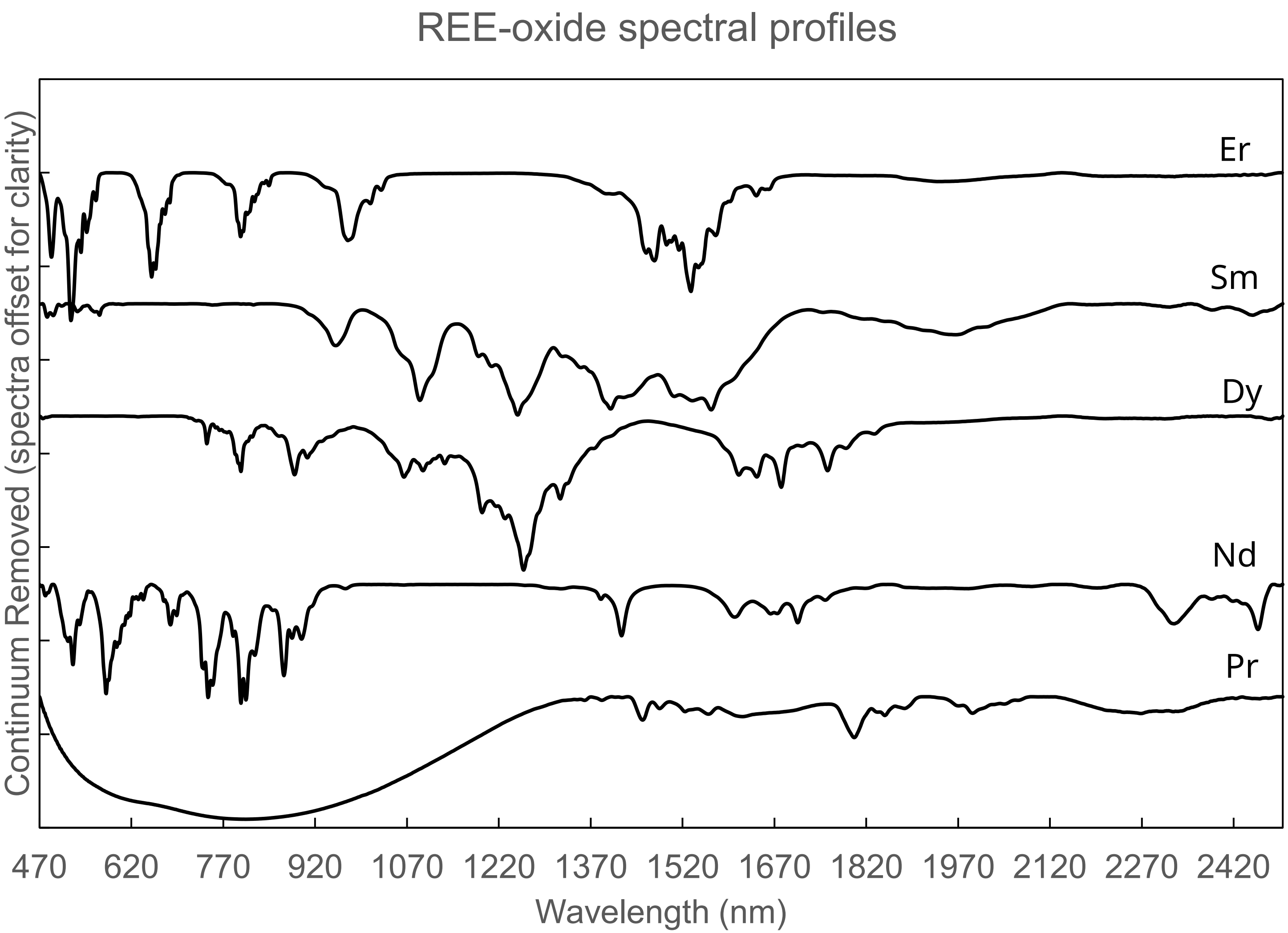
↓

Uneven distribution of deposits

↓

Critical Raw Materials

Reflectance Spectroscopy of REE



REE have distinct spectral signatures in the VNIR-SWIR range.

Absorptions are due to the elements themselves and not the host mineral.

The depth of the absorption feature is roughly related to the concentration.

Objectives

Can explainable AI be used to quantify REE concentrations from reflectance spectra?

- Quantify single REEs using Random Forest Regression
- Verify if the model’s decision-making process is physically meaningful
- Apply the model on images of different scales and resolutions

Materials

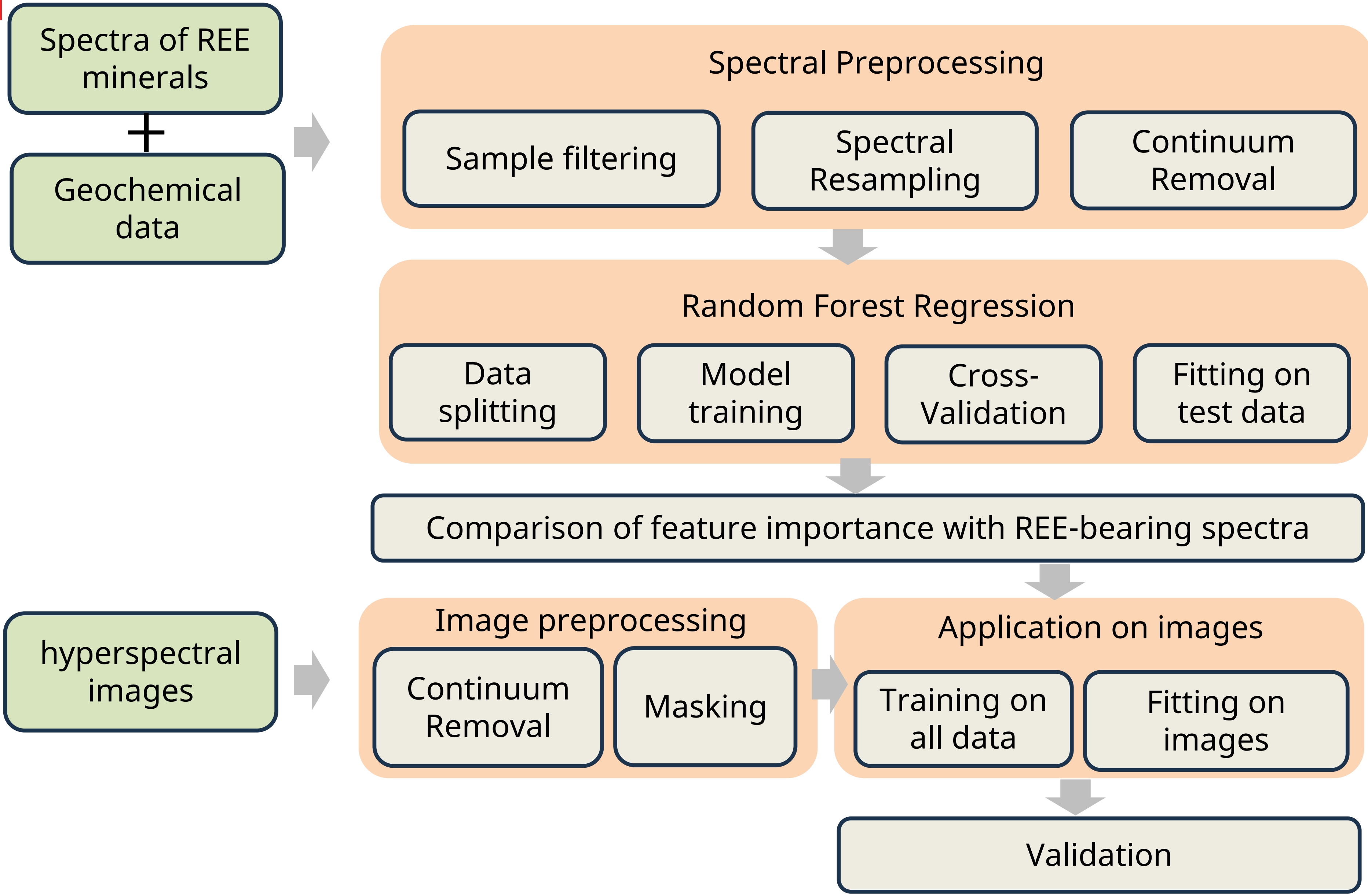
130 samples of 17 different mineral types

Number of samples	Type	Spectroscopic measurement	Geochemical analysis technique	Reference
32	natural	ASD Fieldspec-3	XRF, EMPA, INAA	Neave et al., 2016
41	synthetic	ASD Fieldspec-3	ICP-MS	Tan et al., 2021
33	natural	SPECIM sisuROCK	EMPA	Turner et al., 2014, 2016, 2018
9	natural	ASD Fieldspec-3	ICP-AES	Boesche et al., 2015
15	synthetic	ASD Fieldspec-4	EMPA, SIMS	https://geosciences.ed.ac.uk/about/facilities/all/ionprobe/technical/standards/ree/composition (Unicamp)

Hyperspectral images: SPECIM sisuROCK and HySpeX (lab-derived) and EnMAP

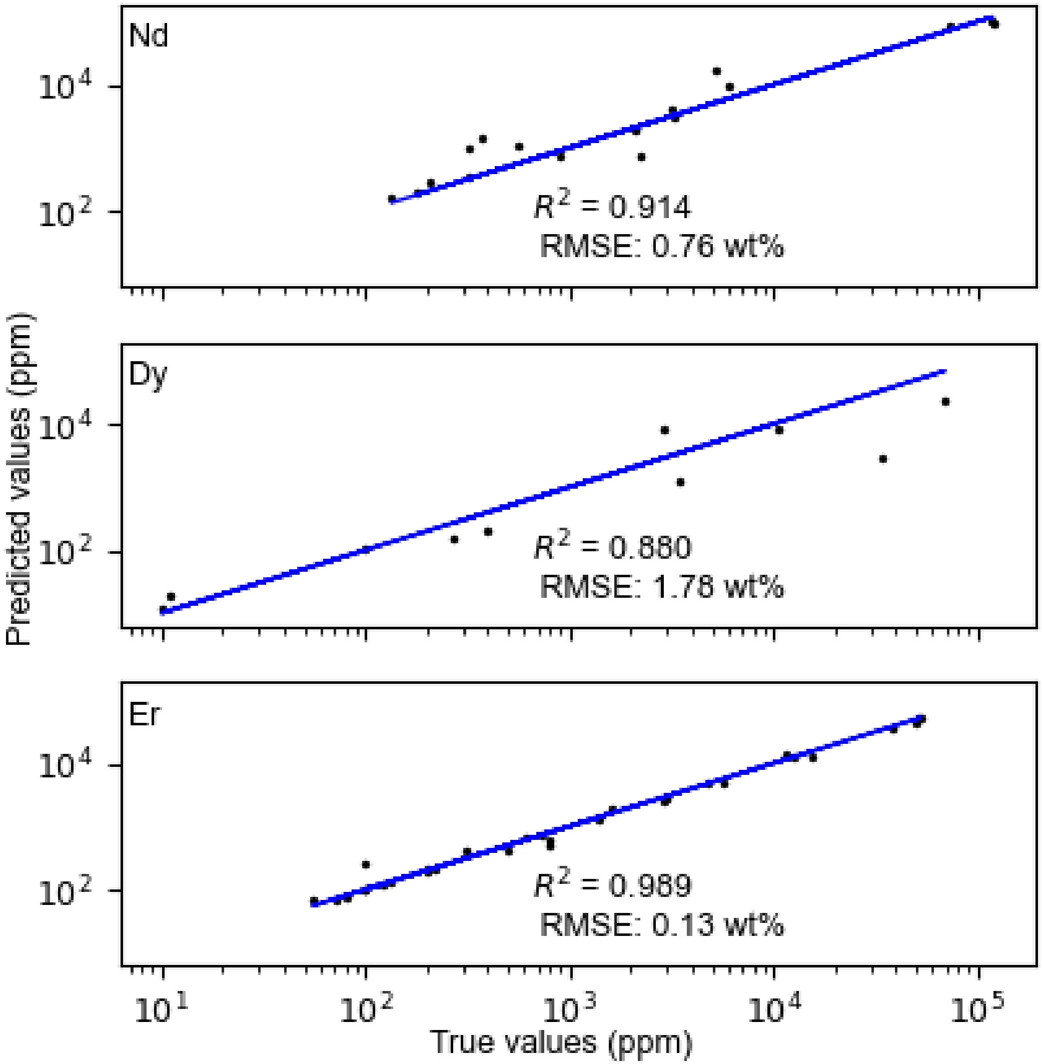
Datasets and images kindly provided by: Dr. David Turner and Dr. Benoit Rivard, Prof. Carlos Roberto de Souza Filho, Dr. Wei Tan.

Methodology

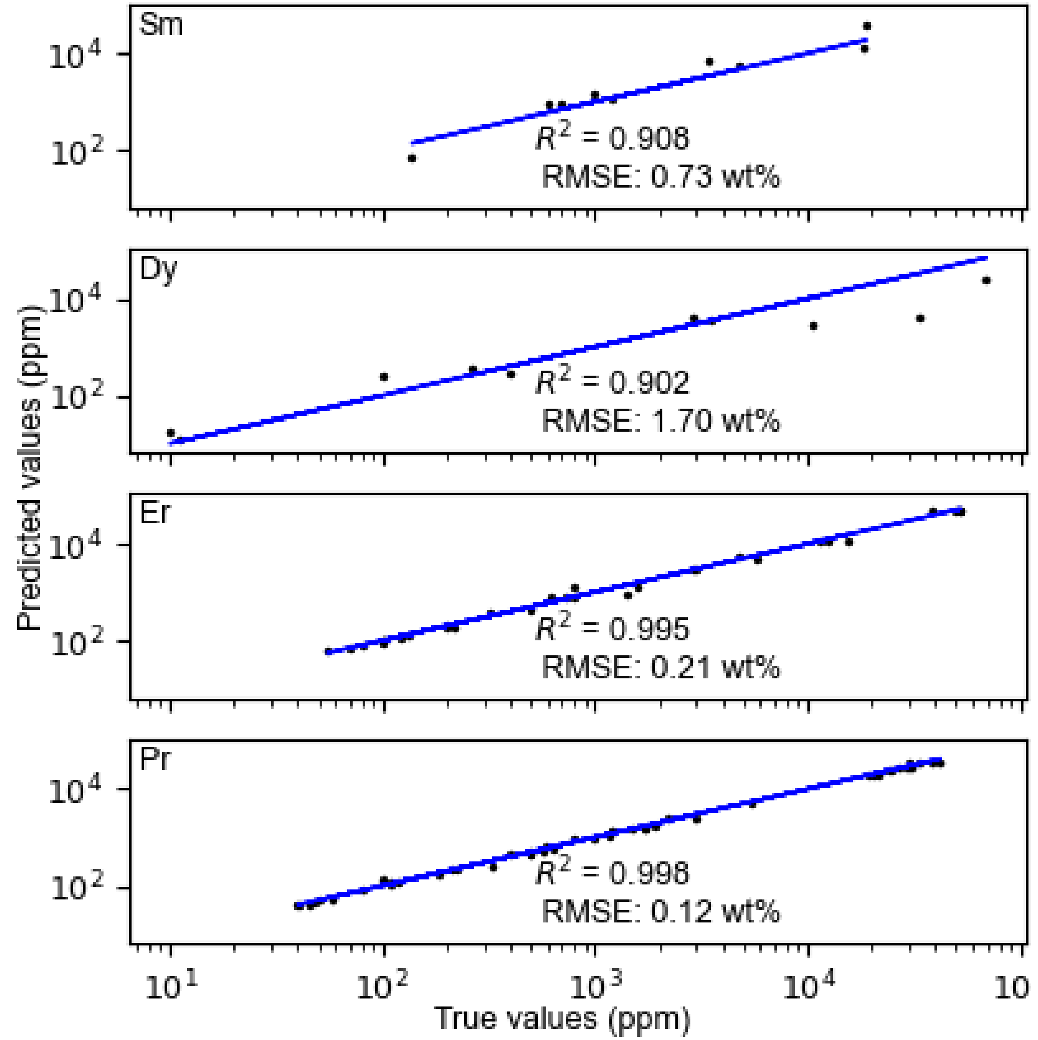


Results – Regression models

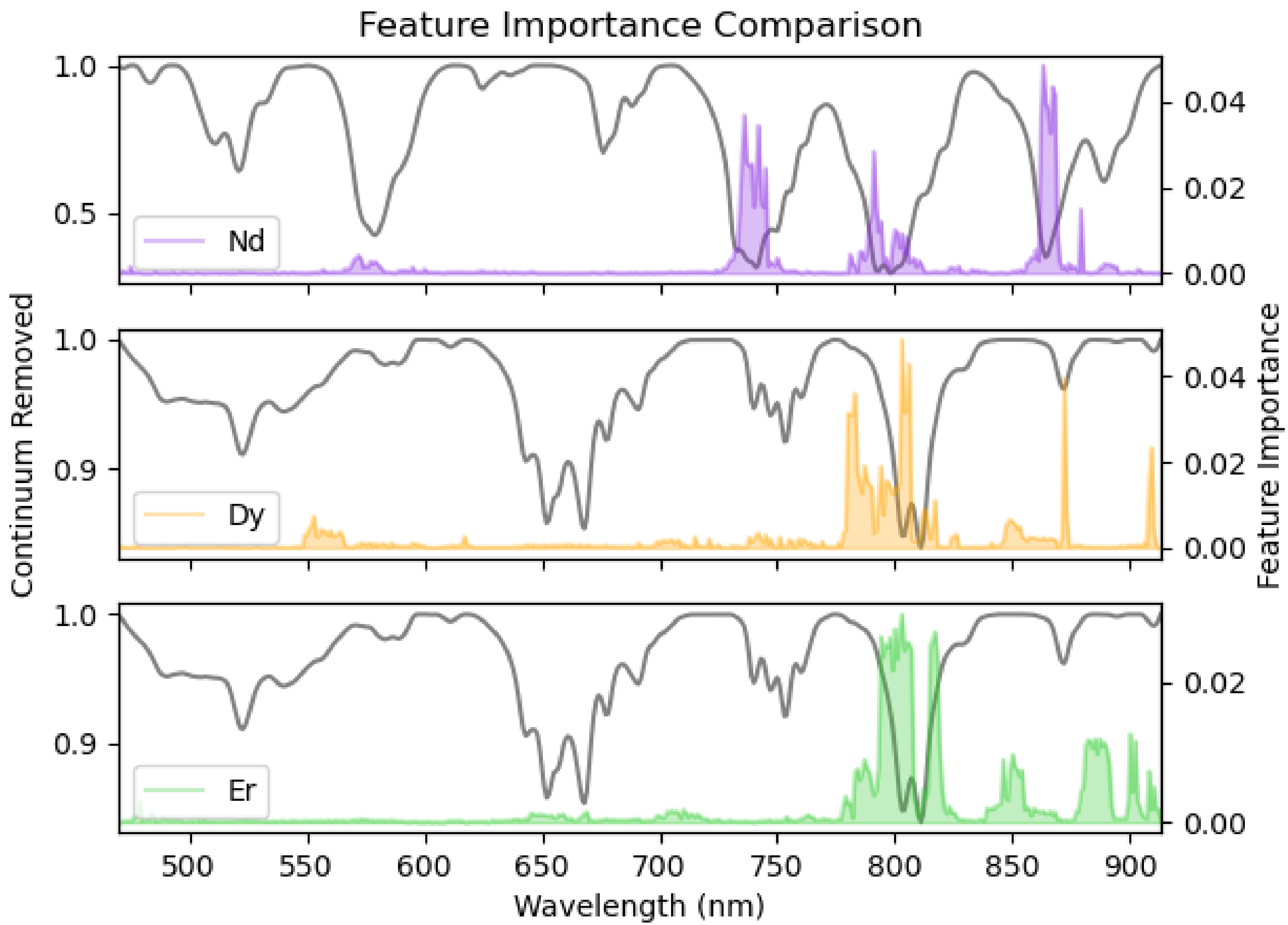
VNIR (470 – 913 nm)



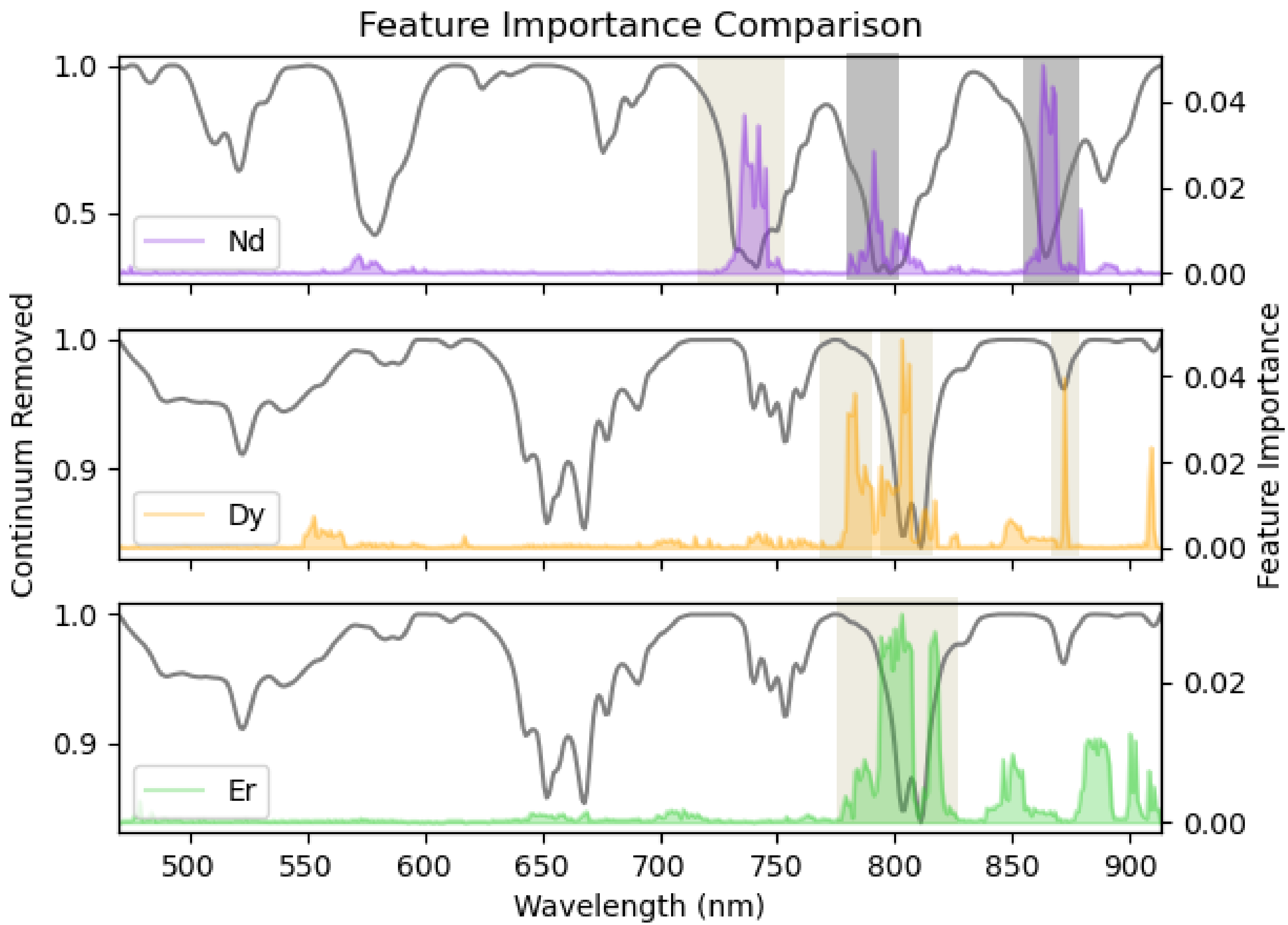
SWIR (1000 – 1700 nm)



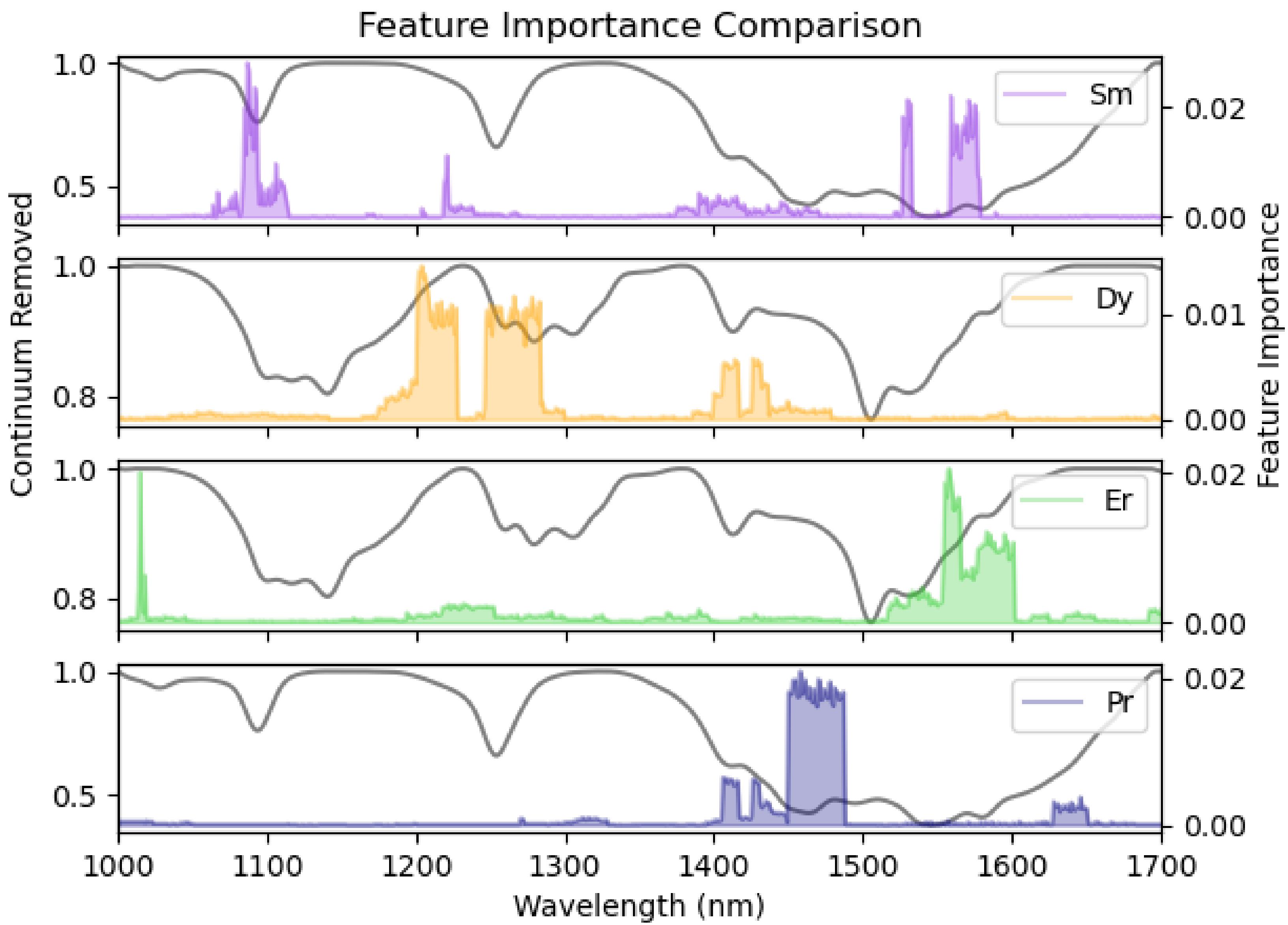
Results – Feature importance: VNIR



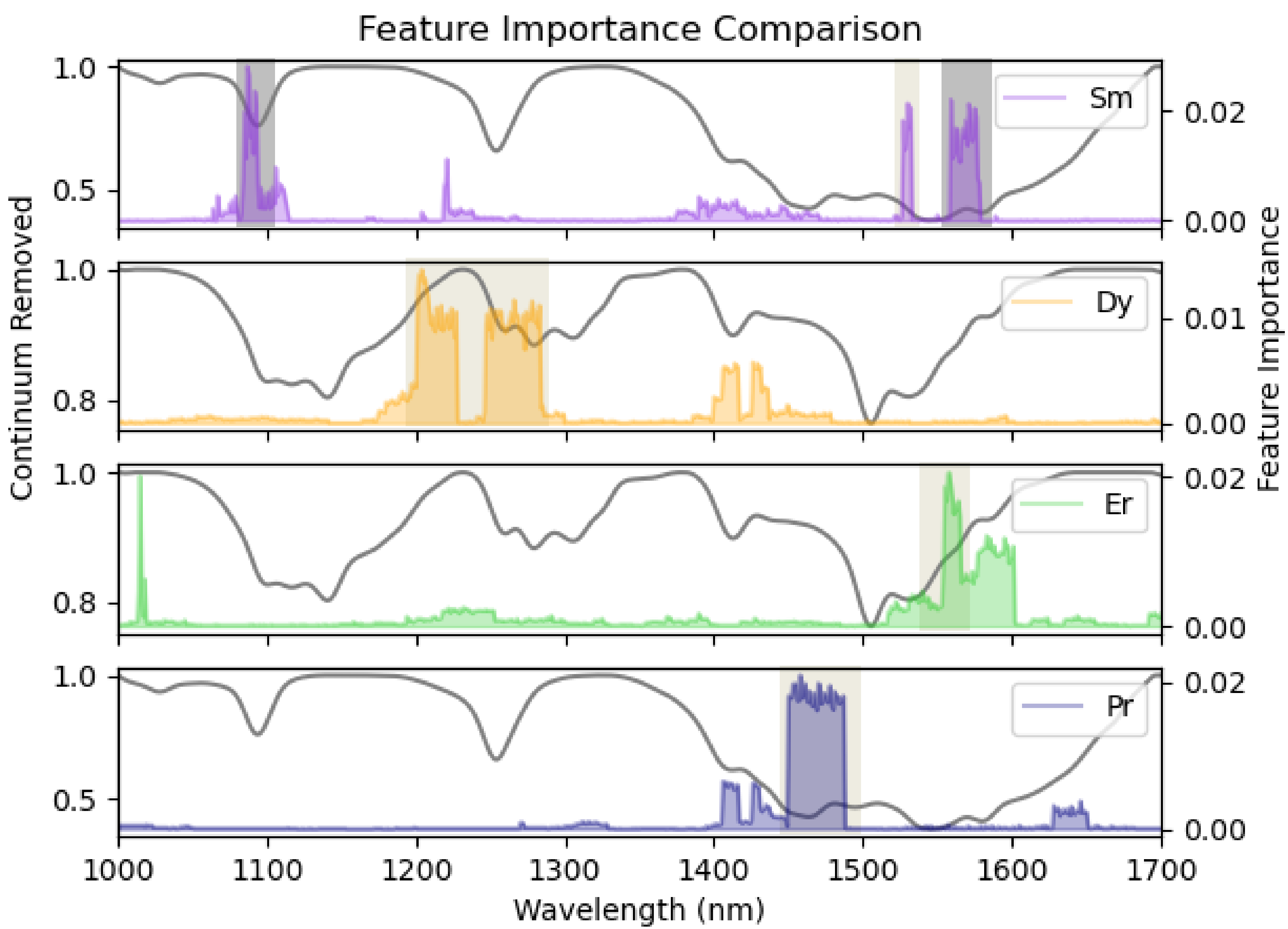
Results – Feature importance: VNIR



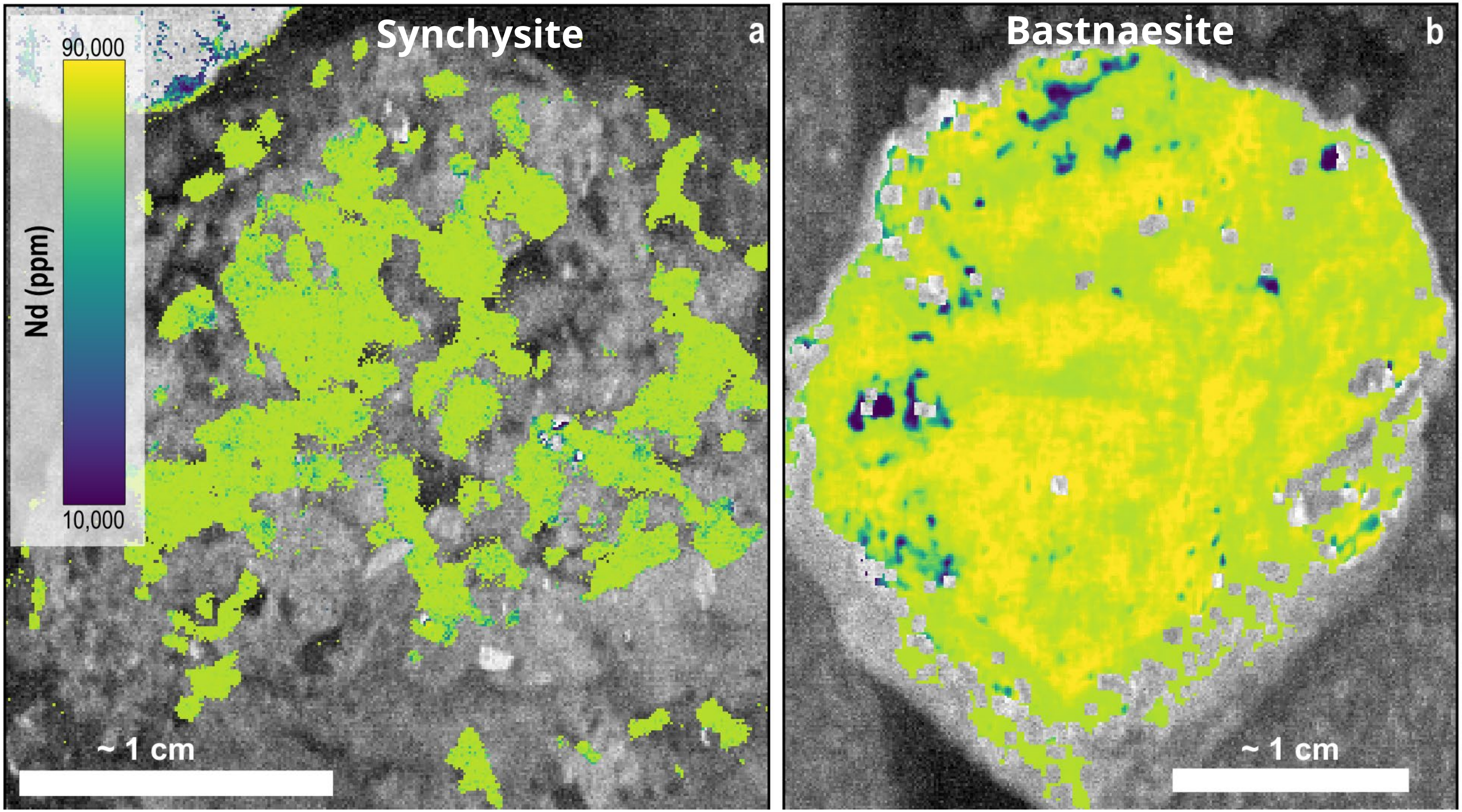
Results – Feature importance: SWIR



Results – Feature importance: SWIR

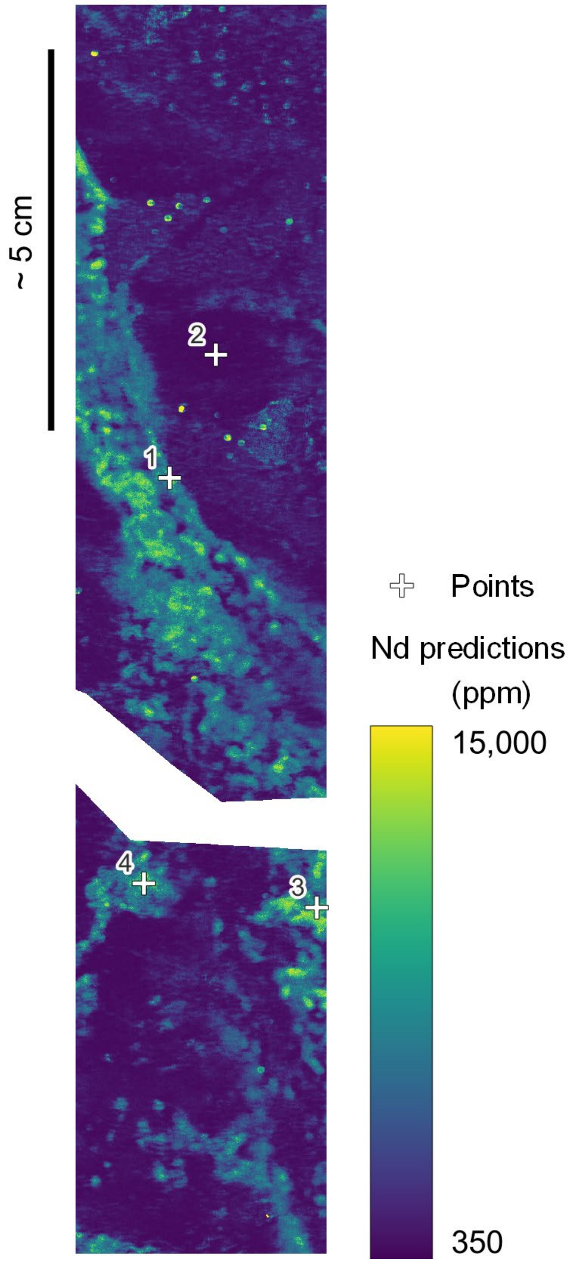


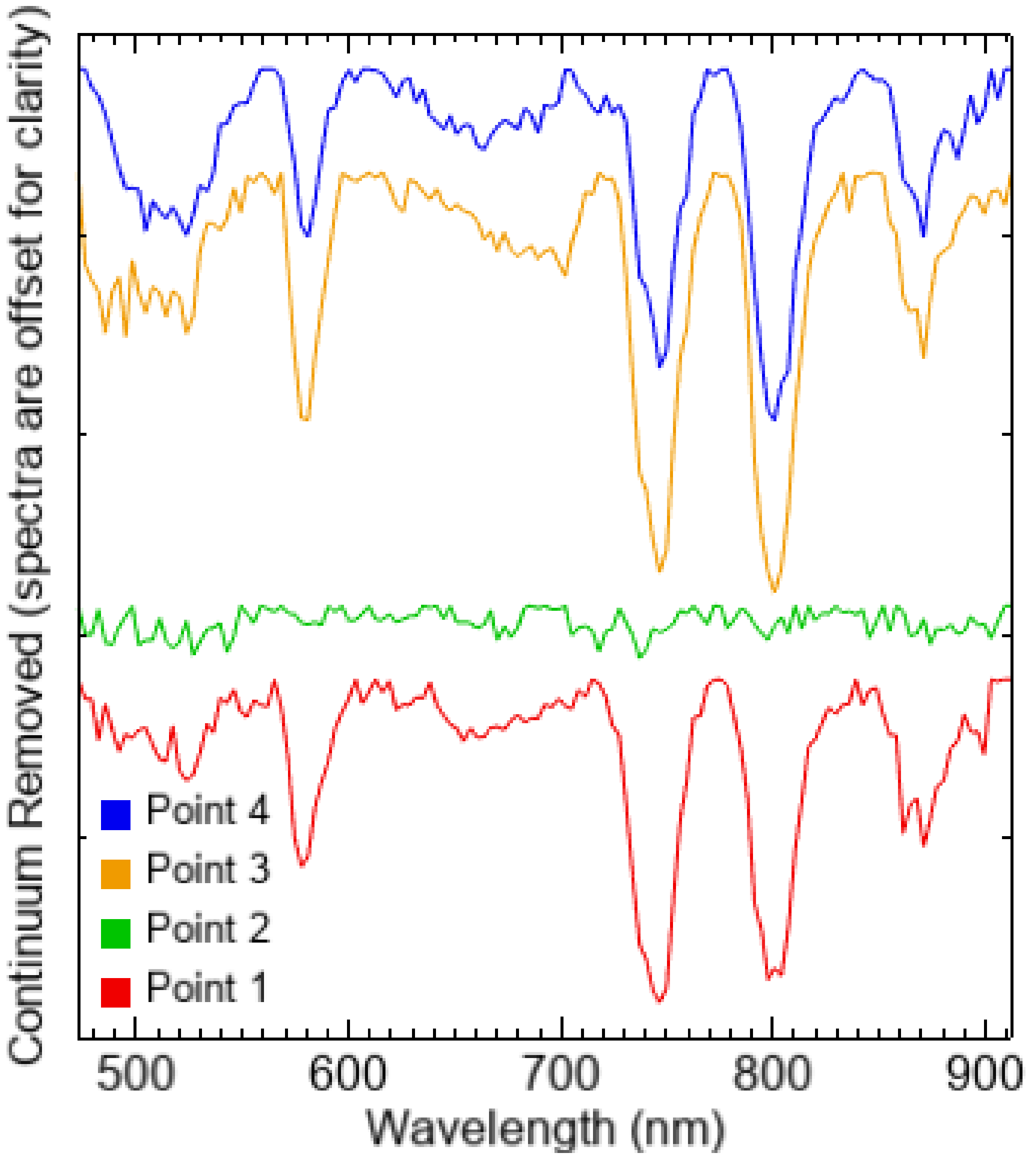
Application to image data: sisuROCK



Mineral	This study	Turner et al. (2014)
Synchysite	7.84 wt%	8.25 wt%
Bastnaesite	8.25 wt%	7.25wt%

Application to image data: HySpeX





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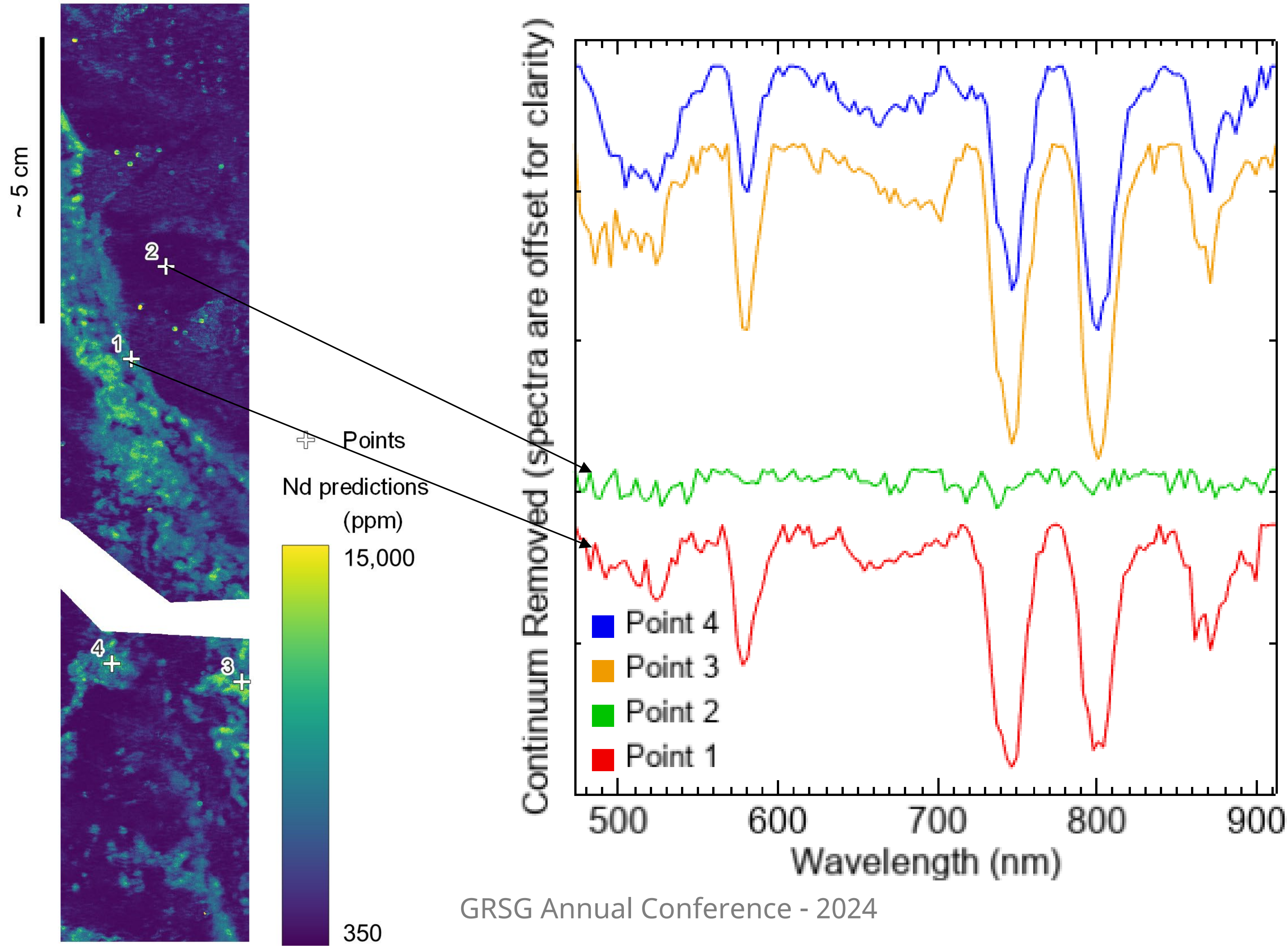
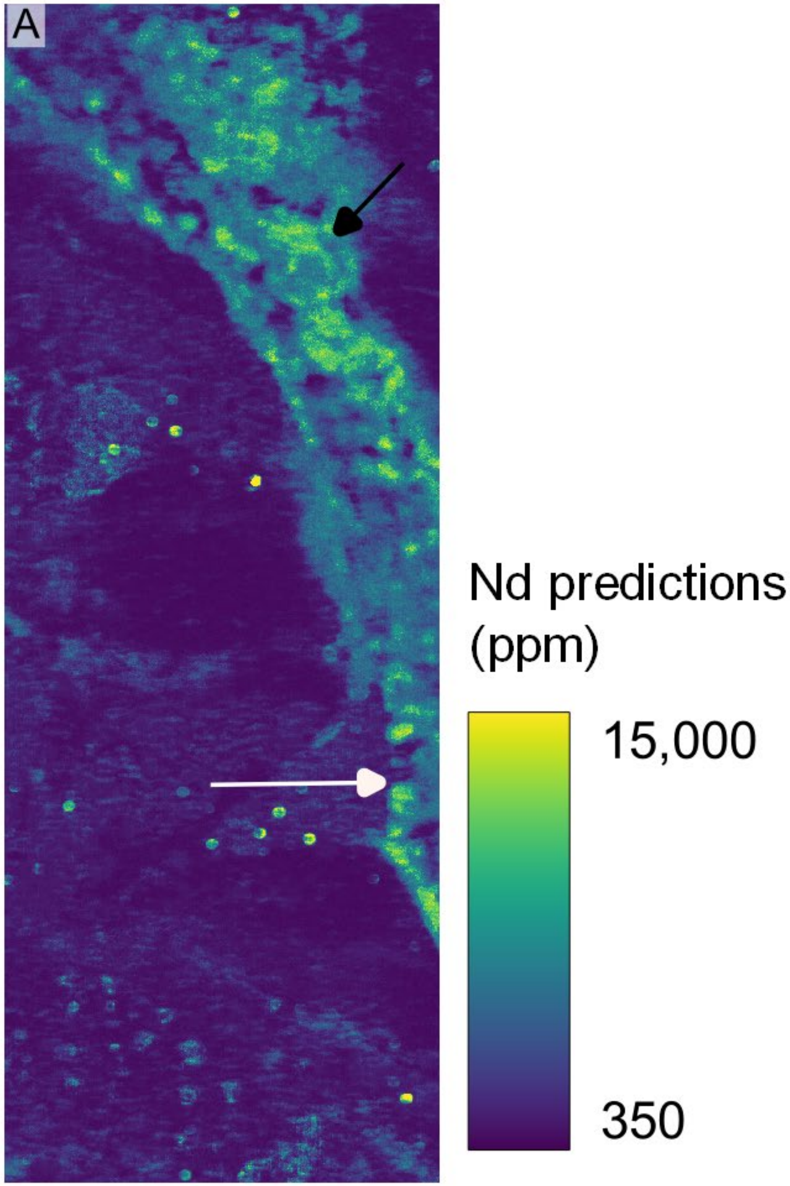
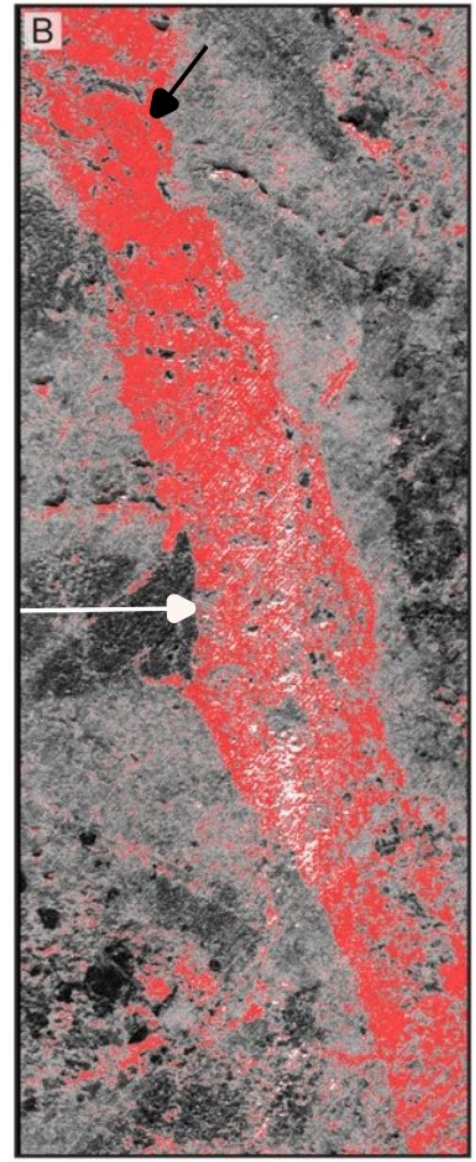


Application to image data: HySpeX

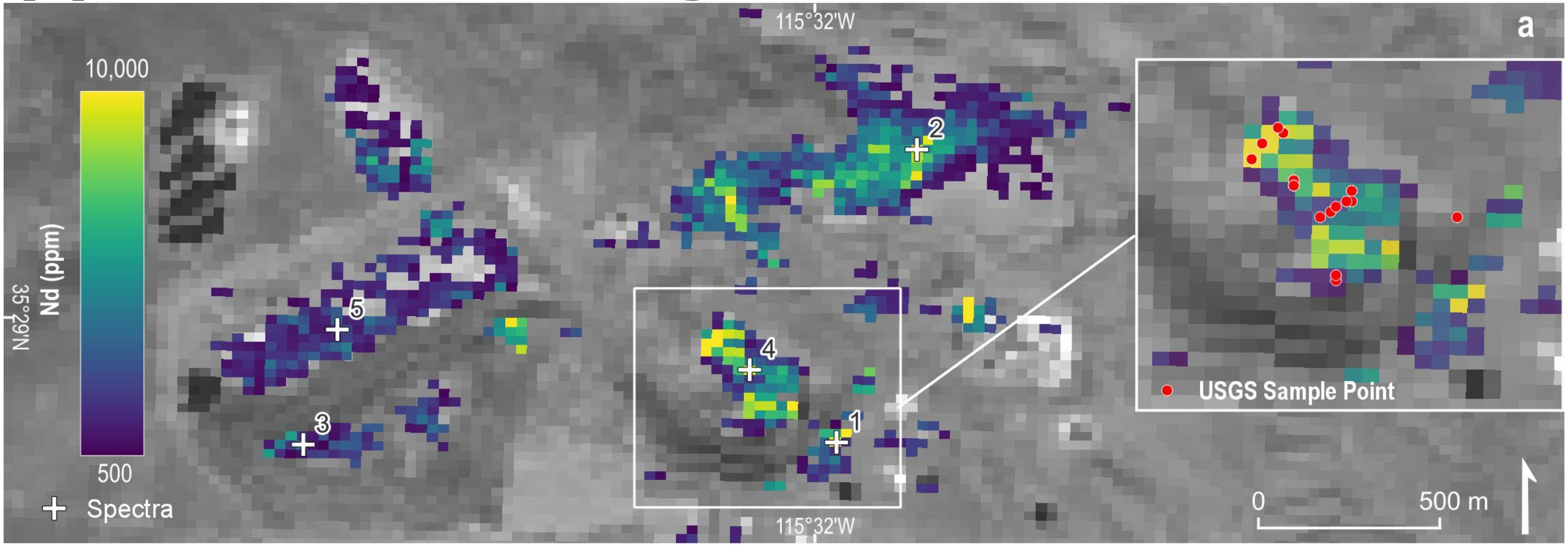


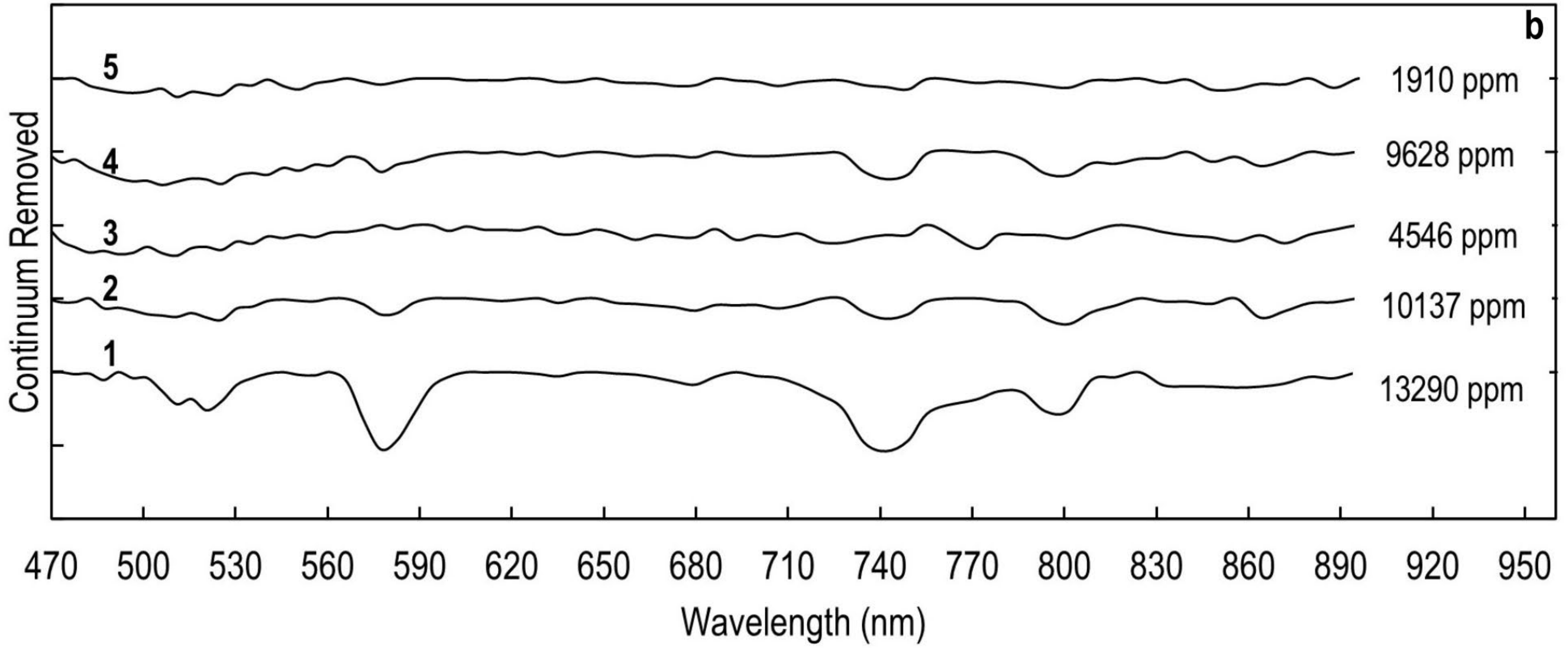
This study



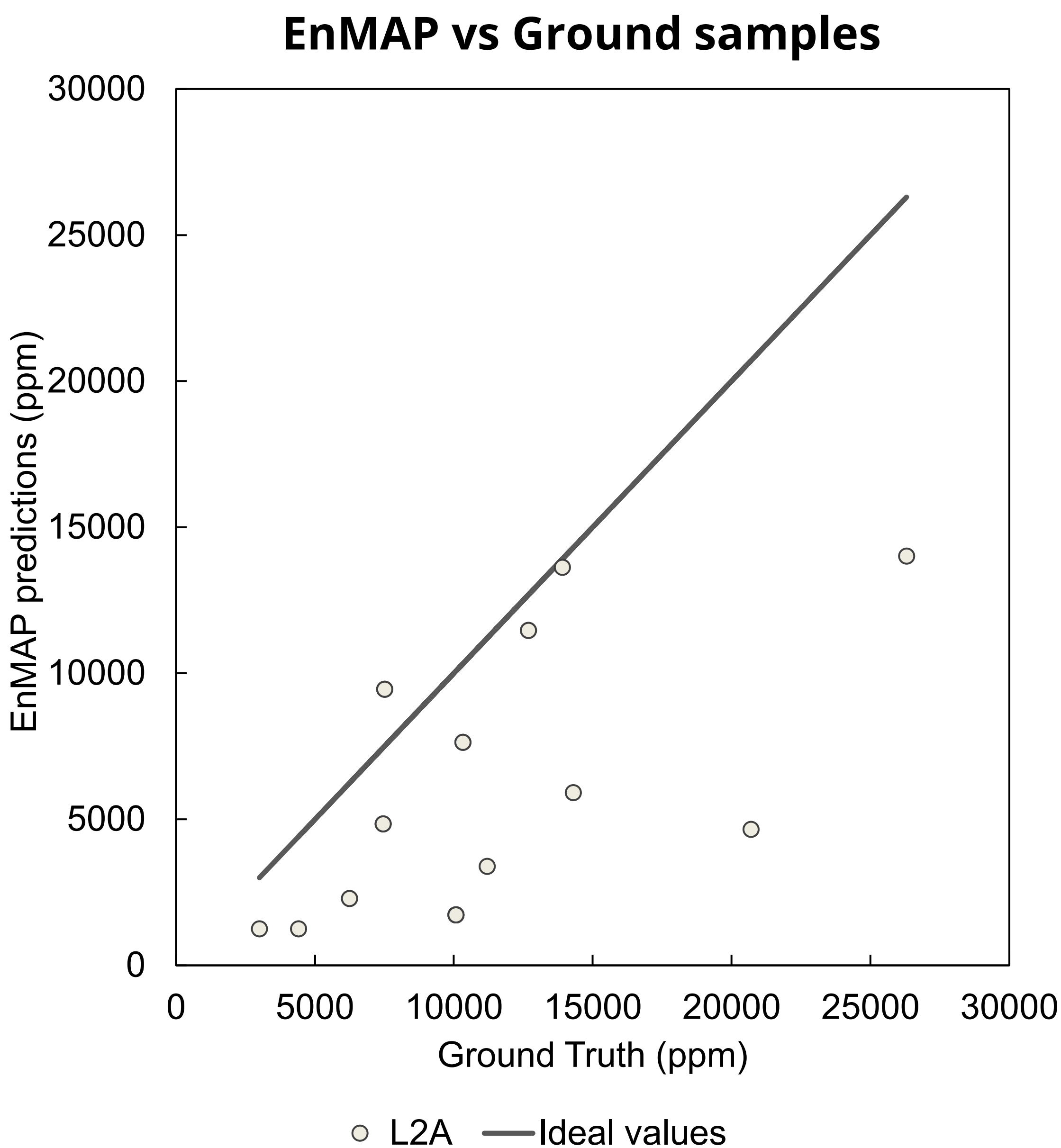
Novaes, 2022

Application to image data: EnMAP, Mt. Pass



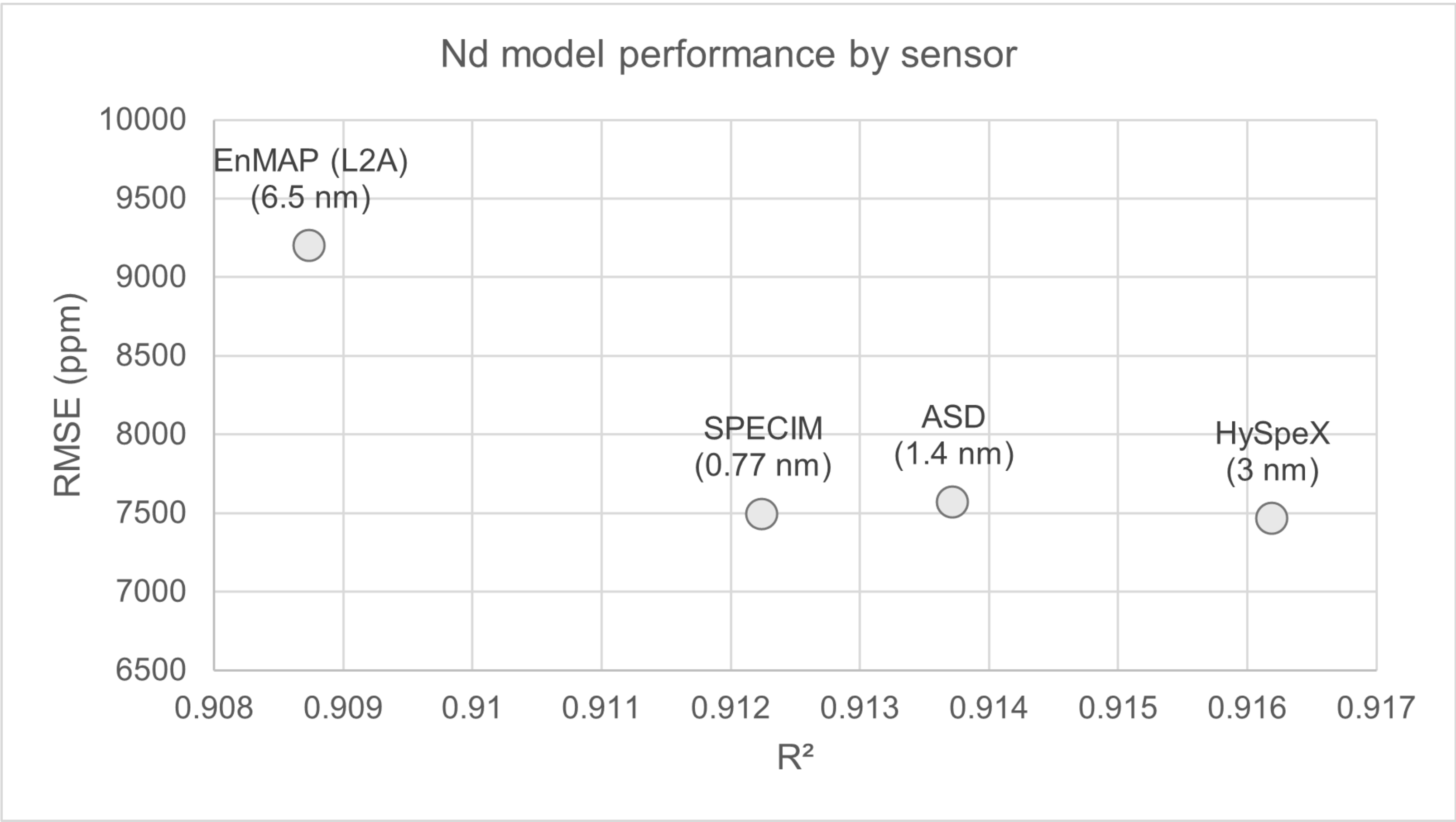


Application to image data: EnMAP, Mt. Pass

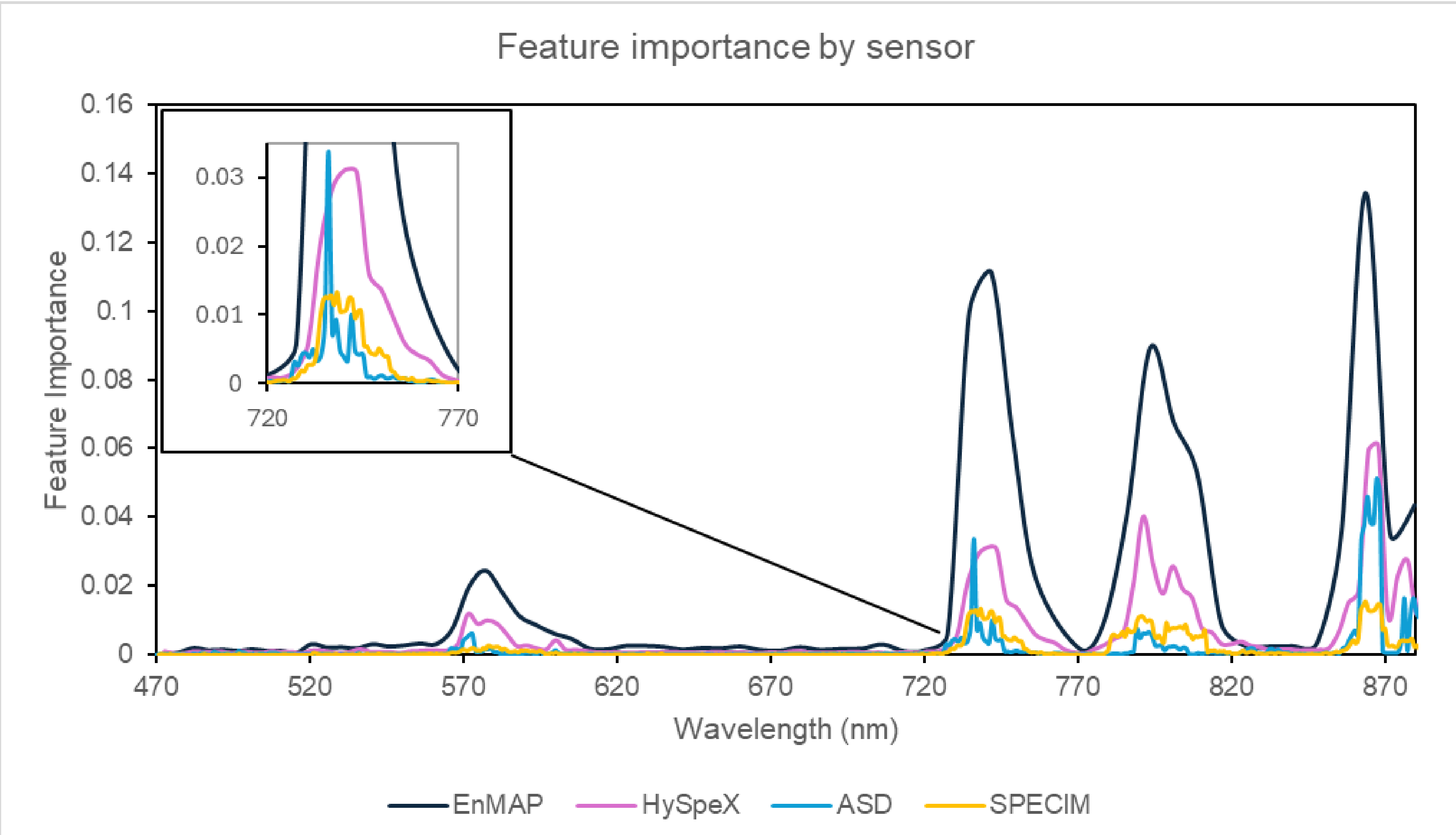


Sample geochemistry from Verplank et al., (2022)

Comparison between different sensors



Comparison between different sensors



Advantages & limitations of the models

Advantages	Limitations
Models are independent of mineralogy	Requires large datasets
The models are scalable to different data resolutions and sensors	Strongly affected by noise (instrumental and atmospheric)
Modeling is effective with datasets from different teams and techniques	Performance deteriorates with an increase in Feox contents.

Conclusions

Random Forest Regression is a robust method for predicting the concentration of REEs in spectral data.

Feature Importance indicates the model's physically meaningful decision-making process, highlighting spectral ranges critical for each individual element, confirming experimental studies.

Application on imaging data shows that the model gives reasonable predictions even at different scales and SNR levels.

Future developments:

- Handling noise and iron oxides effects during modeling.
- Assessing the uncertainty of the model.
- Understanding the effects of mineralogy on model performances.

Thank you for your attention!