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Towards Improved Hydrocarbon Soil Assessment: The Application of Mid-Infrared Spectroscopy and Binary Classification Techniques

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Session: Data Analytics: Use of Machine Learning and Artificial Intelligence Tools for Improved Analysis, Optimization and Decision Making

Motivation

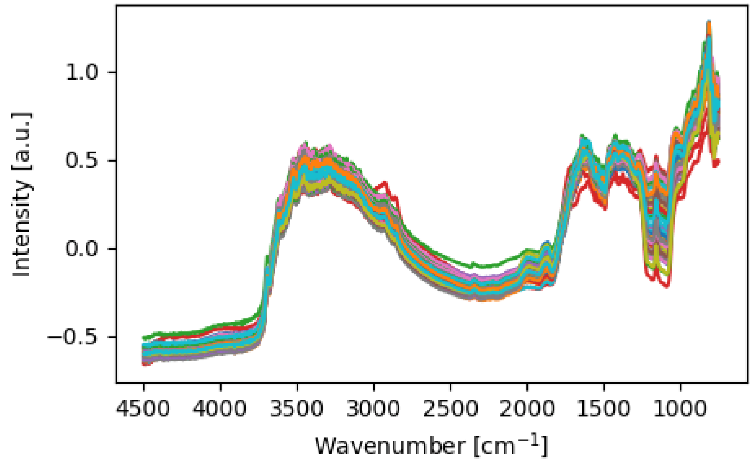
- Rapid on-site assessment is needed for efficient remediation.
- Traditional lab tests are expensive, slow and resource-intensive.
- RemScan is a fast, cost-effective measurement solution.
- Extensive work done to calibrate the instrument.
- New calibration method being developed for RemScan.
- Improve speed and accuracy of measurements.

In-Field Operation

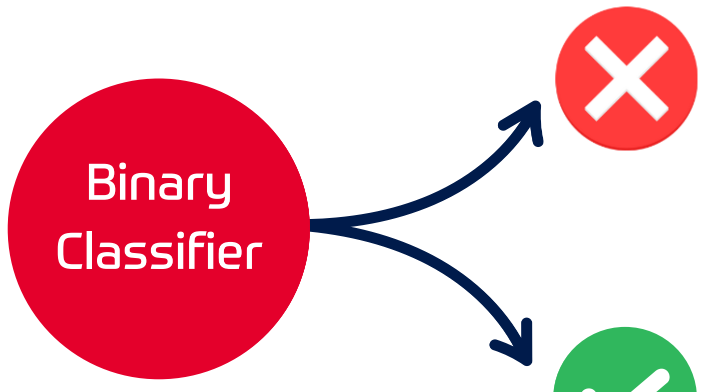
RemScan

Contaminated Soil

Mid-Infrared Spectra



CONTAMINATED

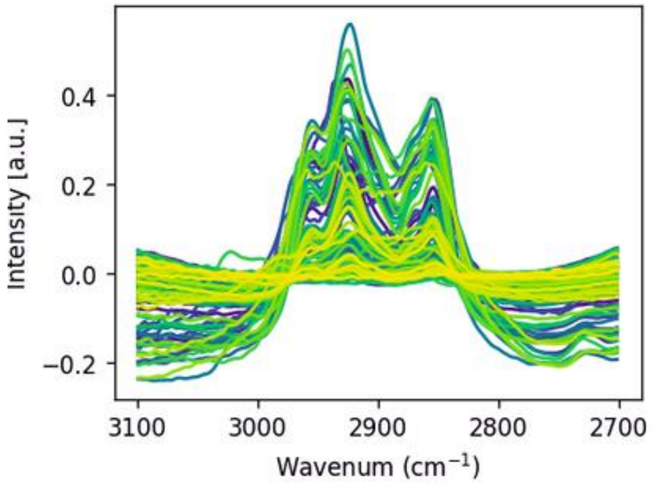


“CLEAN”

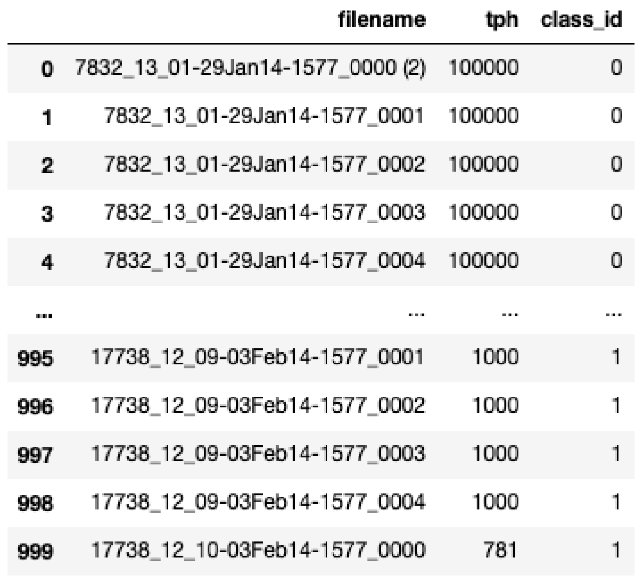
*Common Industry threshold = 1000 ppm/ 0.1% contamination

Methodology

TRAINING SPECTRA



LABELS

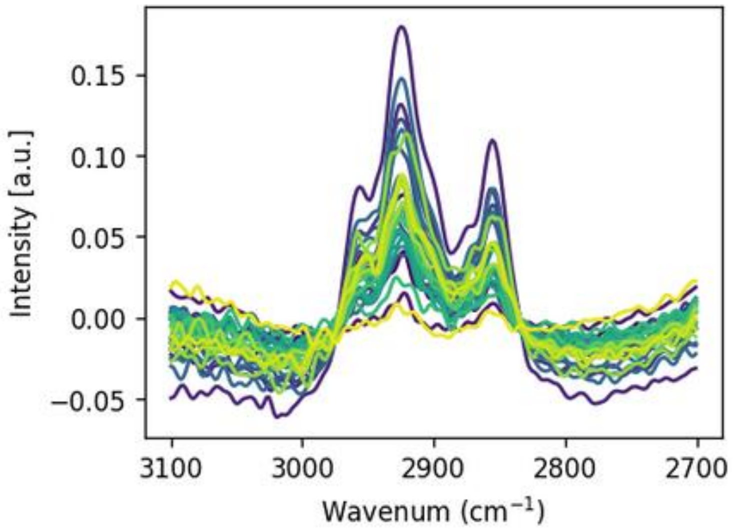


	filename	tph	class_id
0	7832_13_01-29Jan14-1577_0000 (2)	100000	0
1	7832_13_01-29Jan14-1577_0001	100000	0
2	7832_13_01-29Jan14-1577_0002	100000	0
3	7832_13_01-29Jan14-1577_0003	100000	0
4	7832_13_01-29Jan14-1577_0004	100000	0
...	...	...	...
995	17738_12_09-03Feb14-1577_0001	1000	1
996	17738_12_09-03Feb14-1577_0002	1000	1
997	17738_12_09-03Feb14-1577_0003	1000	1
998	17738_12_09-03Feb14-1577_0004	1000	1
999	17738_12_10-03Feb14-1577_0000	781	1

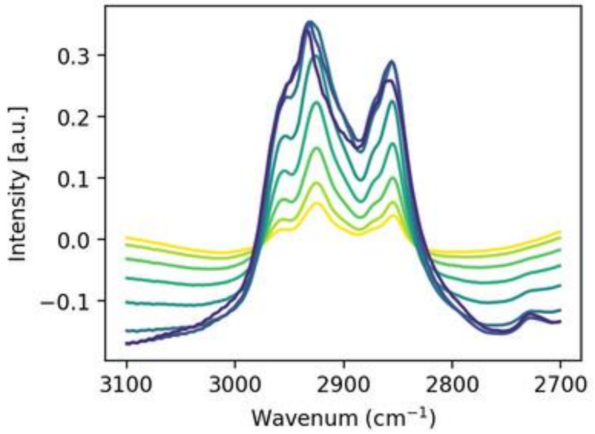
TRAINING MODEL

PREDICTION

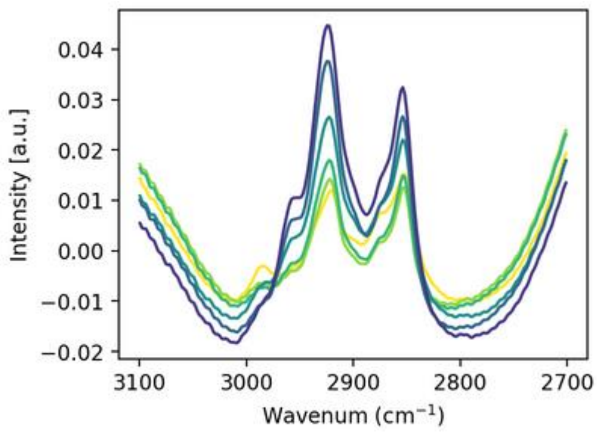
TEST SPECTRA



Contaminated:
TPH > 1000 ppm



Clean:
TPH < 1000 ppm



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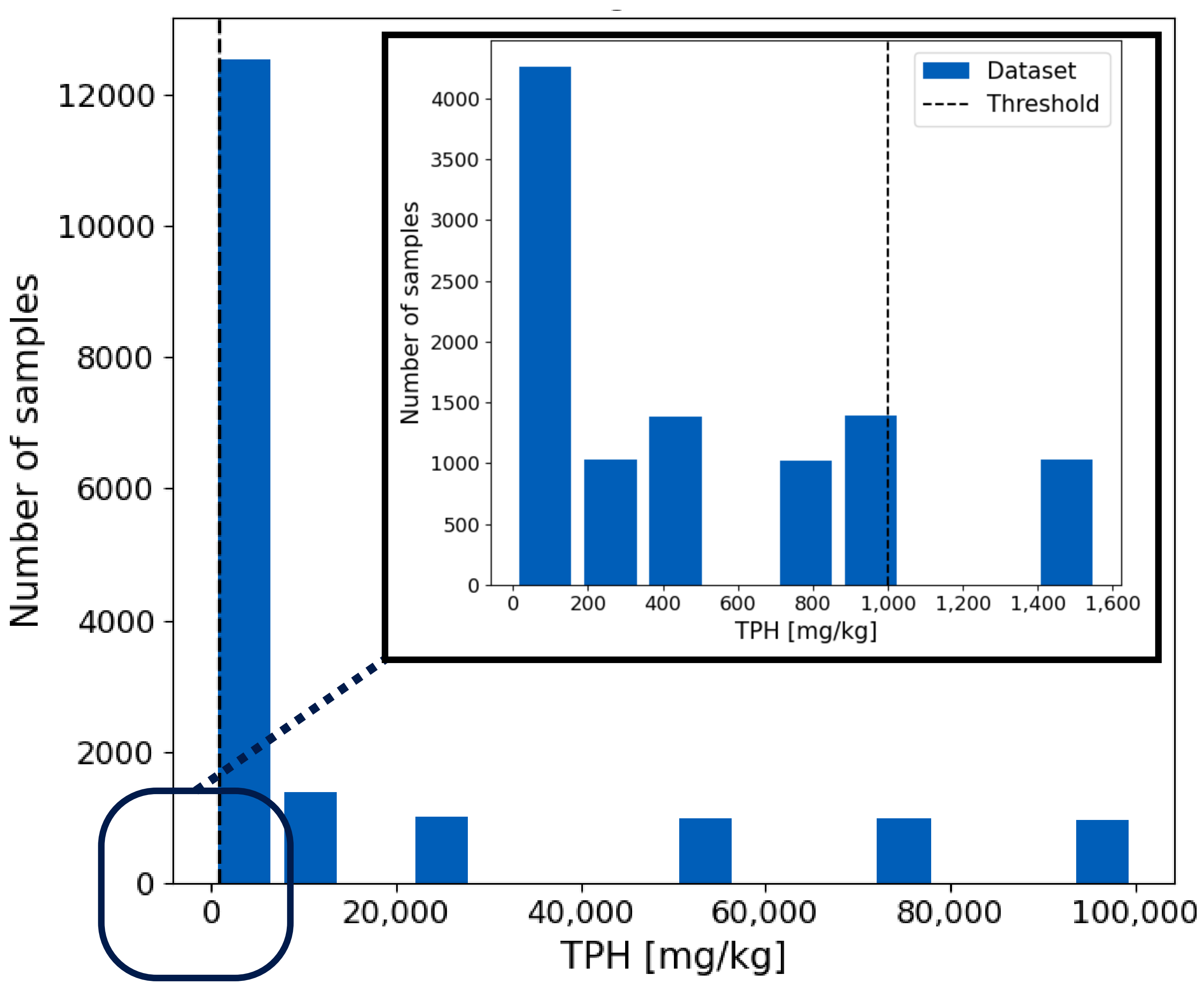
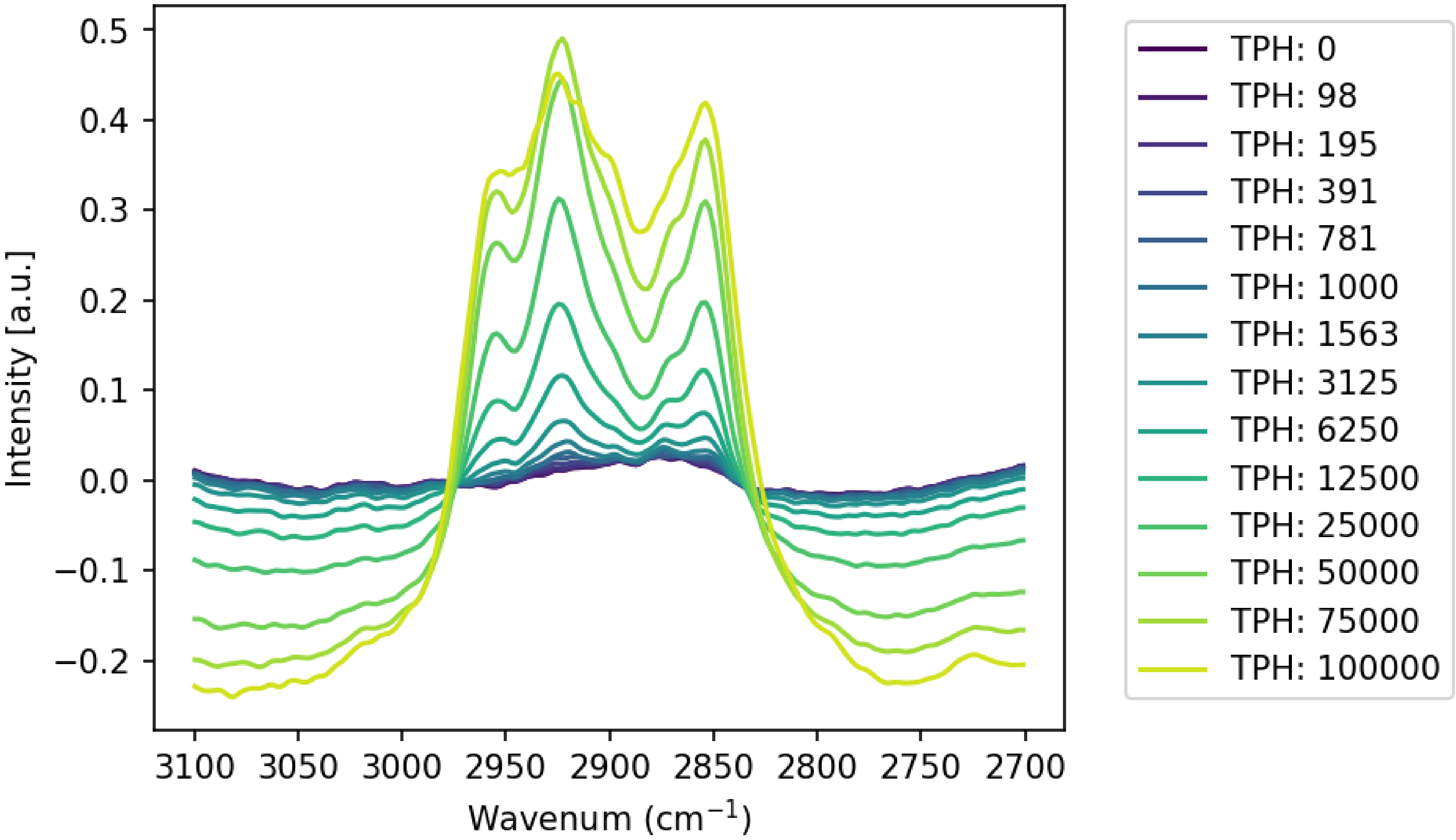
Training Dataset





Total: 17,836

Samples >1000ppm = 8,750

Samples <1000ppm = 9,086

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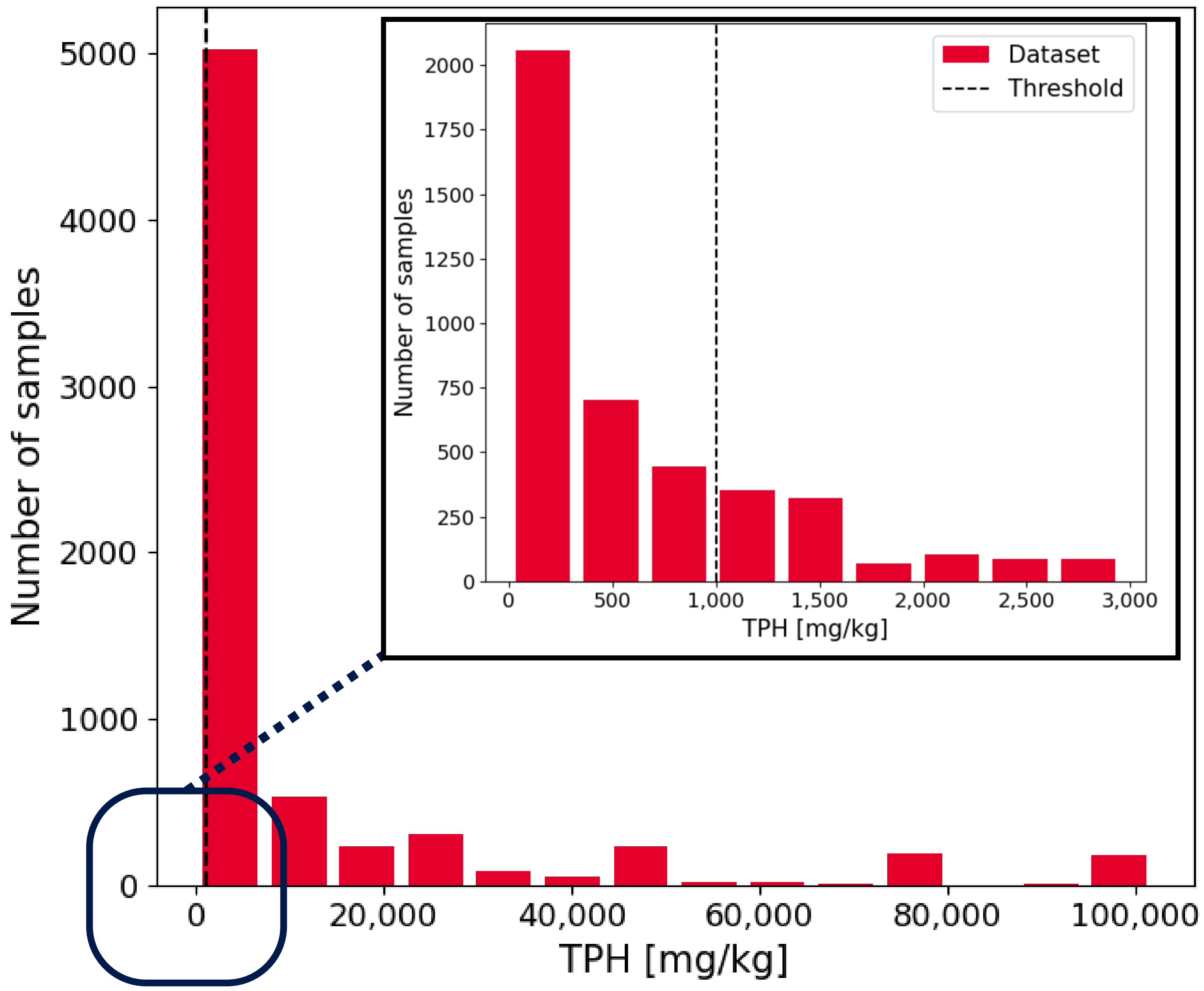
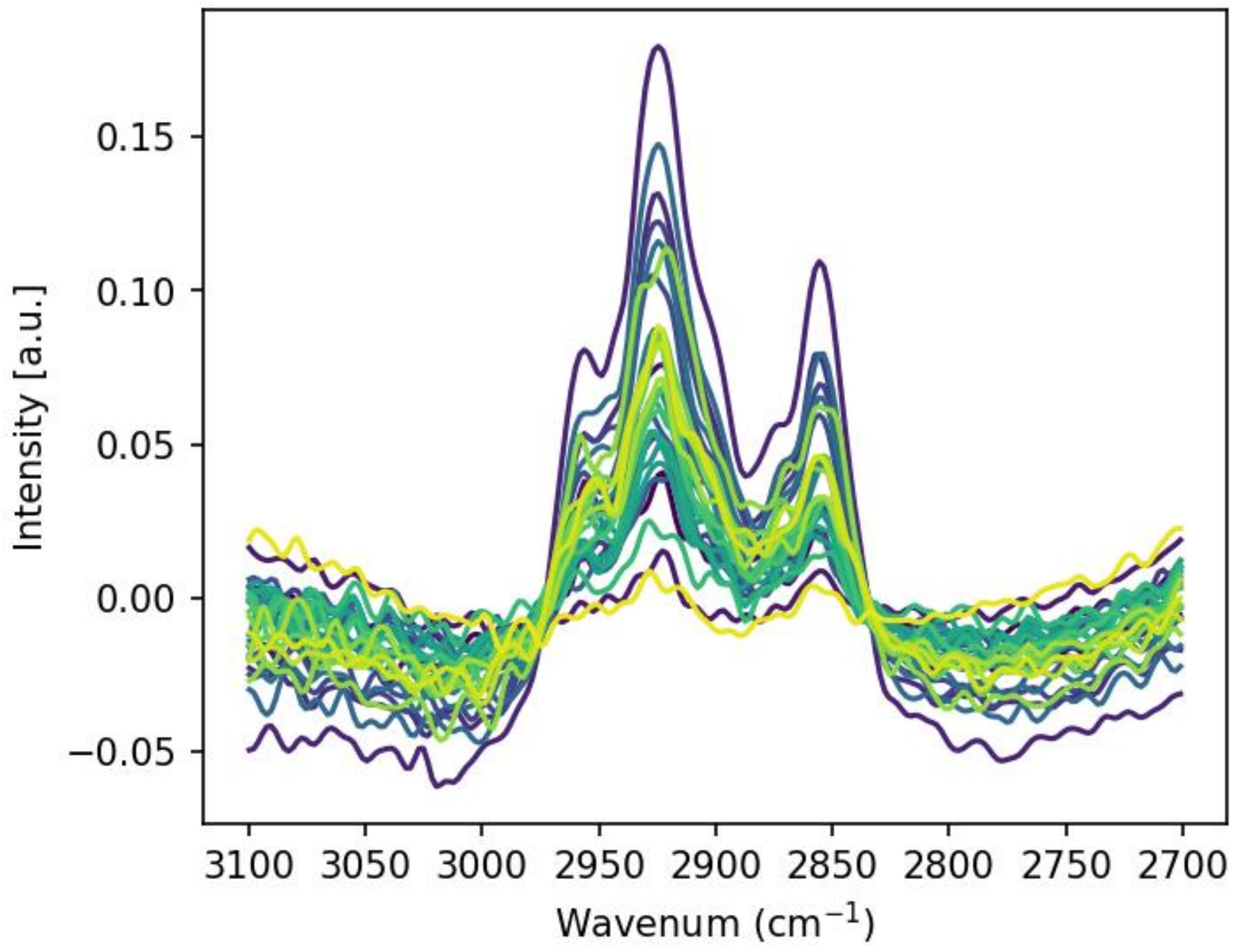
Testing Dataset





Total: 6,880

Samples >1000ppm = 3,485

Samples <1000ppm = 3,398

Confusion Matrix

		PREDICTED	
		CONT.	CLEAN
ACTUAL	CONT.	TP	FN
	CLEAN	FP	TN

CONT. = Contaminated

TP = True Positive (Cont.)
FP = False Positive
TN = True Negative (Clean)
FN = False Negative

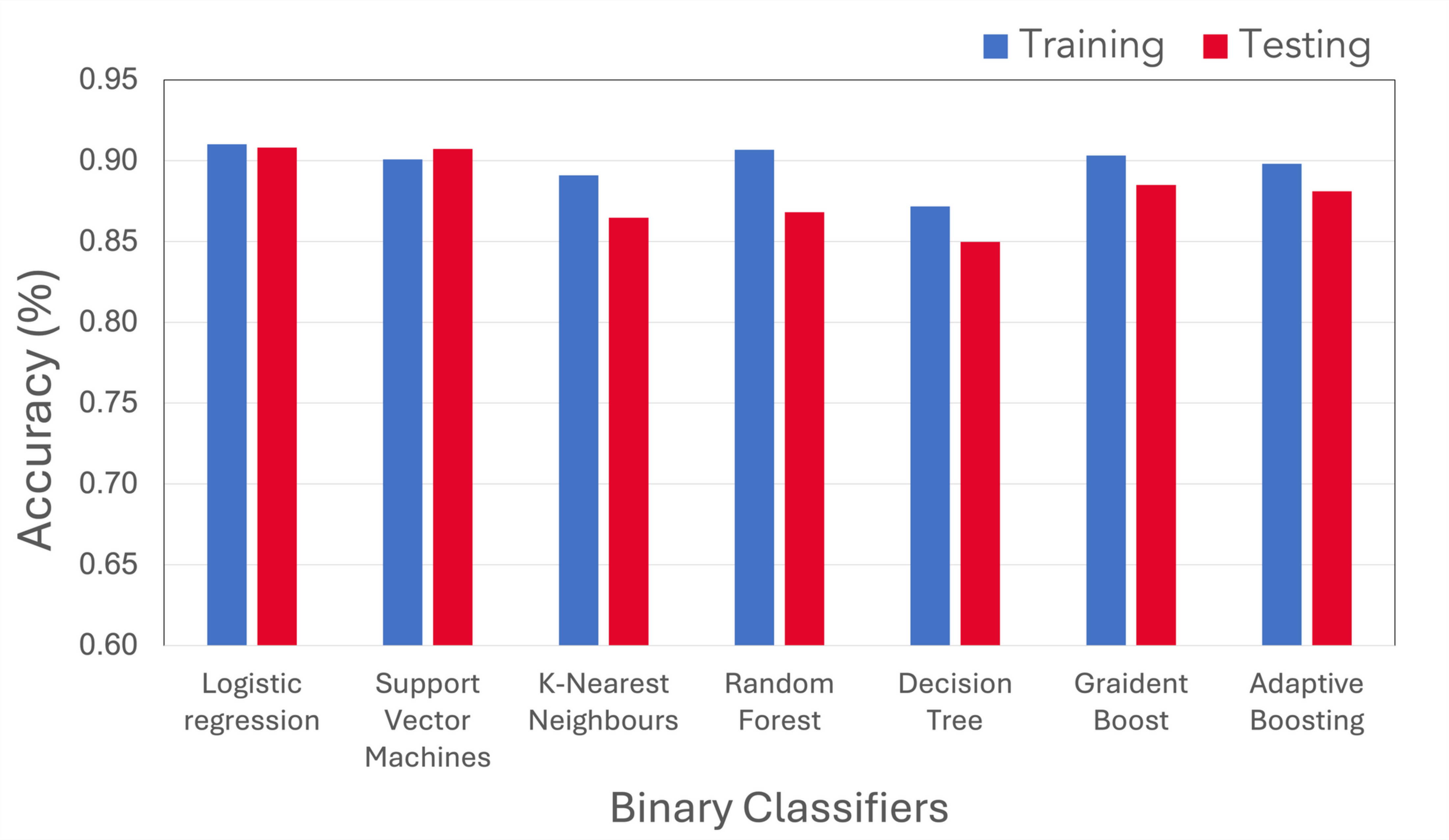
Model refinement

Performance Optimisation

Logistic regression
Training = 90.5 %
Testing = 90.8 %

Random forest
Training = 90.7 %
Testing = 86.8 %

- Used 7 different classifiers
- Three metrics for assessing model performance
  - Accuracy
  - F1 score
  - Matthew's correlation coefficient (MCC)
- Get similar performance across all metrics.



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Model refinement

Data Preparation

PREPROCESSING

- Tested three scenarios
- Best performance: Detrending

FEATURE SELECTION

- Select spectral regions of interest
- Three different combinations tested
- Best performance: Three regions

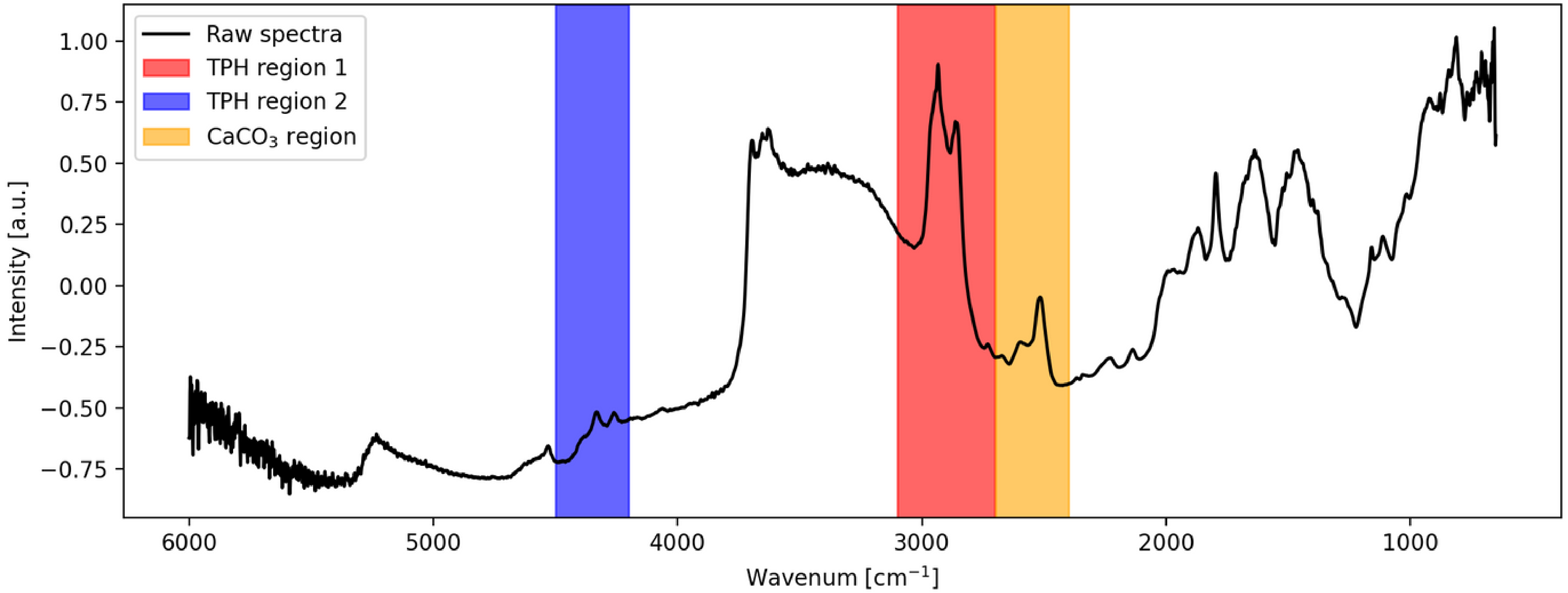


FIG: A typical mid-infrared spectrum of a contaminated sample. The red, blue and orange regions indicate the first TPH region, second TPH region and the calcium carbonate fingerprint region, respectively.

Interfering signals

Calcium Carbonate [$CaCO_3$]

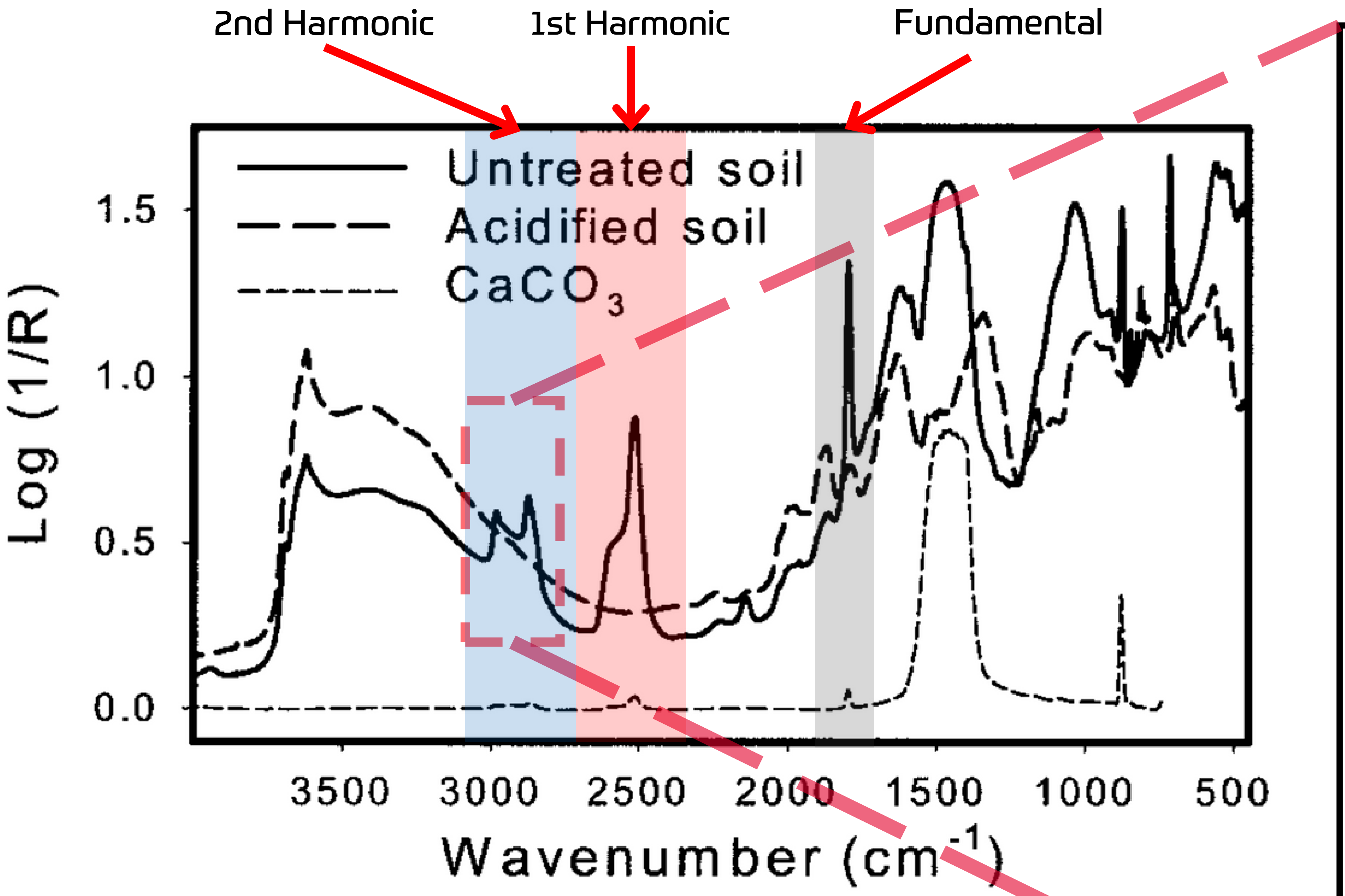
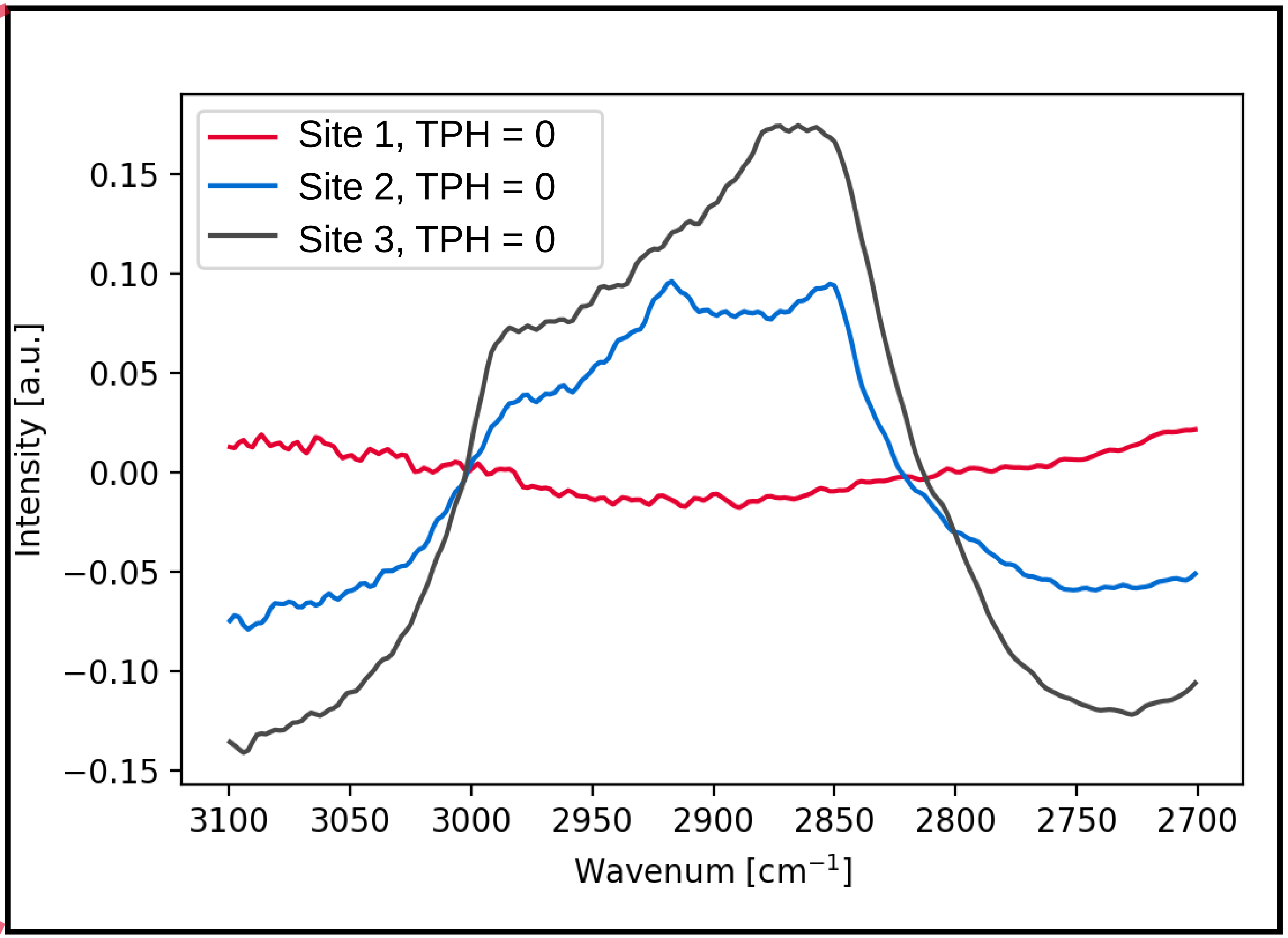


FIG: Comparison of mid-infrared and near-infrared spectra of a highly calcareous soil before and after treatment with acid for removal of carbonates. The carbonate (i.e., CaCO3) spectrum is included for additional comparison.

Reference: G. McCarty et al., Mid-Infrared and Near-Infrared Diffuse reflectance spectroscopy for Soil Carbon Measurements.

DOI: 10.2136/sssaj2002.6400



Interfering signals

Soil Organic Carbon (SOC)

- Known overlap between TPH-sensitive IR peak & natural organic matter

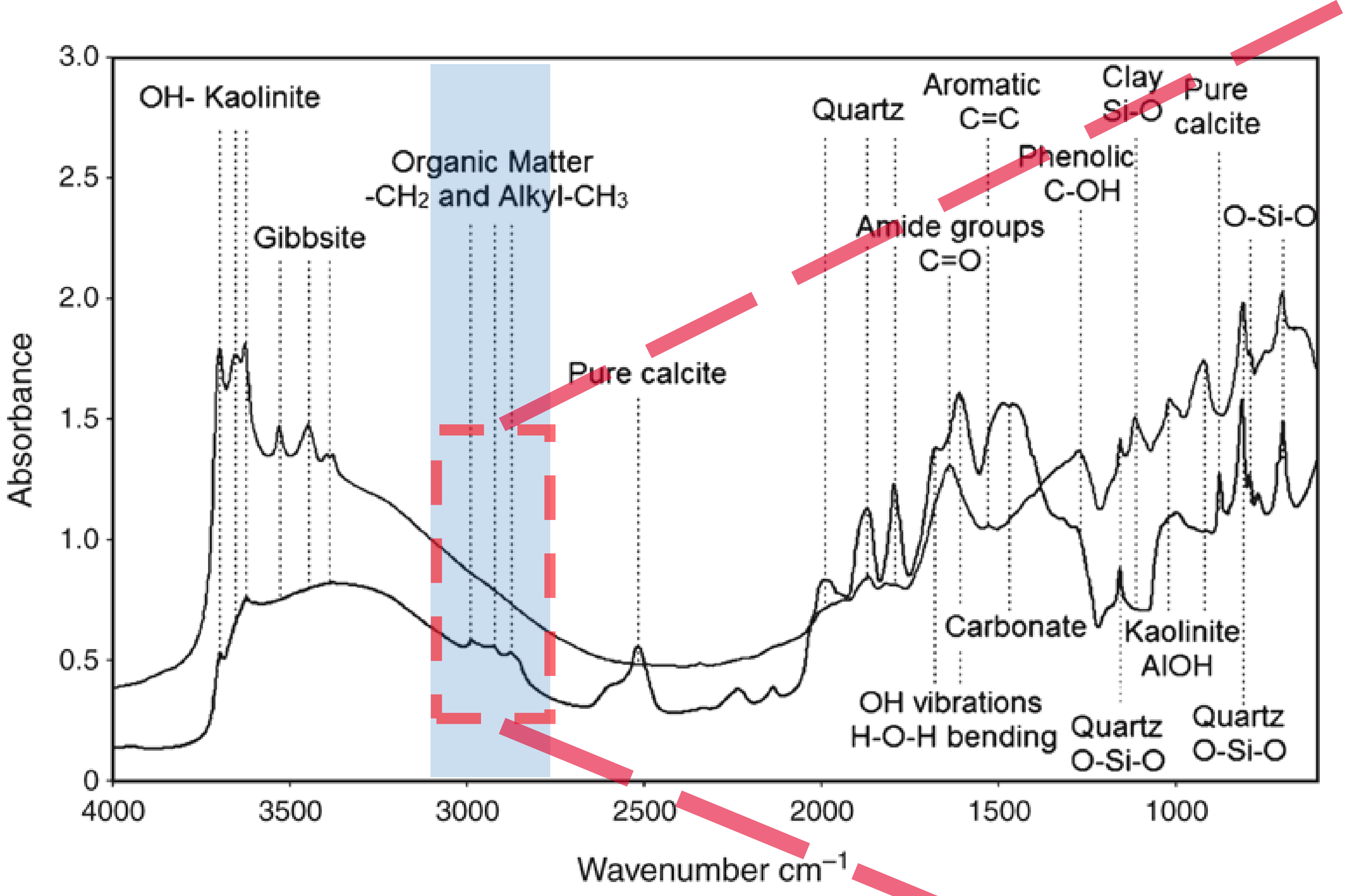
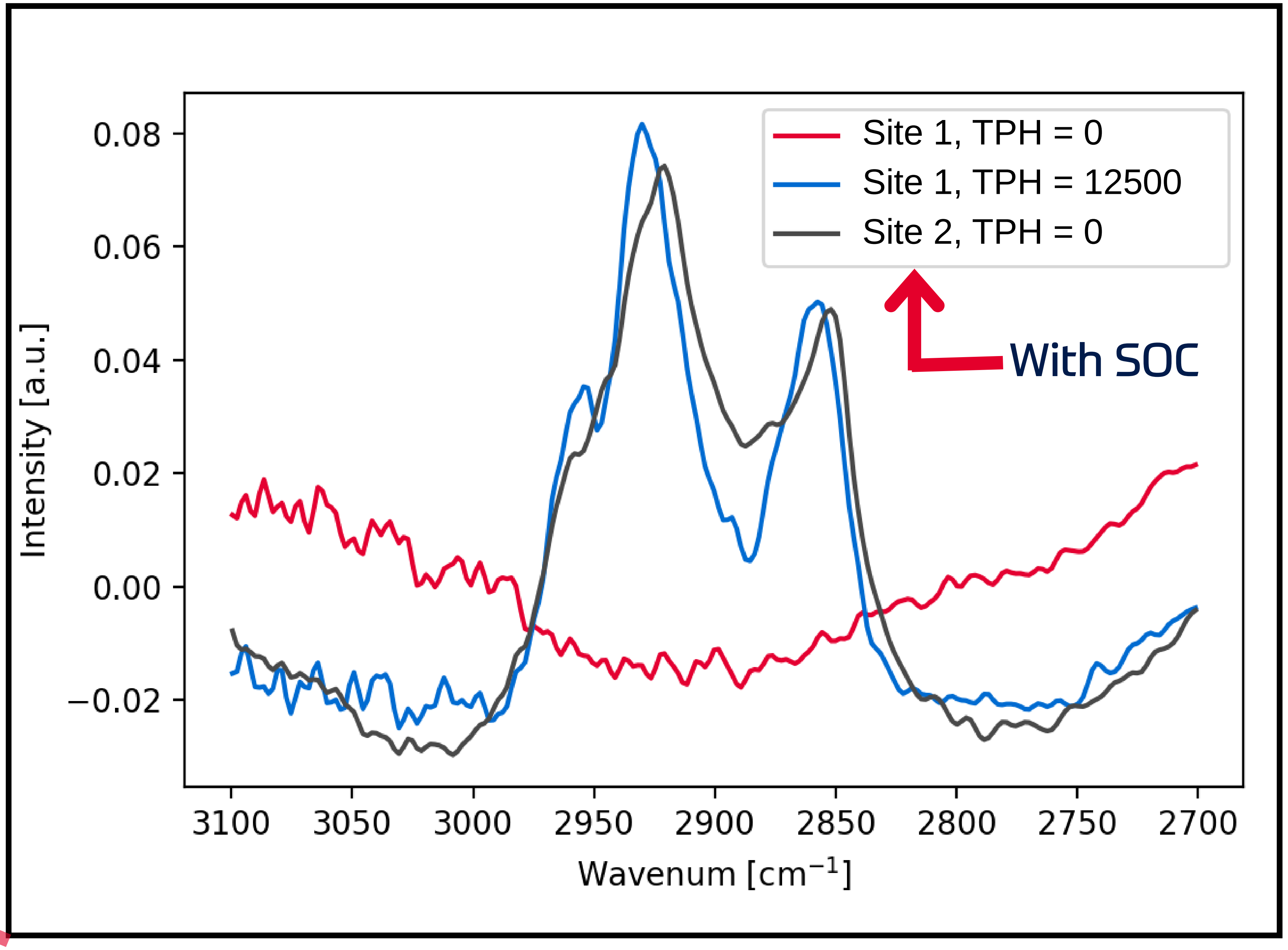


FIG: Representative soil mid-IR spectrum showing absorptions related to the mineral and organic composition of soil.

Reference: F. Le Guillou et al., How does grinding affect the mid-infrared spectra of soil and their multivariate calibrations to texture and organic carbon?.

DOI: 10.1071/SR15019



Interfering signals

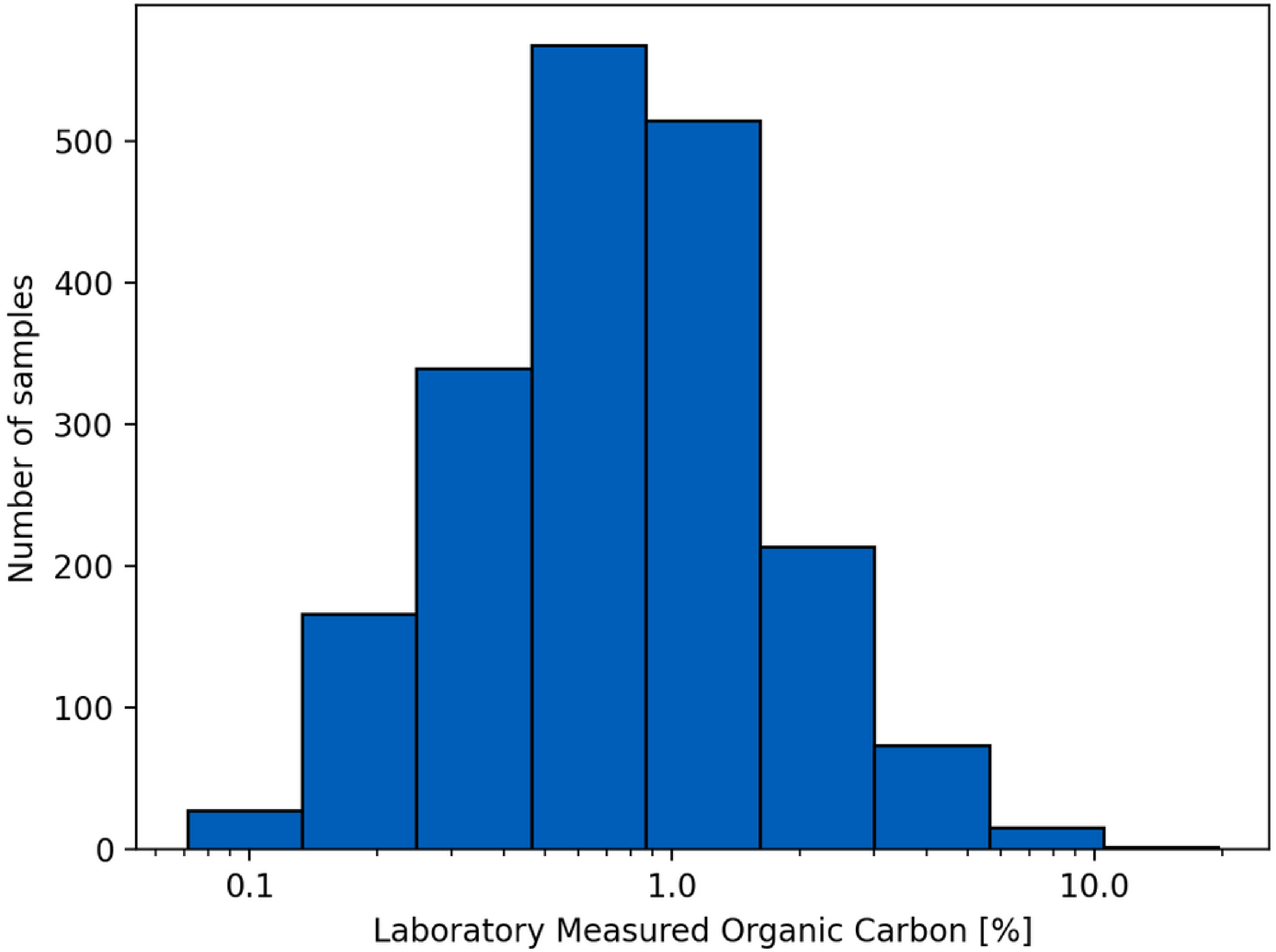
Soil Organic Carbon (SOC)

- Clean samples collected across Australia
- SOC content measured by accredited laboratory [Dry Combustion]

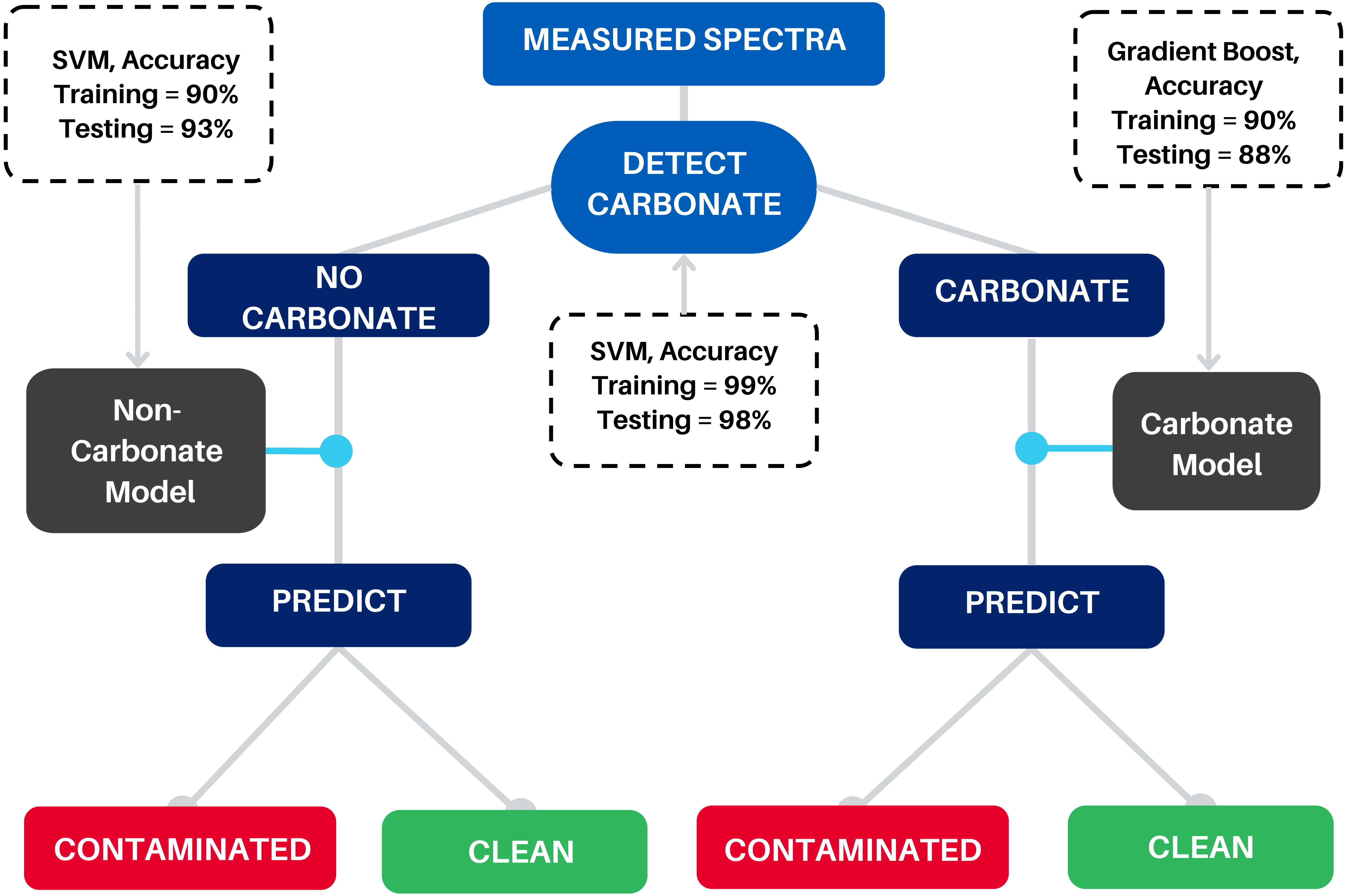
- Classifier: Support Vector Machines (SVM)
  - Accuracy: 99%
  - Confusion matrix

Predictions

$$\text{Actual}\quad \begin{array}{ccc} & \text{Cont.} & \text{Clean} \\ \text{Cont.} & 0 & 0 \\ \text{Clean} & 2 & 1919 \end{array}$$



Model Workflow



Model Summary

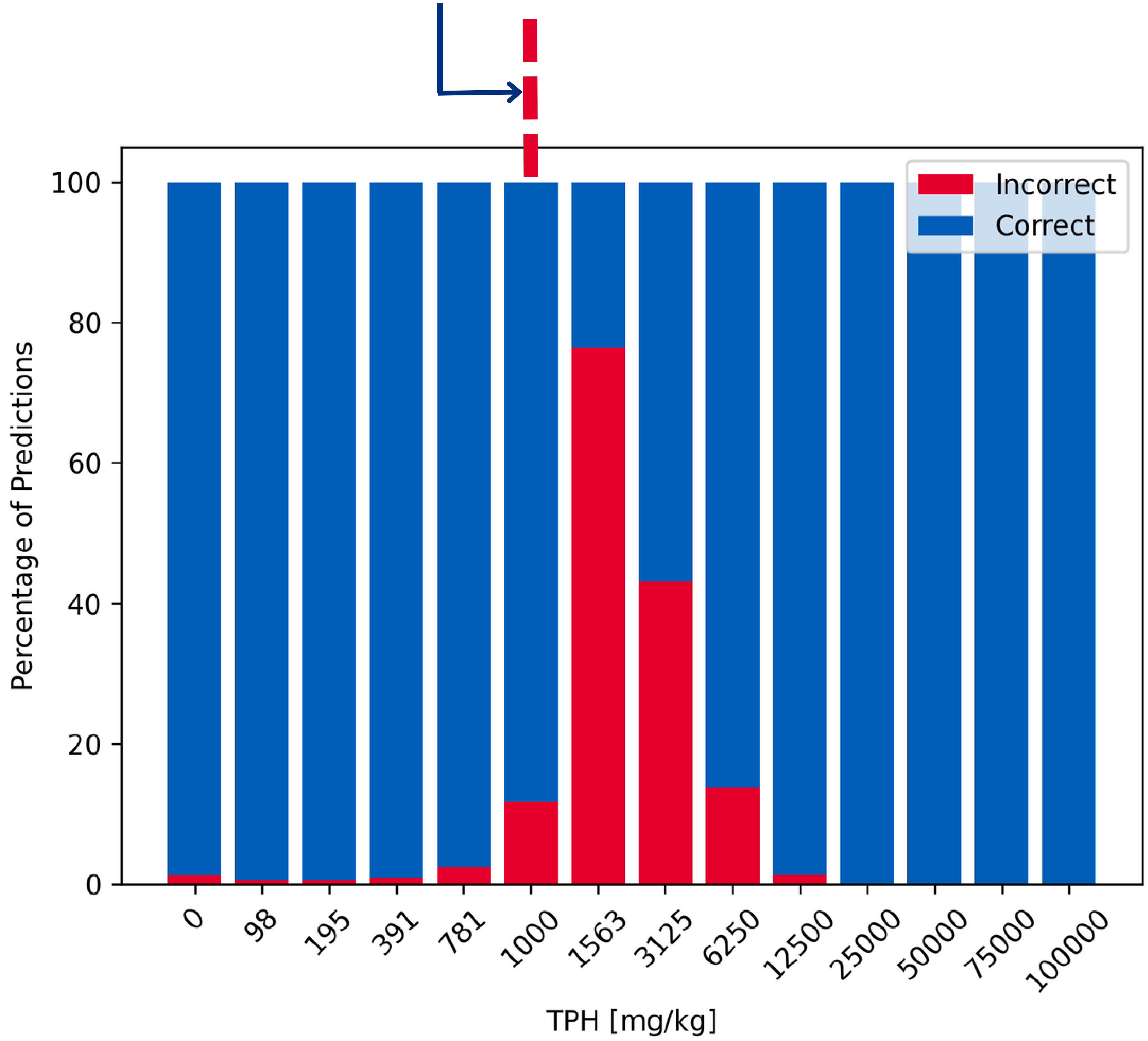
NON-CARBONATE MODEL

- Filtered dataset
  - Training = 13,984
  - Testing = 5,008
- Preprocessing = Detrend

- Best Classifier = SVM
- Accuracy
  - Training = 90%
  - Testing = 93%

- Highest misclassified samples just above the threshold
- Misclassified samples at lower TPH values likely due to SOC.

Decision boundary



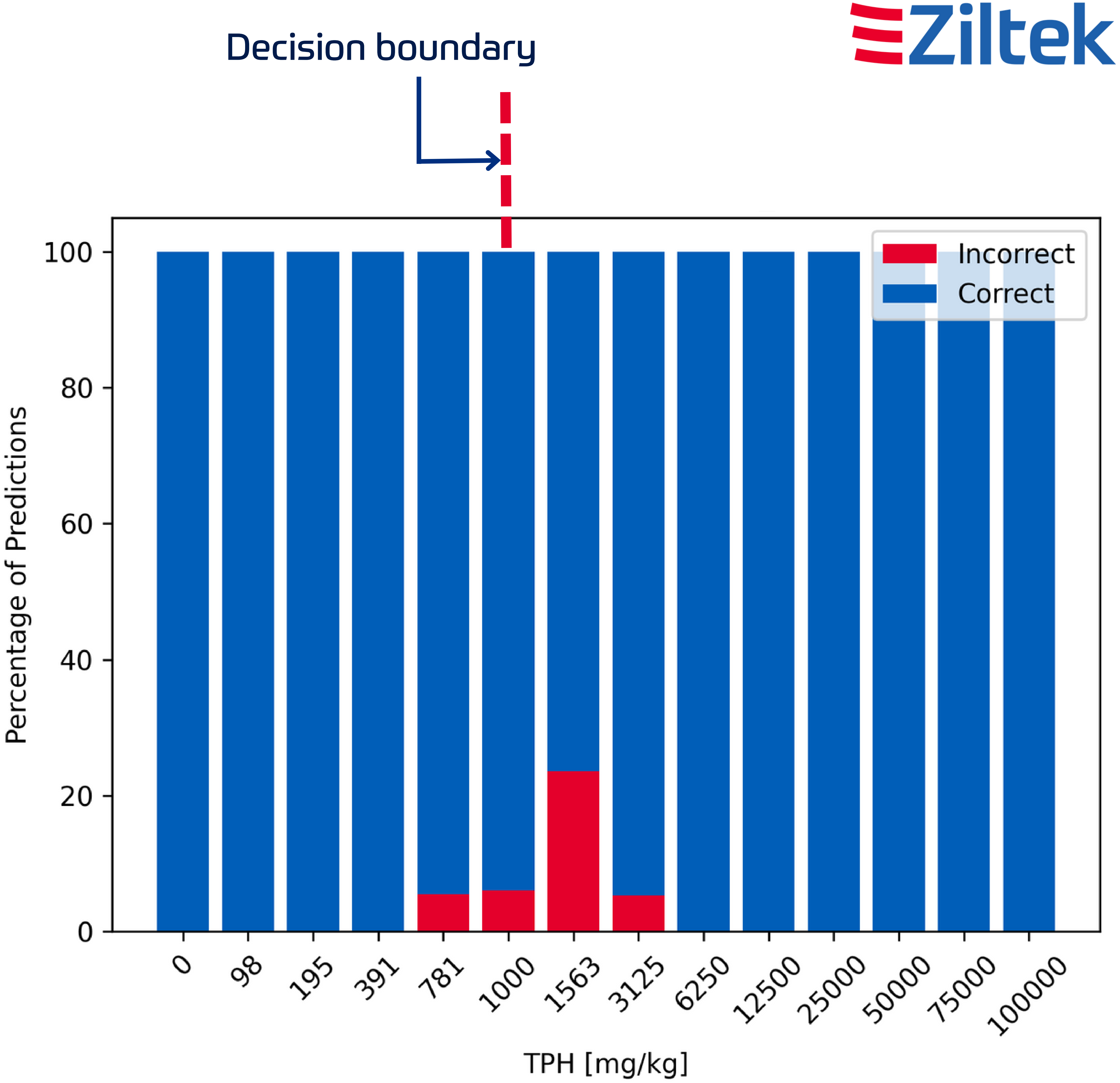
Model Summary

CARBONATE MODEL

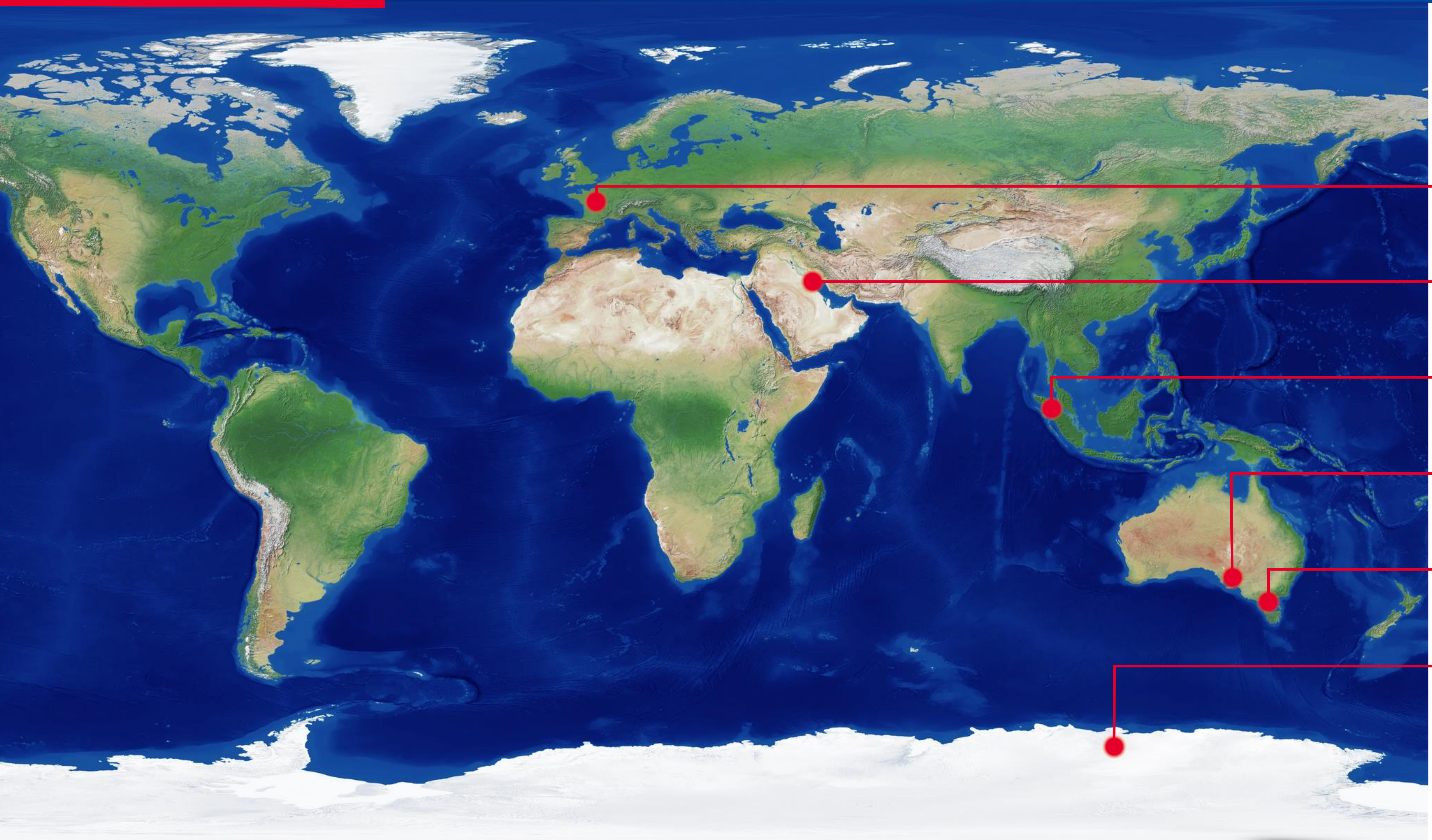
- Model built exclusively on carbonate samples.
    - Training = 3,852
    - Testing = 1,872
- Preprocessing: Detrend

- Best Classifier = Gradient Boost
- Accuracy
    - Training = 90.1%
    - Testing = 88.4%

- Require more samples for future optimisation.



Test Results



- France
- Kuwait
- Indonesia
- Adelaide
- Victoria
- Antarctica

Results

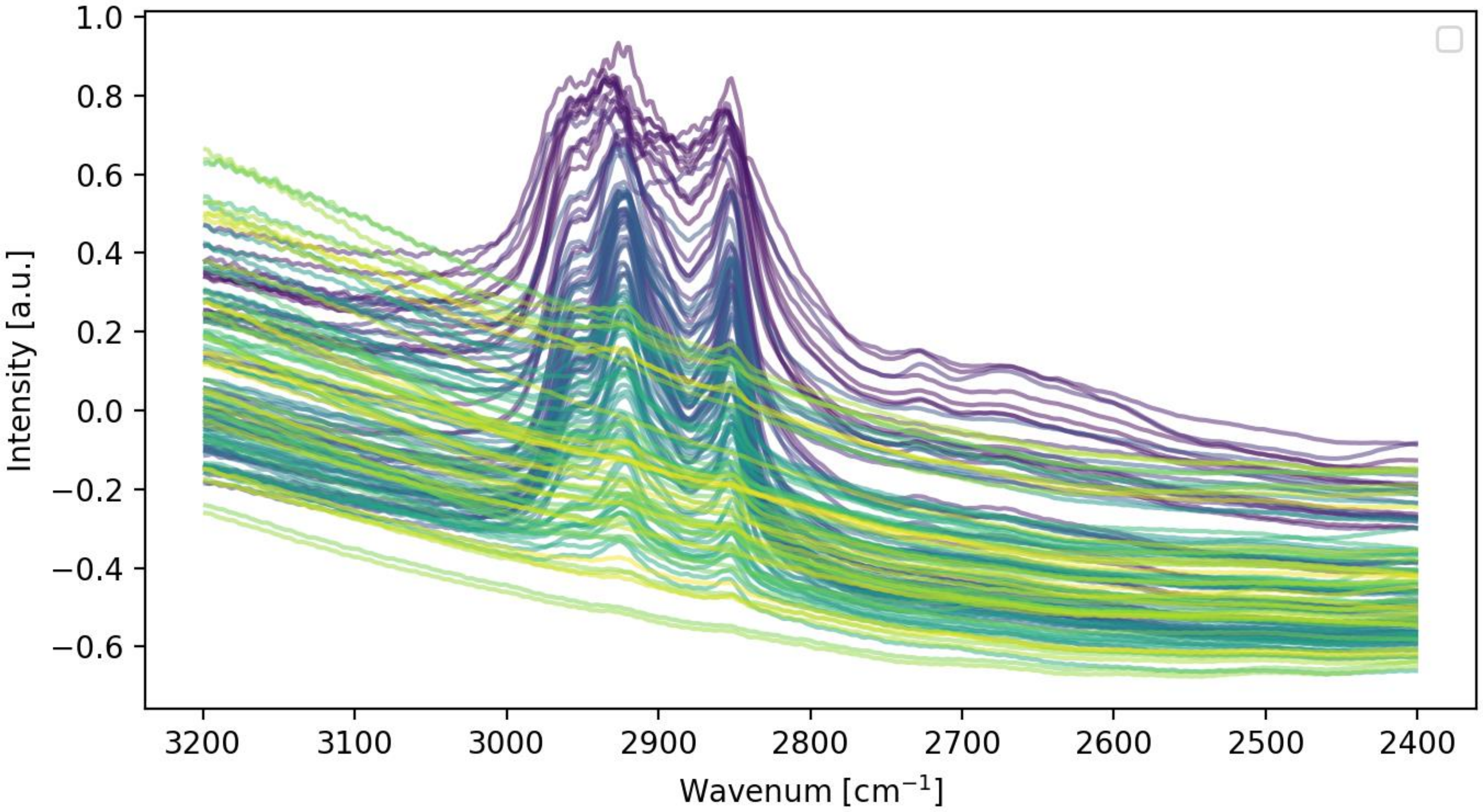
TEST CASE 1 - Indonesia

CONFUSION MATRIX $\begin{bmatrix} 1218 & 10 \\ 80 & 730 \end{bmatrix}$

- Project Details
  - Sumatran oil fields
  - Contaminant: Crude Oil
  - Large scale, multi-year project

- Model: Non-Carbonate
- Number of samples: 2038
  - Class A: 1218 (>1000)
  - Class B: 810 (<1000)

- Classifier: SVM
  - Accuracy: 95%
  - F1 Score: 0.94
  - MCC: 0.90



Results

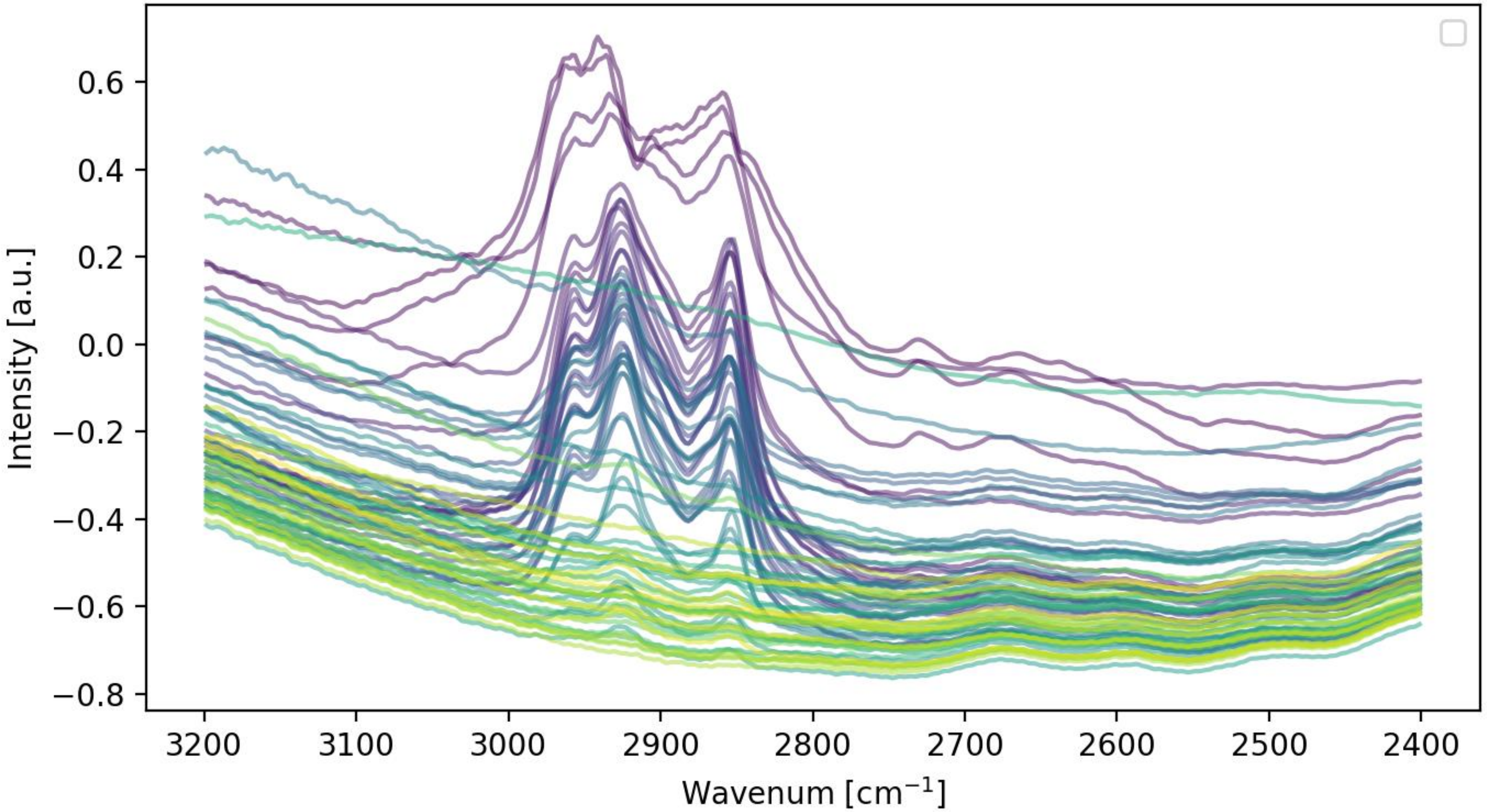
TEST CASE 2 - Coastal Victoria

CONFUSION MATRIX $\begin{bmatrix} 117 & 0 \\ 0 & 361 \end{bmatrix}$

- Project Details
  - Coastal Wilderness
  - Contaminant: Crude Oil
  - Medium scale, 18 months project

- Model: Non-Carbonate
- Number of samples: 538
  - Class A: 361 (>1000)
  - Class B: 177 (<1000)

- Classifier: SVM
  - Accuracy: 100%
  - F1 Score: 1.0
  - MCC: 1.0



Results

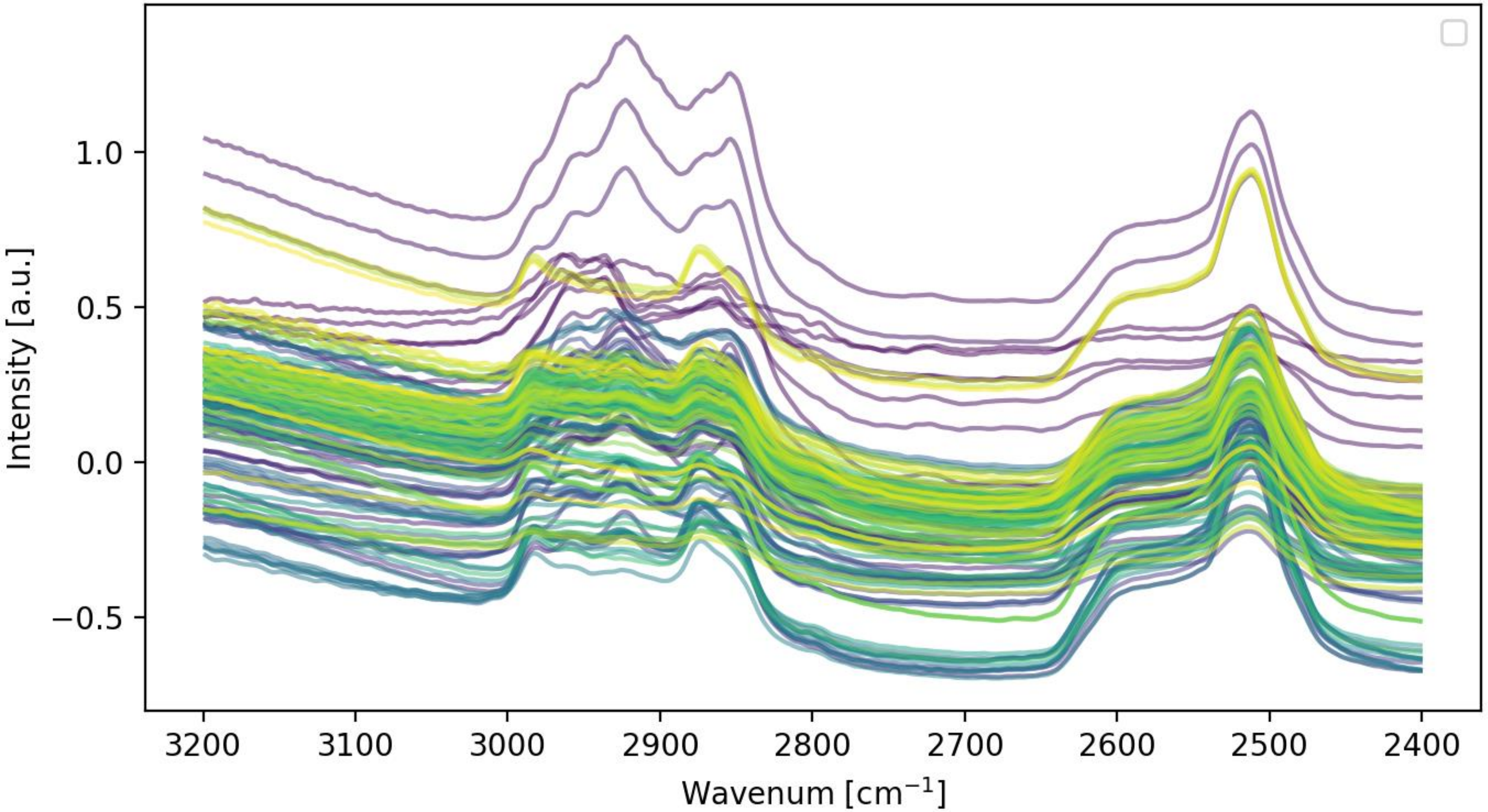
TEST CASE 3 - France

CONFUSION MATRIX $\begin{bmatrix} 389 & 83 \\ 29 & 396 \end{bmatrix}$

- Project Details:
  - Industrial site
  - Contaminant: Diesel
  - Small scale, several weeks

- Model: Carbonate
- Number of samples: 897
  - Class A: 472 (>1000)
  - Class B: 452 (<1000)

- Classifier: Gradient Boost
  - Accuracy: 88%
  - F1 Score: 0.88
  - MCC: 0.76



HIGH CARBONATE CONTENT !!!

Results

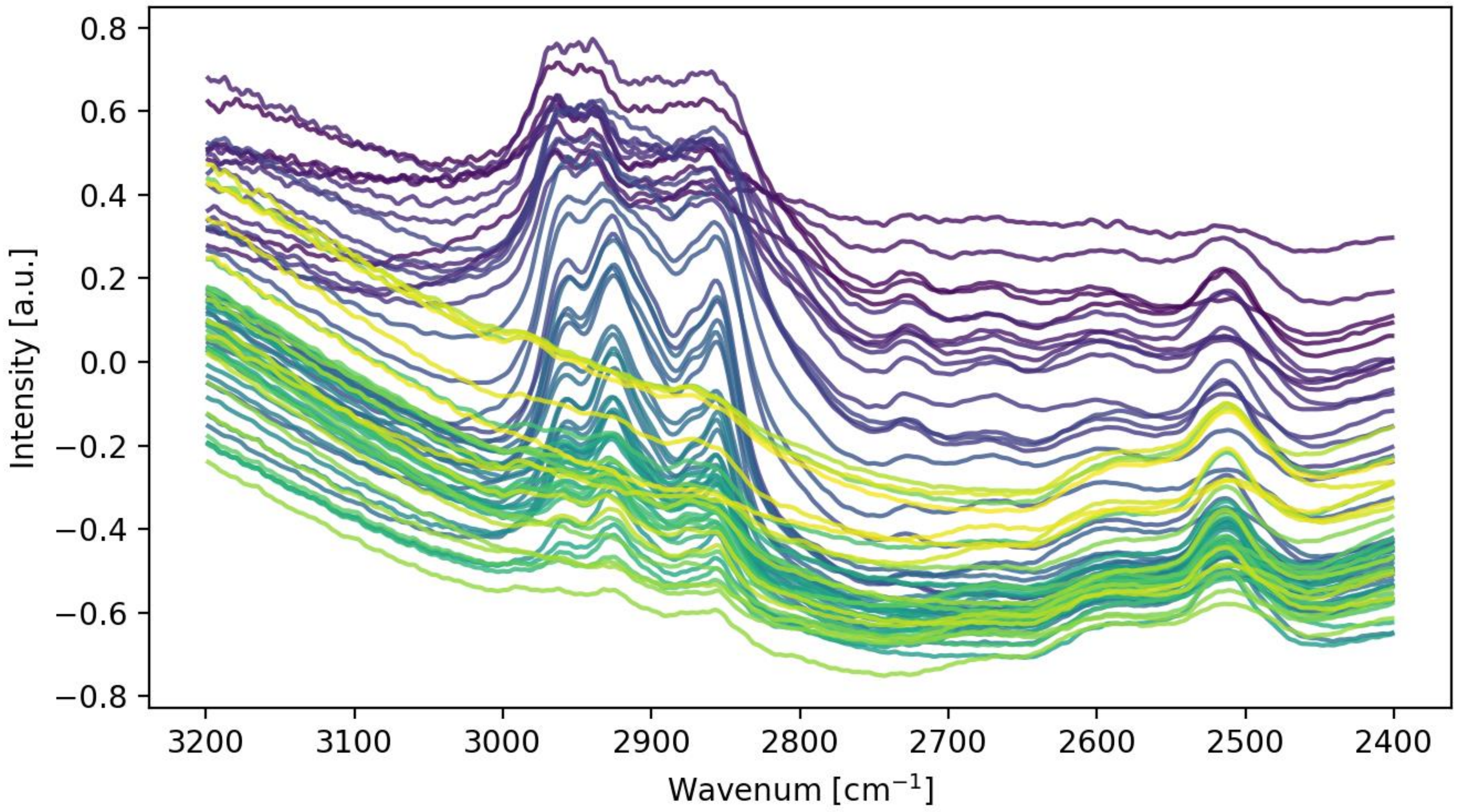
TEST CASE 4 - Kuwait

CONFUSION MATRIX $\begin{bmatrix} 204 & 0 \\ 25 & 125 \end{bmatrix}$

- Project Details
  - Kuwaiti oil fields
  - Contaminant: Weathered Crude Oil
  - Large scale, multi-year project

- Model: Carbonate
- Number of samples: 354
  - Class A: 204 (>1000)
  - Class B: 150 (<1000)

- Classifier: Gradient Boost
  - Accuracy: 93%
  - F1 Score: 0.91
  - MCC: 0.86



Results

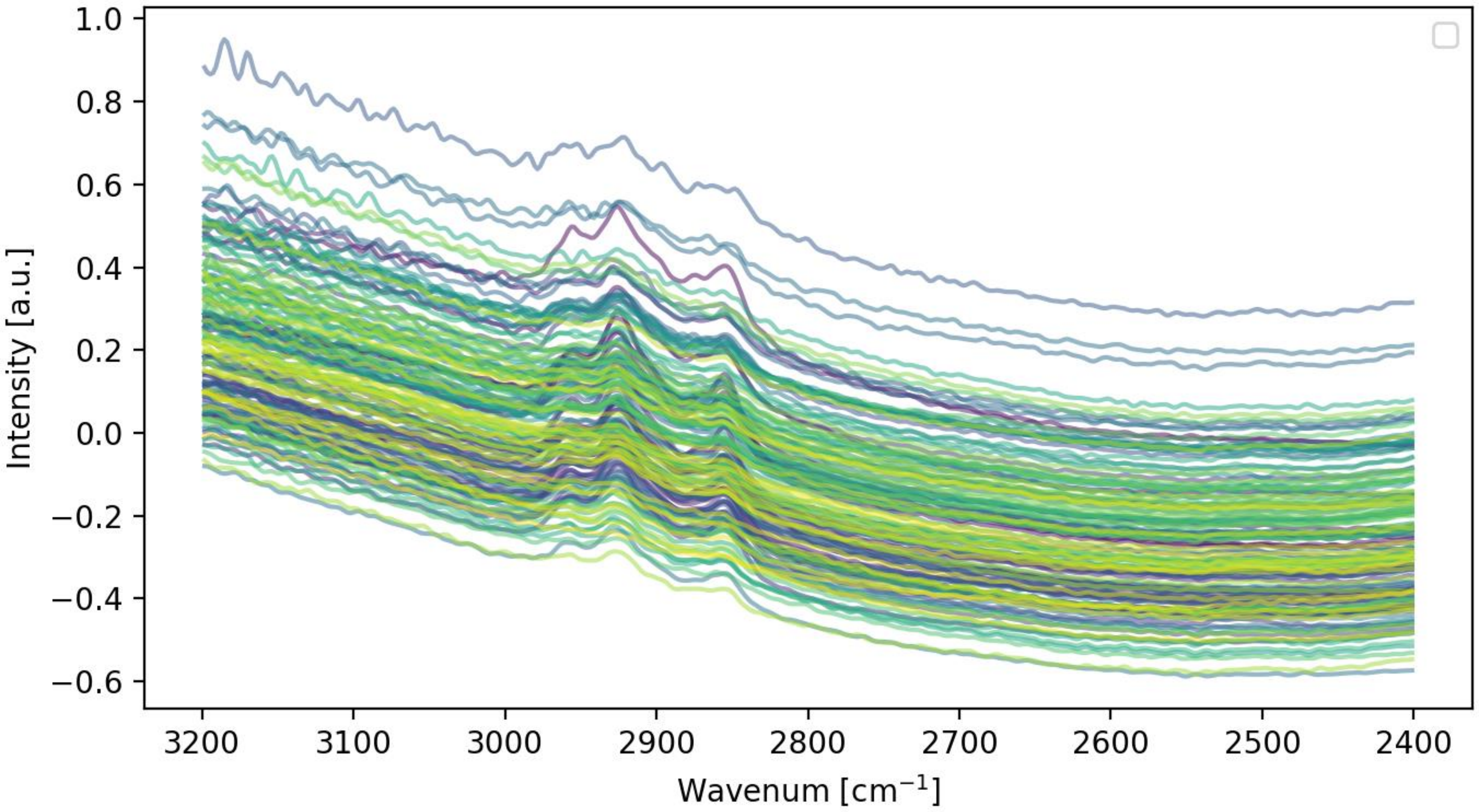
TEST CASE 5 - Antarctica

CONFUSION MATRIX $\begin{bmatrix} 275 & 10 \\ 60 & 392 \end{bmatrix}$

- Project Details:
  - Research facility
  - Contaminant: Antarctic Diesel
  - One week

- Model: Non-carbonate
- Number of samples: 737
  - Class A: 452 (>1000)
  - Class B: 285 (<1000)

- Classifier: SVM
  - Accuracy: 91%
  - F1 Score: 0.92
  - MCC: 0.81



Results

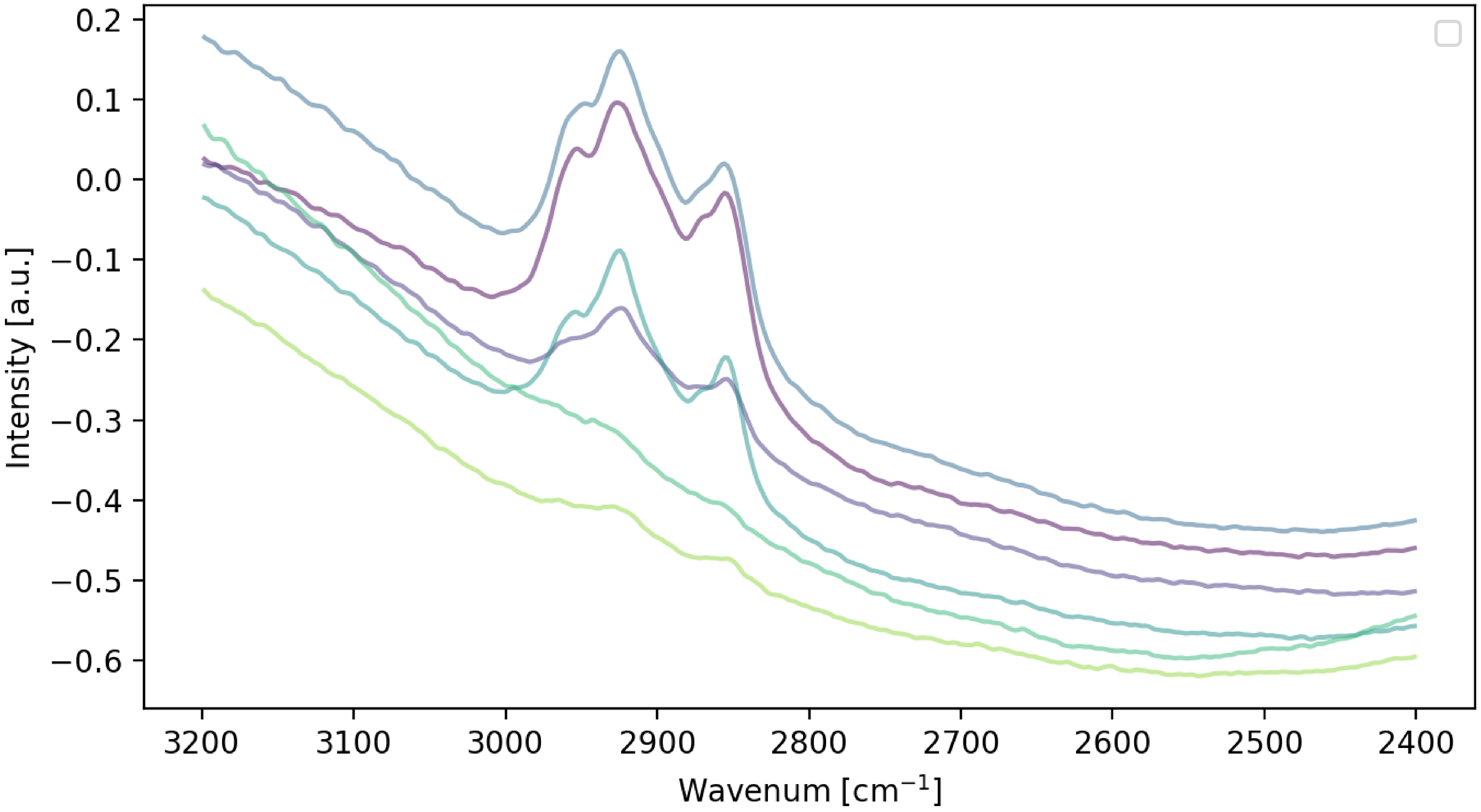
TEST CASE 6 - Metro Adelaide

CONFUSION MATRIX $\begin{bmatrix} 20 & 0 \\ 0 & 12 \end{bmatrix}$

- Project Details:
  - Industrial site
  - Contaminant: Diesel
  - Small scale, several weeks

- Model: Non-carbonate
- Number of samples: 32
  - Class A: 20 (>1000)
  - Class B: 12 (<1000)

- Classifier: SVM
  - Accuracy: 100%
  - F1 Score: 1
  - MCC: 1



USE CASE

PETROL STATION CLEANUP

- Decommissioned petrol stations require cleanup
- Typical backfill soils:
  - Dolomite
  - Sand

- Clean soil samples collected from suppliers.
- Spiked with a known level of contaminant.
- Binary classifiers used to access sample contamination.

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USE CASE

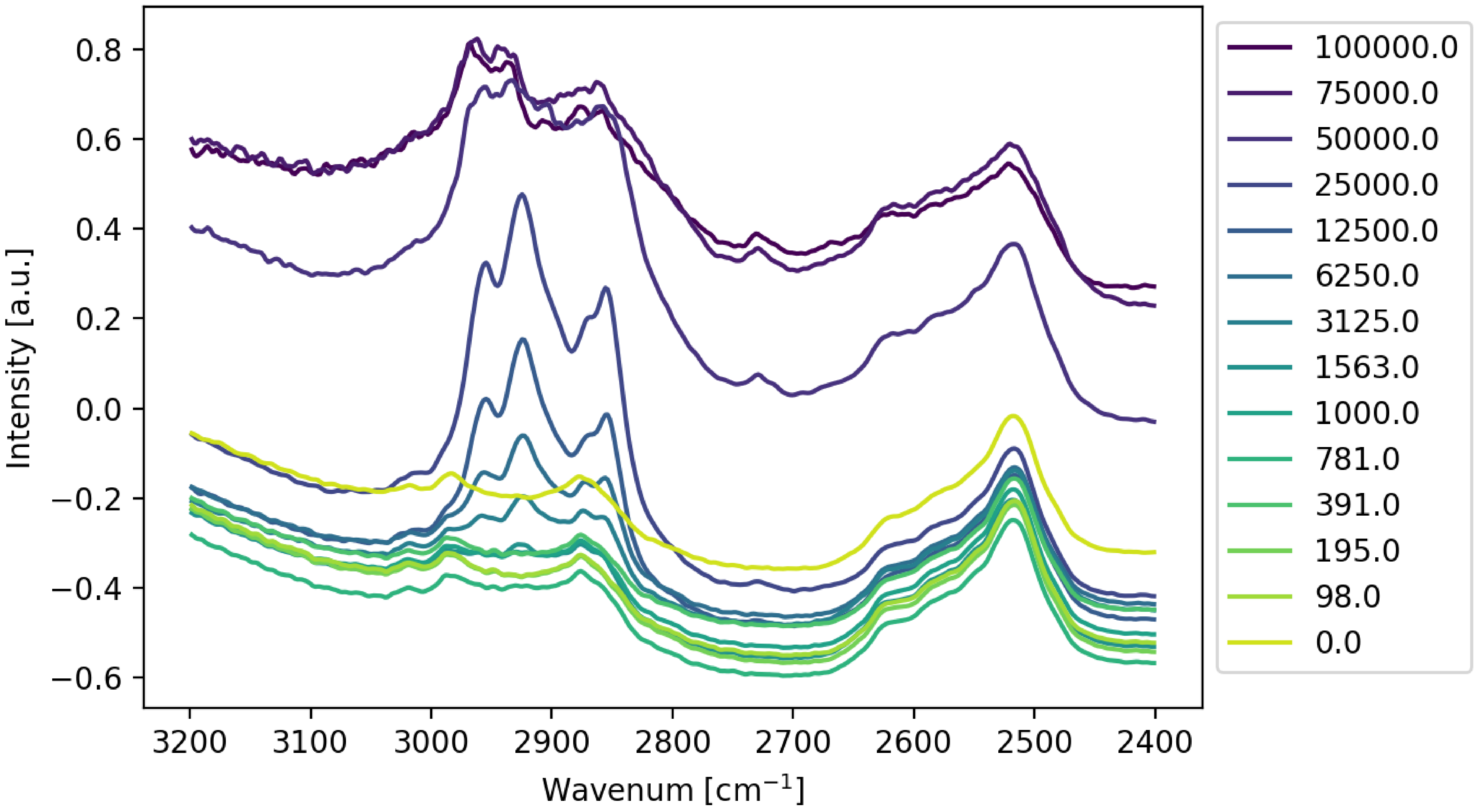
Calibration series: DOLOMITE

CONFUSION MATRIX $\begin{bmatrix} 75 & 15 \\ 0 & 90 \end{bmatrix}$

- Sample details
  - Contaminant: Diesel
  - Calibration standard

- Model: Carbonate
- Number of samples: 180
  - Class A: 90 (>1000)
  - Class B: 90 (<1000)

- Classifier: Gradient Boost
  - Accuracy: 92%
  - F1 Score: 0.93
  - MCC: 0.85



USE CASE

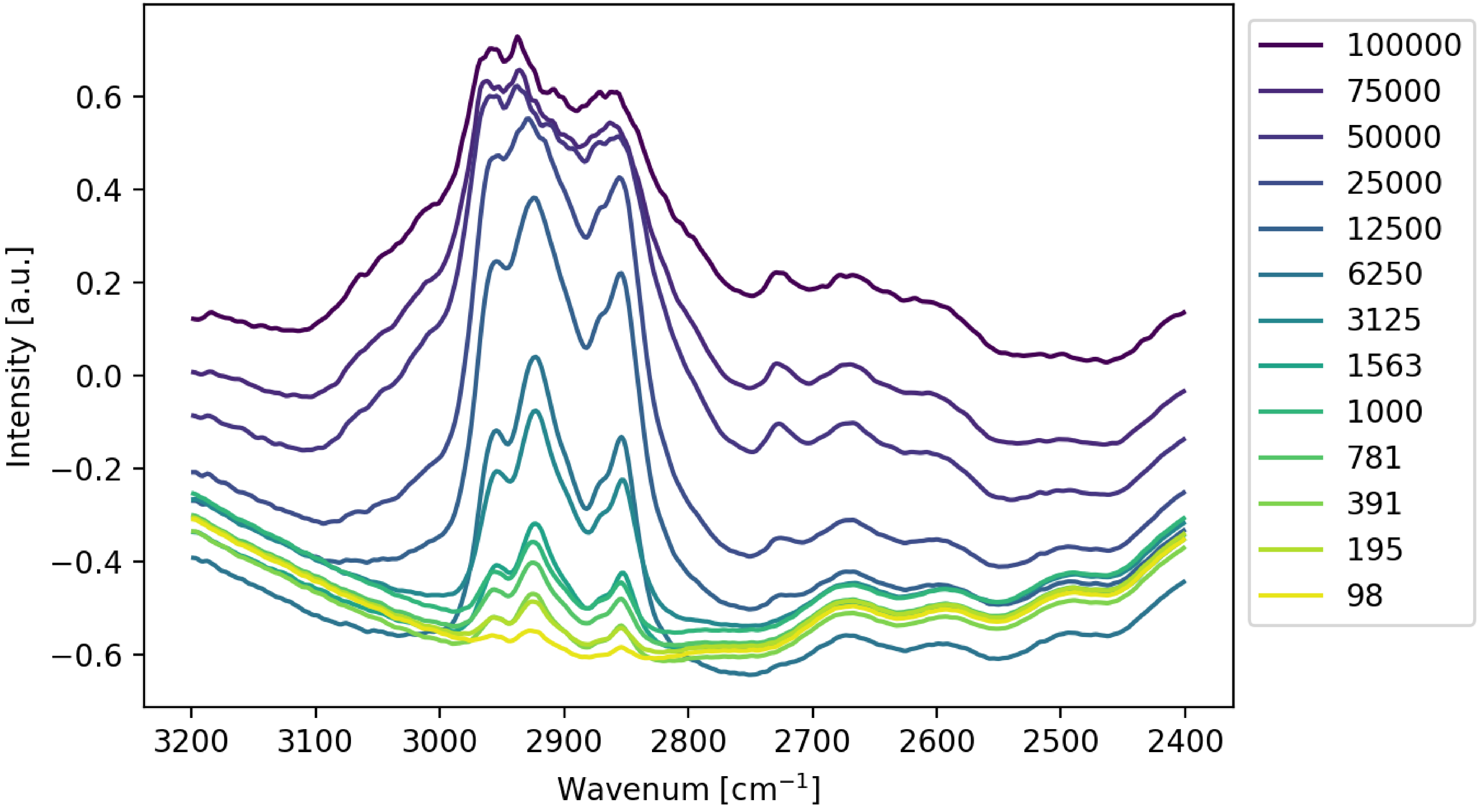
Calibration series: SAND

CONFUSION MATRIX $\begin{bmatrix} 90 & 0 \\ 0 & 60 \end{bmatrix}$

- Sample details
  - Contaminant: Diesel
  - Calibration standard

- Model: Non-Carbonate
- Number of samples: 150
  - Class A: 90 (>1000)
  - Class B: 60 (<1000)

- Classifier: SVM
  - Accuracy: 100%
  - F1 Score: 1.0
  - MCC: 1.0



Conclusion

- Developed binary classifier for rapid-assessment of hydrocarbon-contaminated soils.
- Potential issues identified
  - Calcium Carbonate
  - Soil Organic Carbon
  - Misclassified samples around threshold
- Developed a robust method for handling carbonate signatures.
- Organic carbon signature unlikely to be an issue for soils with SOC $\leq$ 10%.
- Classifier performance accessed on historical customer data with Diesel Range Organics and heavier contaminants.
- Results are promising with prediction accuracy around 90%.
- Future work will involve
  - Training data refinement
  - Refining model structure to catch edge cases
  - Testing lighter hydrocarbons (e.g., Gasoline)

ZILTEK TEAM

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Thank You

QUESTIONS?

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