Building regional calibrations for prediction of soil health properties using Mid-Infrared range FTIR spectroscopy

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DALHOUSIE UNIVERSITY

Centre for Sustainable Soil Management

The mission of the Centre for Sustainable Soil Management (CSSM) is to:

- Advance scholarship and research in soil science;
- Provide a focal point for soil science education and training in the Atlantic region; and
- Serve as a national data hub for data intensive mapping, understanding, and use of soil-landscape information and the impact of management on those landscapes.

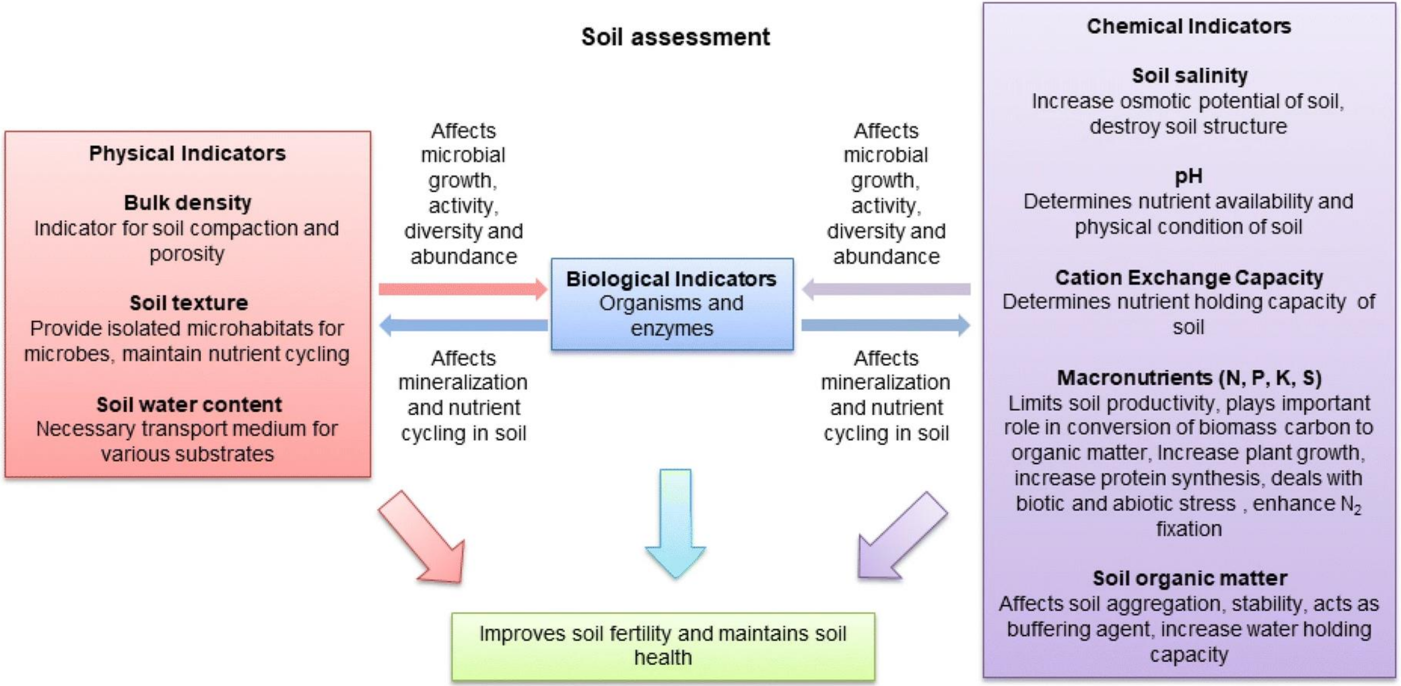
https://www.sustainablesoils.ca/

Soil "Health" vs. Soil "Quality"

Soil Health is the the continued capacity of soil to function as a vital living system, within ecosystem and land-use boundaries, to sustain biological productivity, promote the quality of air and water environments, and maintain plant, animal, and human health (Pankhurst et al., 1997).

Soil Quality the capacity of a soil to function, within ecosystem and land use boundaries, to sustain productivity, maintain environmental quality, and promote plant and animal health. (Linn and Doran, 1994)

Importance and Need for Soil Health Monitoring



Maurya, S., Abraham, J.S., Somasundaram, S. *et al.* Indicators for assessment of soil quality: a mini-review. *Environ Monit Assess* **192**, 604 (2020).

Barriers in Monitoring Soil Health Parameters

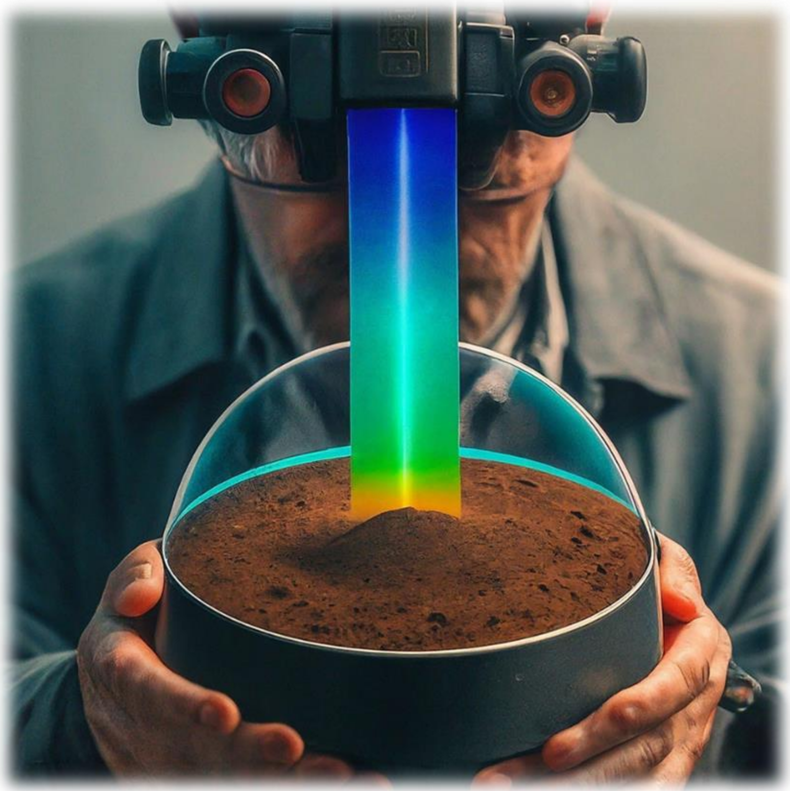
High Cost

Long Turnaround Time

- **Infrequent Soil Testing**
- **Blanket Fertilizer Recommendation**
- **Delayed Sustainable Practices**
- **Hindered Soil Map Update**

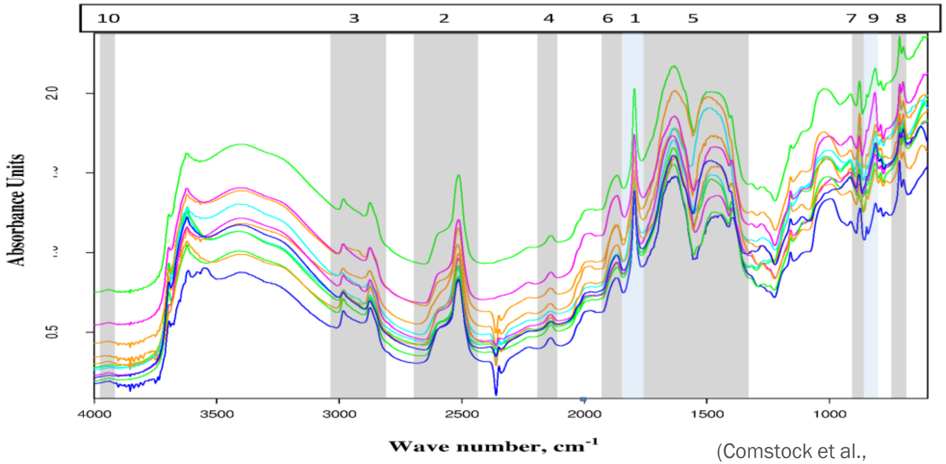
The development of cost-effective, rapid techniques like Mid-infrared (MIR) spectroscopy as an alternative for routine soil analysis and health monitoring

The Future is Spectroscopy!

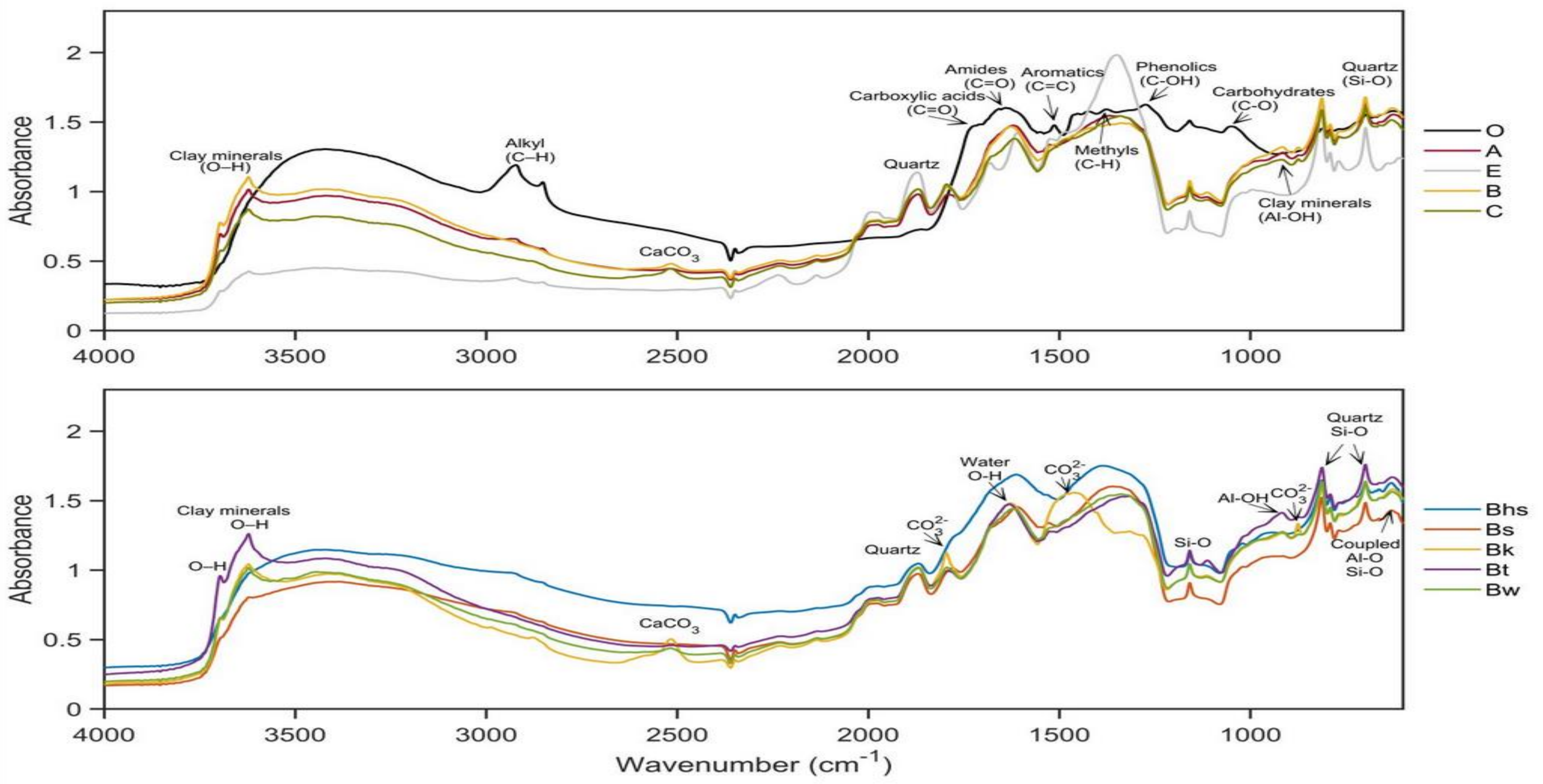


MIR Spectroscopy

Mid-infrared spectroscopy has been validated as a valuable tool for generating estimates of soil properties when high quality reference values are available for development of appropriate calibrations (or models).



(Comstock et al., 2019)


Absorbance
Clay minerals (O–H)
Alkyl (C–H)
CaCO3
Quartz
Carboxylic acids (C=O)
Amides (C=O)
Aromatics (C=C)
Methyls (C-H)
Phenolics (C-OH)
Carbohydrates (C-O)
Clay minerals (Al-OH)
Quartz (Si-O)
O
A
E
B
C
Clay minerals O–H
O–H
Water O-H
CO3 2-
Si-O
Al-OH
Coupled Al-O Si-O
Quartz Si-O
Bhs
Bs
Bk
Bt
Bw
Wavenumber (cm-1)

Spectroscopy Research Program Goals

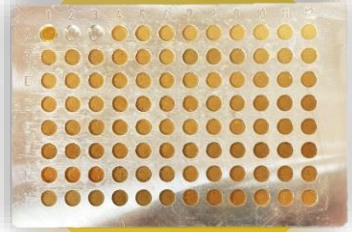
Le sol du jour

Objectives

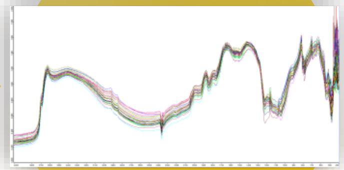
- Develop calibrations for different soil properties for Atlantic Canada, Ontario, and Quebec
- Compare calibrations against USDA NRCS spectral database and calibrations
- Field test strength of calibrations for different soil properties
- Build regional, eventually national, spectral database and library

Rationale for Using Soil Spectroscopy

Non-Destructive



Sustainable



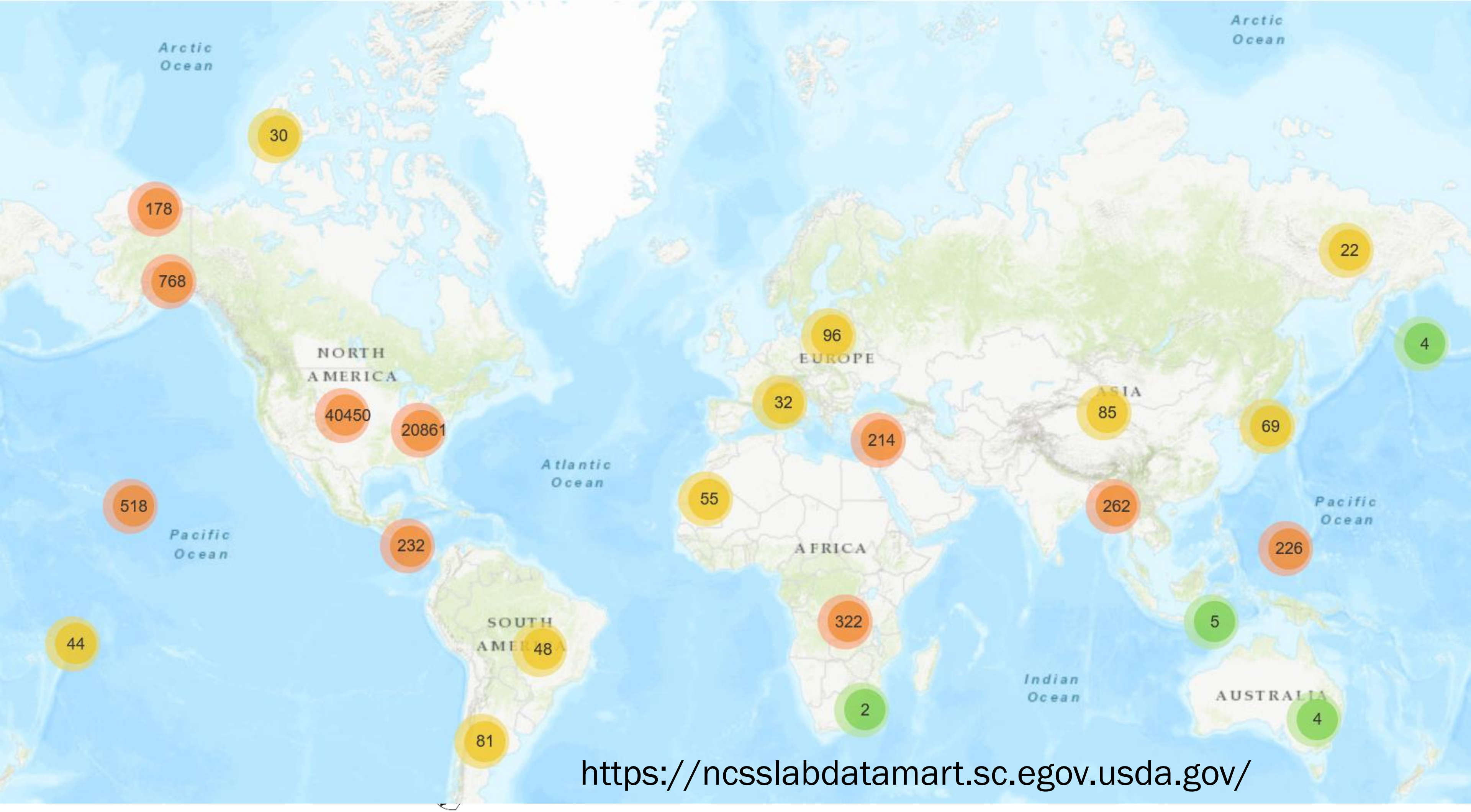
- pH
- Total Organic Carbon
- Total Nitrogen
- Lime Rate
- Cation Exchange Capacity
- Organic Matter
- Carbonate
- Fe & Al Oxide Content

Throughput Time

> 2X Faster

Cost Per Sample

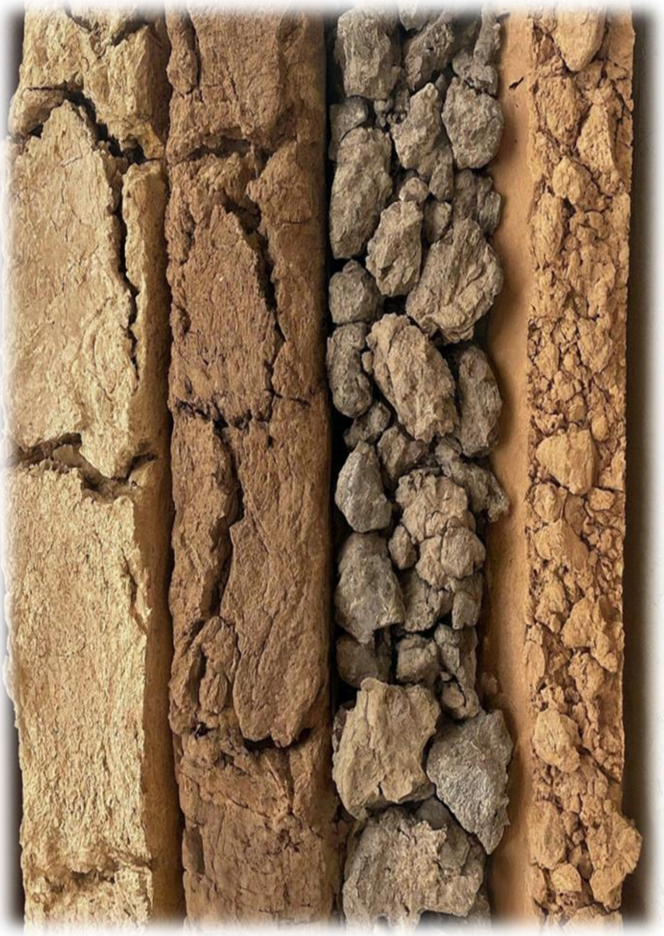
~ 80% Cheaper



https://ncsslabdatamart.sc.egov.usda.gov/

Challenges and Priorities

- Soil properties being measured may include differences in:
  - ***Representative sampling***, project objectives differ
  - Methodological approaches (or modifications to existing ones)
  - ***Instrument hardware***
  - Pre-processing, storage of soils, i.e. sieving, grinding
  - ***Influence of sample preparation for spectroscopy (MIR)***
  - Data Leakage



Soil Sample Analysis

Soil Pre-processing

Soil samples were air-dried and sieved to 2 mm

Fine Grinding

Soil samples were finely ground to <180 um

Chemometrics

Spectra were pre-processed and models were generated using partial linear squares regression (PLSR)

Conventional Analysis

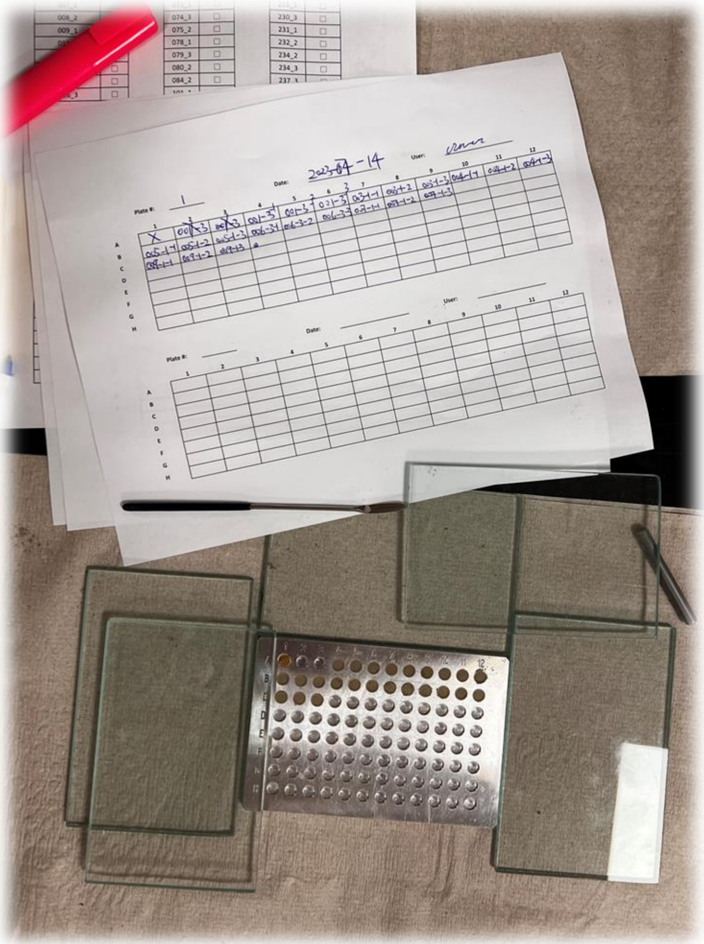
Soil samples were analyzed for various soil health parameters (pH, CEC, C, N, moisture content, texture, etc)

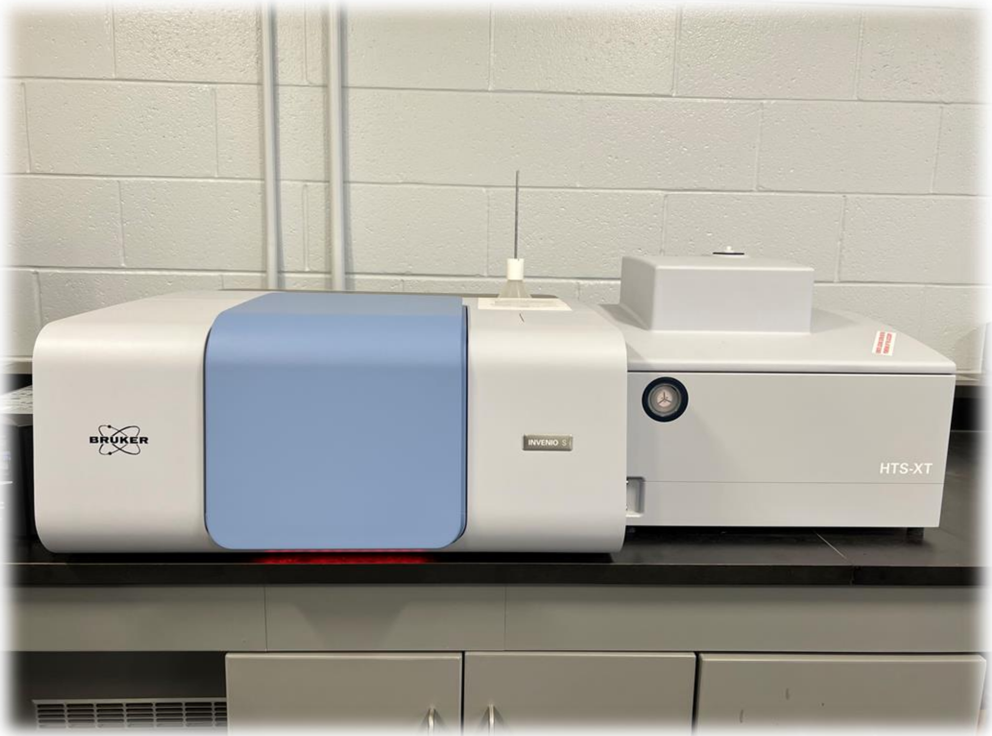
MIR Scanning

Soil samples were packed to 96-well plates and scanned using Bruker Invenio-S with HTS-XT in the MIR range between 4000 cm^{-1} and 400 cm^{-1}


1 2 3 4 5 6 7 8 9 10 11 12
A
B
C
D

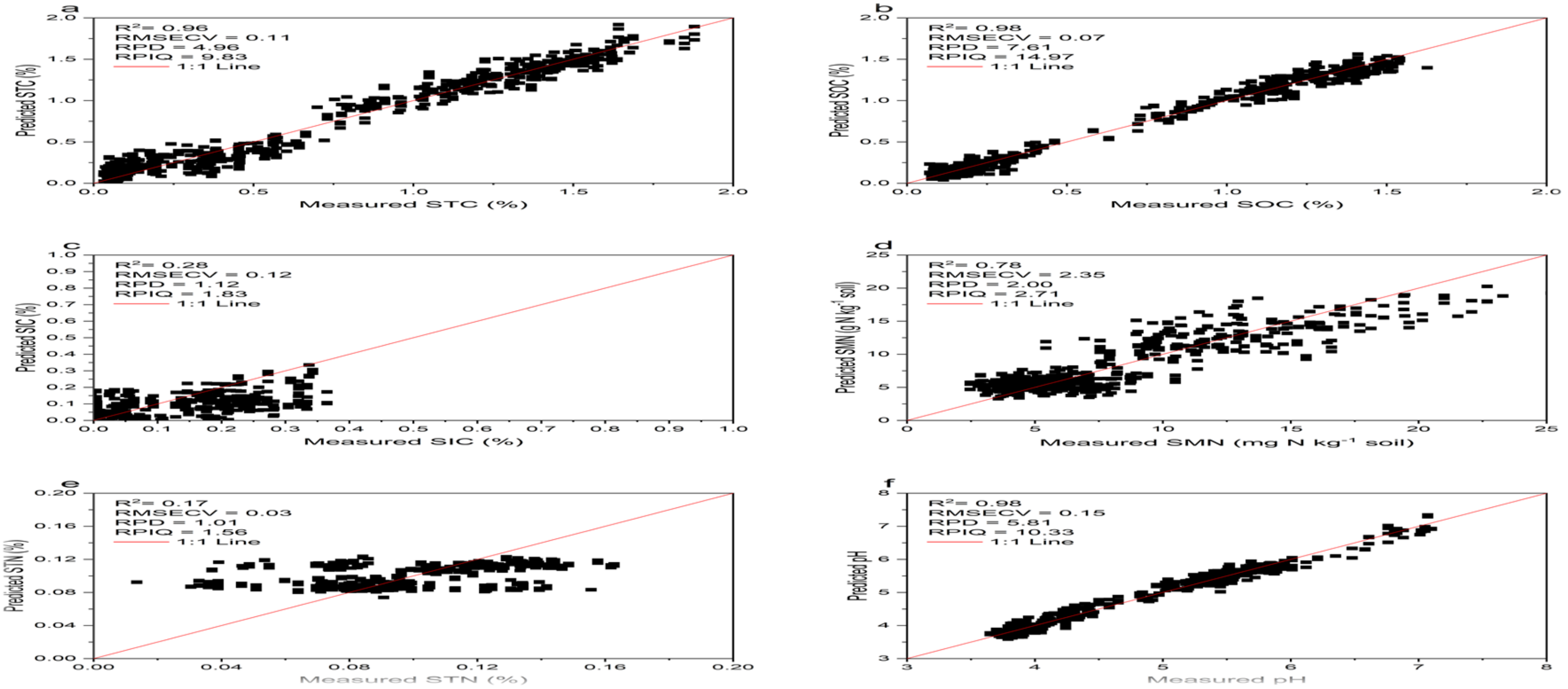

1 2 3 4 5 6 7 8 9 10 11 12
A
B
C
D




BRUKER
INVENIO S
HTS-XT

Zheya Lin, G.W. Price, David L. Burton, Derek H. Lynch	Modelling soil carbon and nitrogen in biosolids amended soils with mid-infrared (MIR) diffuse reflectance spectroscopy

Modeling soil properties in vertical profile

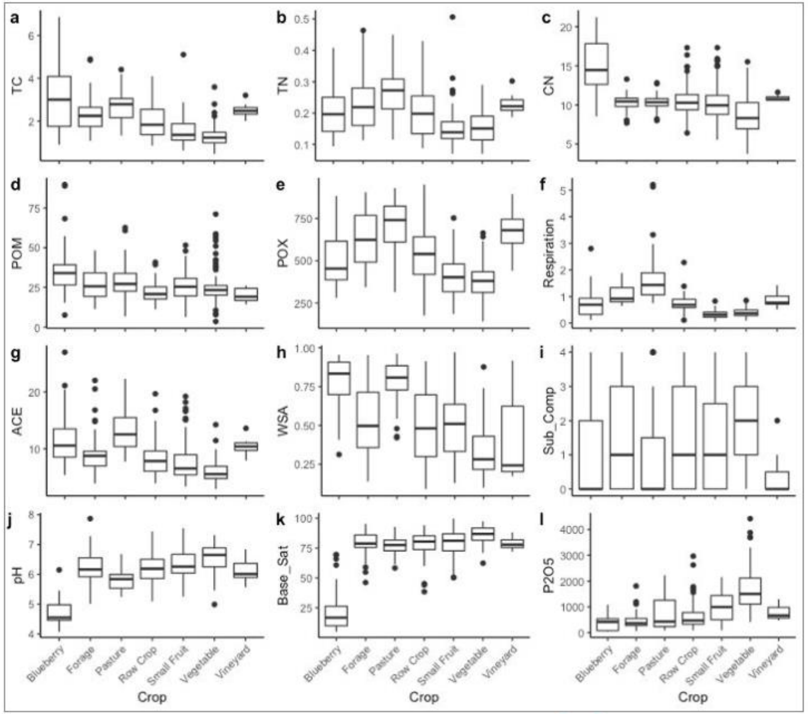


Overview of Nova Scotia Soil Health Database

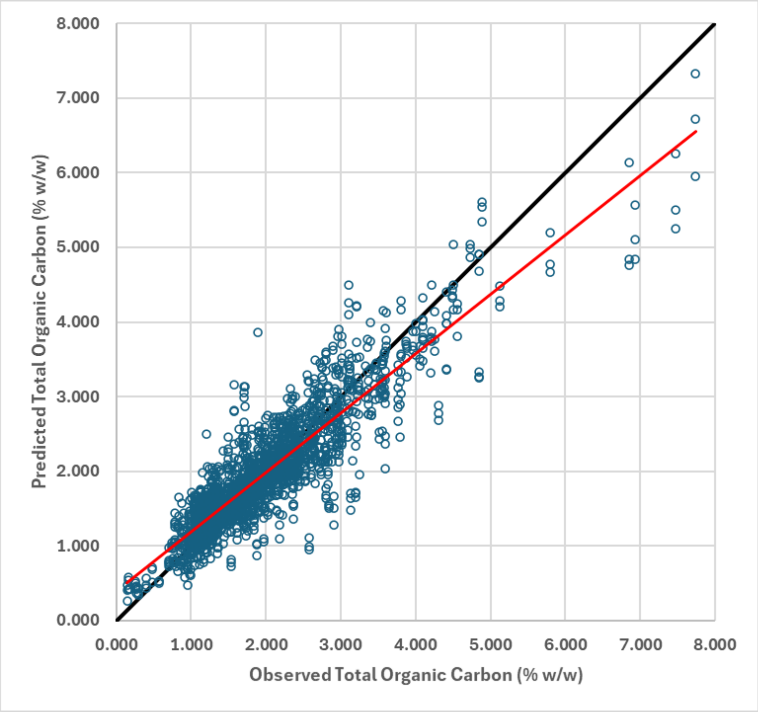
Cropping System	Count
Field Crop	918
Vegetable	327
Small Fruit	309
Pasture	267
Forage	222
Orchard	132
Wild Blueberry	60
Vineyard	60
Total	**829**

Modeling soil health properties across agricultural land uses

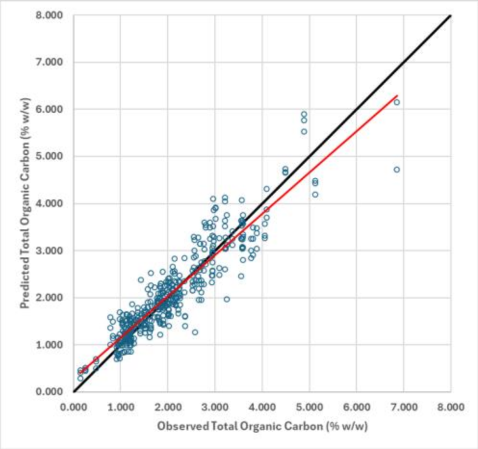
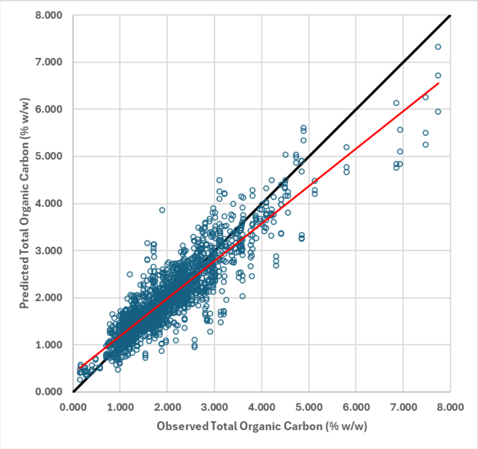
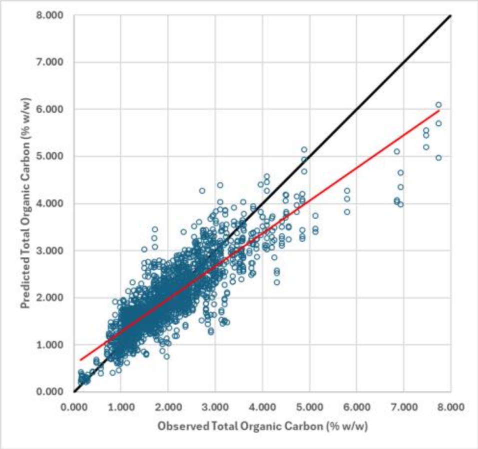
Fine-Tuning Mid-Infrared Spectroscopy Model Optimization and Regional Calibrations for Soil Health Prediction Models Properties
W. Shu, G. Price, D. Lynch, D. Burton, B, heung



[Influence of cropping system and soil type on soil health](#)
CB Marshall et al. 2021

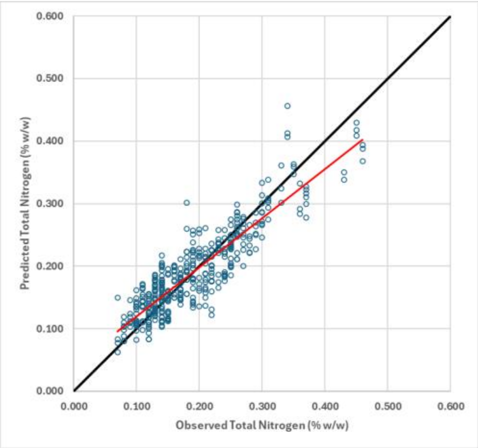


Total Organic Carbon (TOC) – 687 Samples (2061 Spectra)

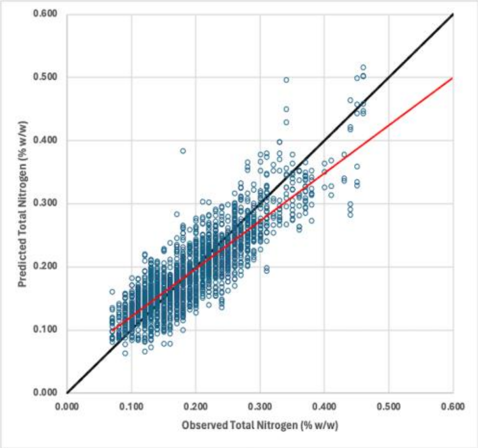
	80/20 Split	10-Fold CV	LGOCV
			
RMSEP	0.393	0.407	0.479
R^2	0.849	0.808	0.737
RPIQ	3.686	2.652	2.253

Total Nitrogen (TN) – 687 Samples (2061 Spectra)

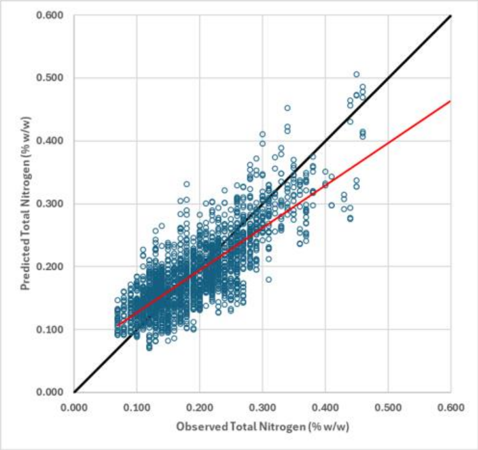
80/20 Split



10-Fold CV



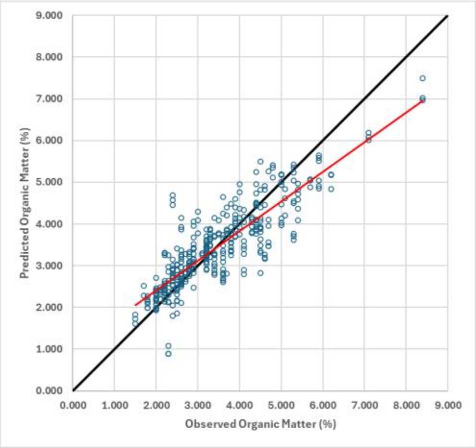
LGOCV



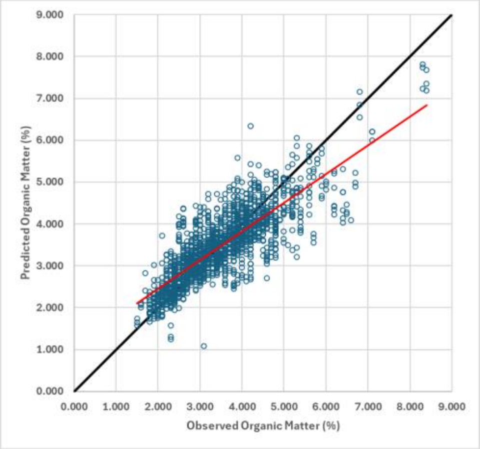
	80/20 Split	10-Fold CV	LGOCV
RMSEP	0.035	0.037	0.044
R^2	0.801	0.752	0.652
RPIQ	3.167	2.708	2.274

Soil Organic Matter (OM) – 603 Samples (1809 Spectra)

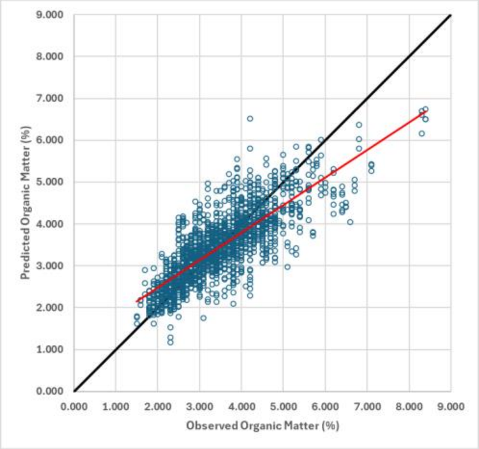
80/20 Split



10-Fold CV

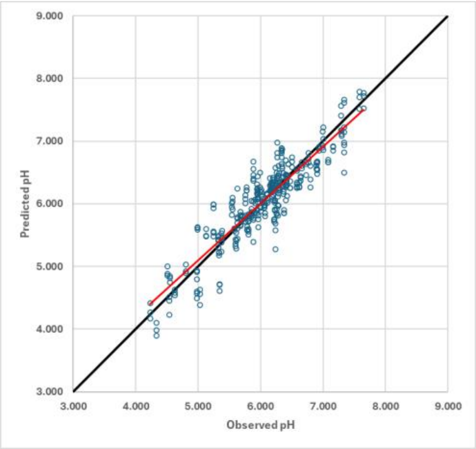
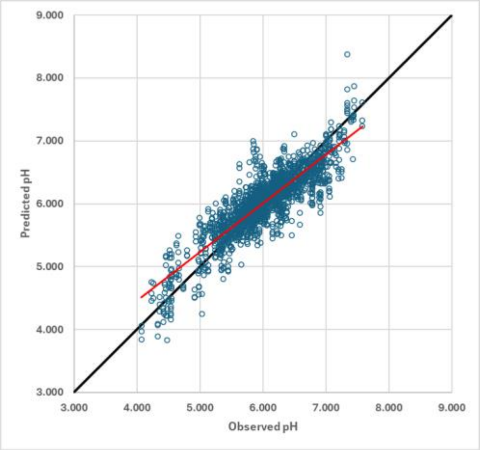
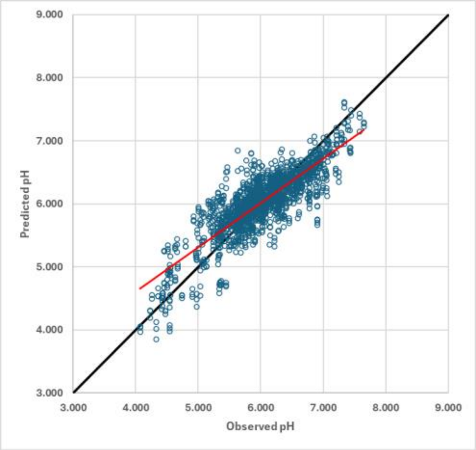


LGOCV

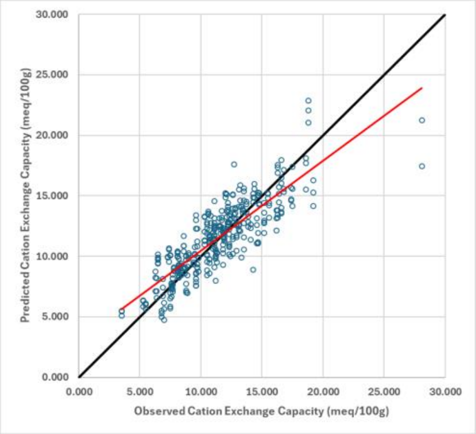
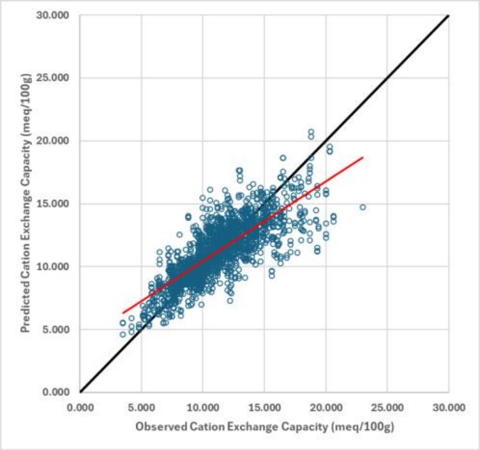
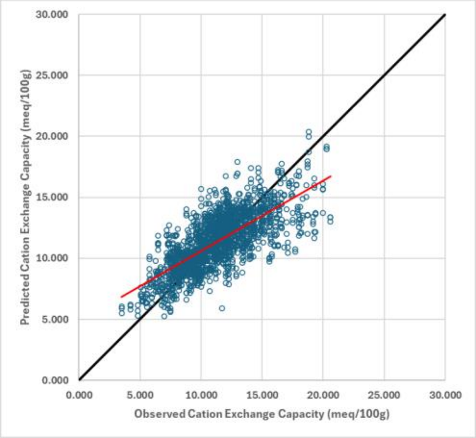


	80/20 Split	10-Fold CV	LGOCV
RMSEP	0.618	0.571	0.609
R^2	0.738	0.680	0.639
RPIQ	2.995	2.452	2.300

Soil pH – 603 Samples (1809 Spectra)

	80/20 Split	10-Fold CV	LGOCV
			
RMSEP	0.284	0.295	0.331
R^2	0.831	0.764	0.707
RPIQ	2.467	2.498	2.203

Cation Exchange Capacity (CEC) – 603 Samples (1809 Spectra)

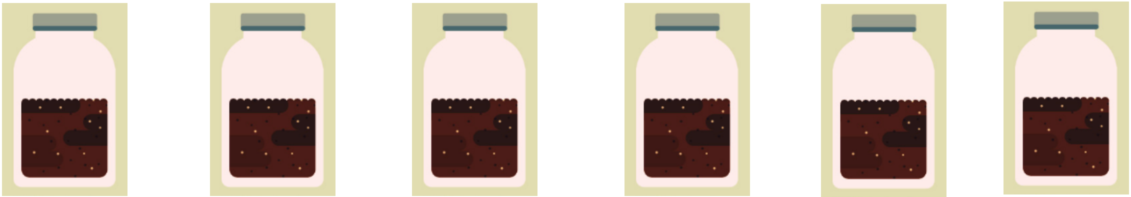
	80/20 Split	10-Fold CV	LGOCV
			
RMSEP	1.852	1.827	1.999
R^2	0.710	0.622	0.541
RPIQ	2.444	2.135	1.951

Soils amended with Organic Matter Sources

-Marshland cropping area Truro (0-15cm)
-Gleyed Regosol, silt loam - silty clay loam
-Air-dried, ground <2mm, mixed
-100g of soil

4 rates – 1, 2, 3, and 4 % C and experiment had 4 replicates

In-vessel Compost | SSO row compost | Manure + Bedding | N-Viro Biosolid | Straw | Control



Each time period - subsamples will be measured for TC & TN, spectral scan

- Soil health analyses

OA	C%	N %	C:N
Manure	31.71	1.90	16.65
Straw	40.39	1.92	21.06
Hotrot	20.43	1.84	11.08
Colchester	13.30	1.77	7.50
ATB	23.68	1.44	16.50

Incubate — 1 Month — 3 Months — 6 Months — 9 Months — 12 Months

Soil amendment dynamics and calibrations

Application of mid-infrared spectroscopy to a controlled soil incubation examining the effects of organic amendments on total carbon and total nitrogen
<u>S. Downie</u>, G. Price, B. Heung, W. Shu

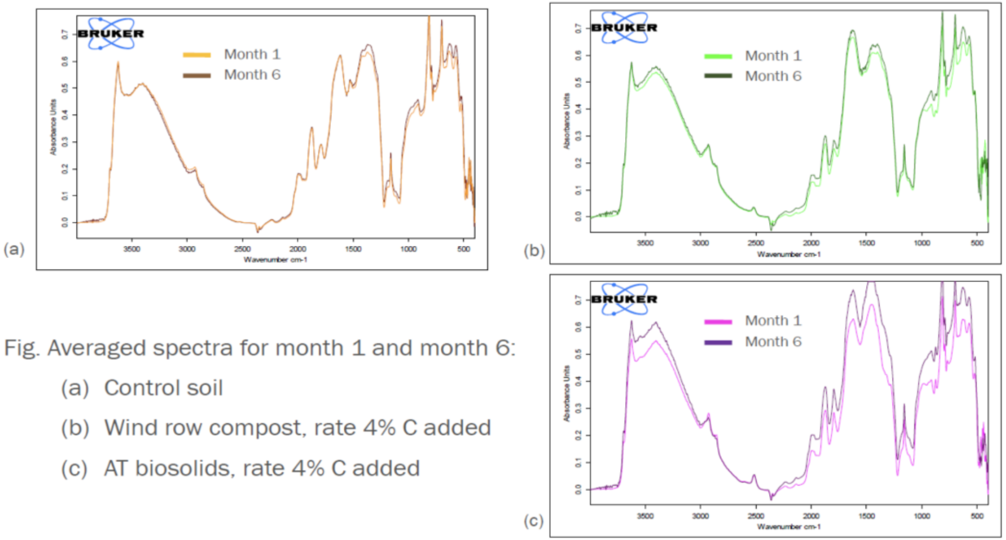
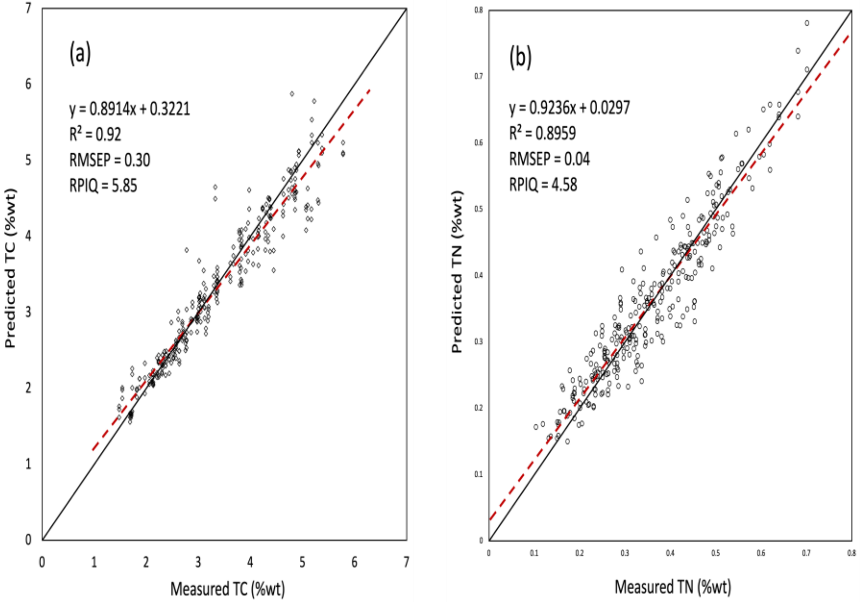


Fig. Averaged spectra for month 1 and month 6:

(a) Control soil

(b) Wind row compost, rate 4% C added

(c) AT biosolids, rate 4% C added



Model with an RPD of:

- 2-3 is FAIR
- >3 is GOOD
- >5 is EXCELLENT

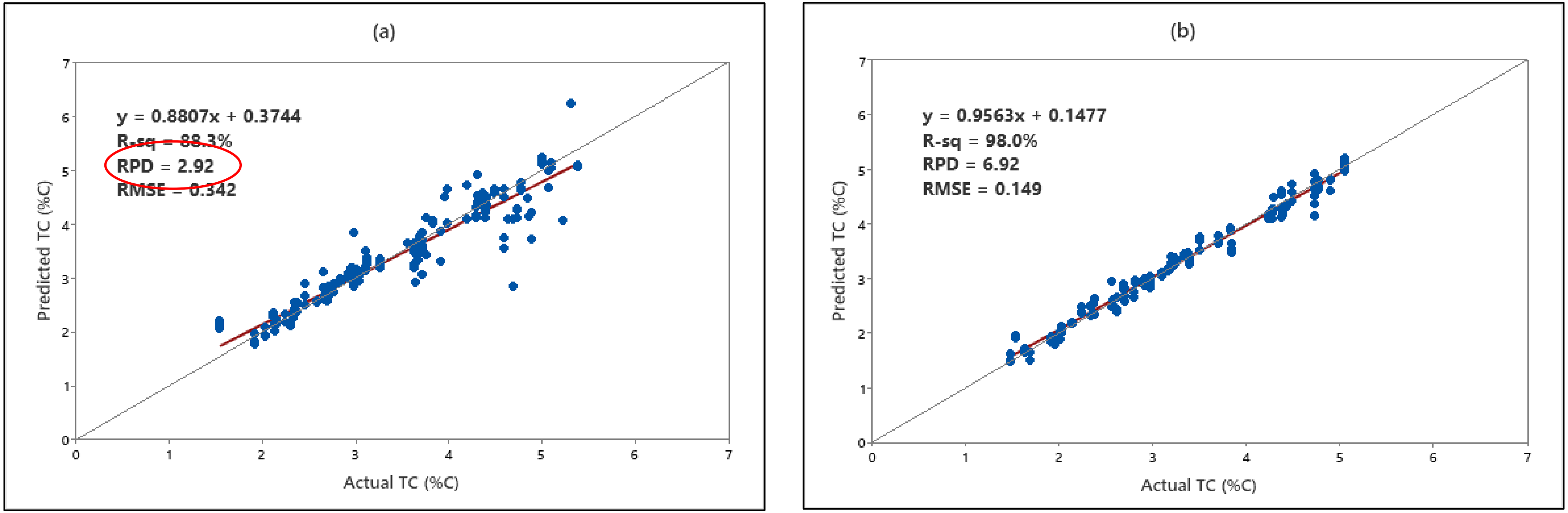
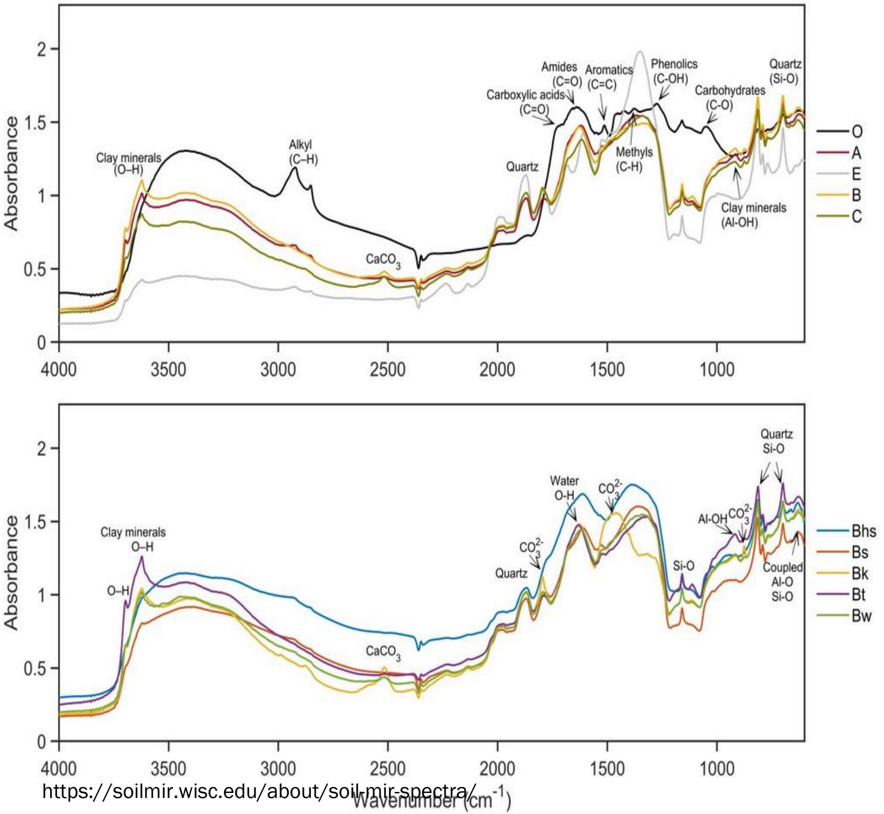
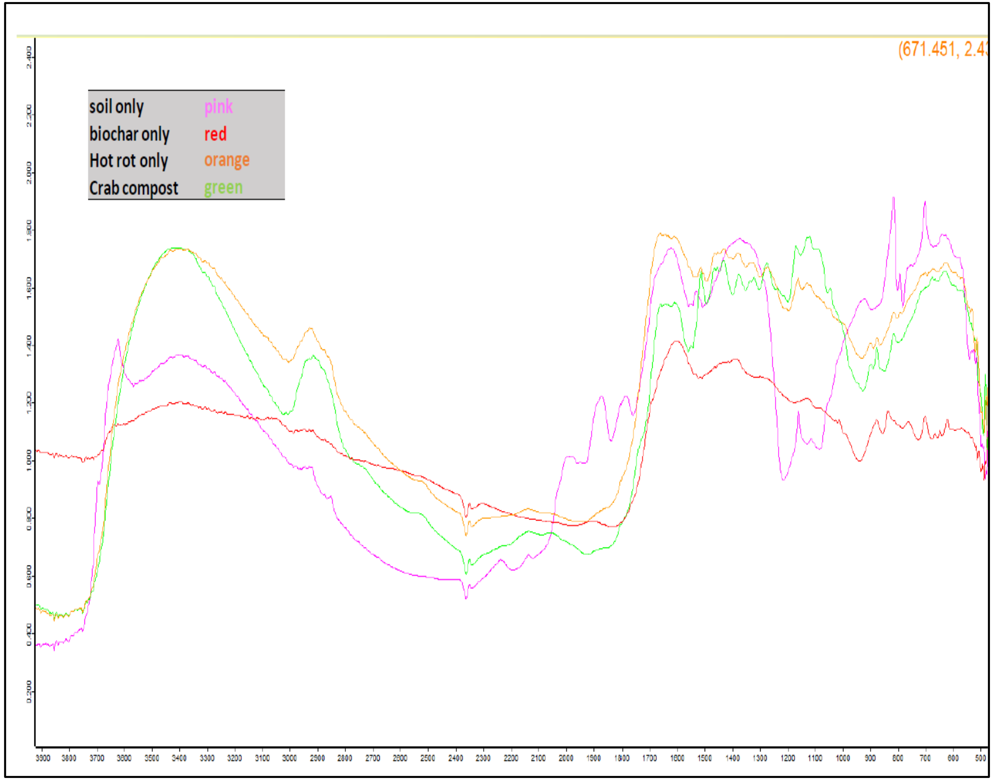


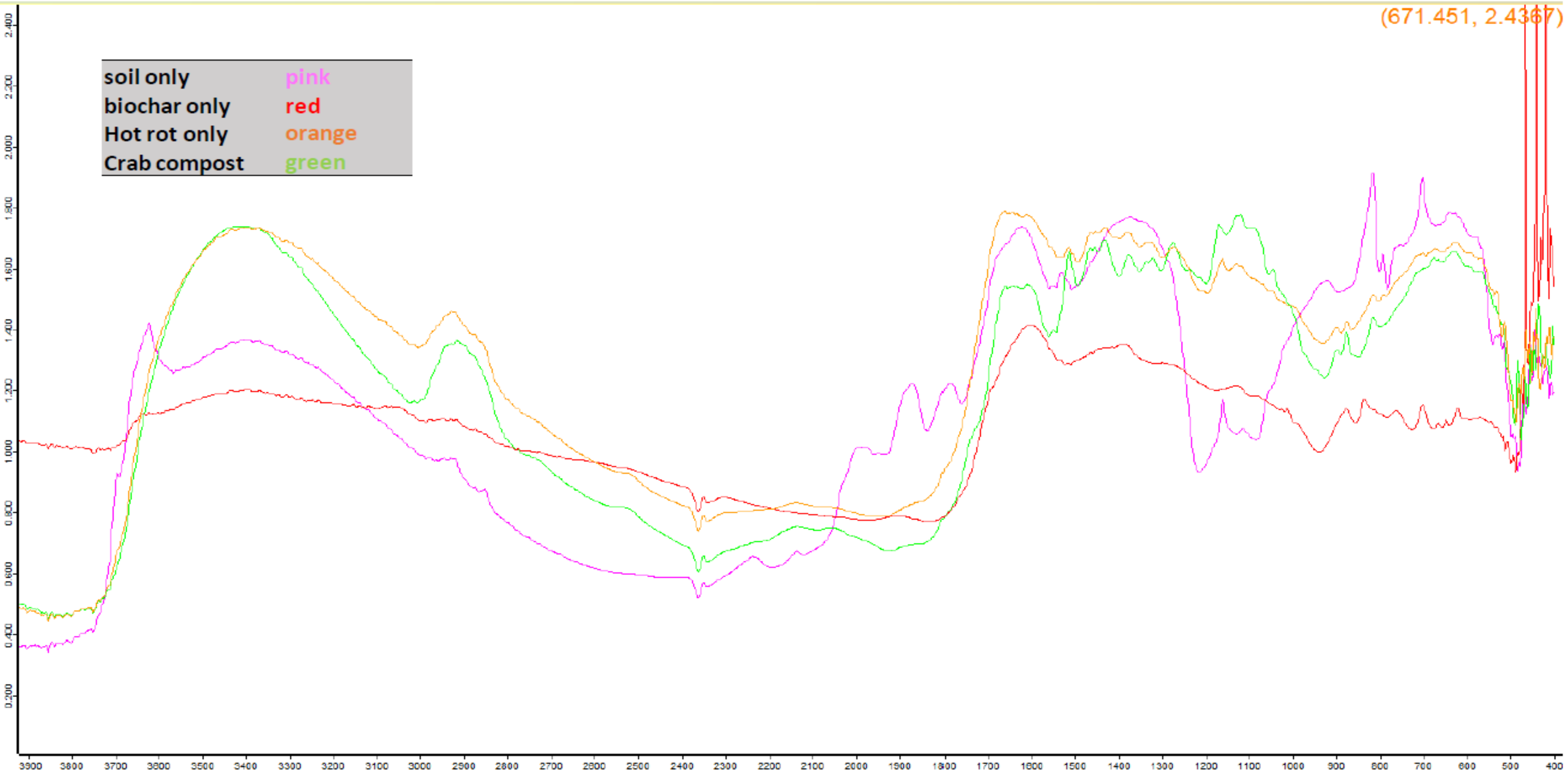
Fig 3. PLS prediction of total C (%) versus actual measures, and respective regression equations and coefficients of determination (R^2) for models developed with each treatment replicated four times for the period (a) 0 to 6 months (n = 166), and (b) 1-6 months (n = 147).

‘Fingerprinting’ and Bond Composition

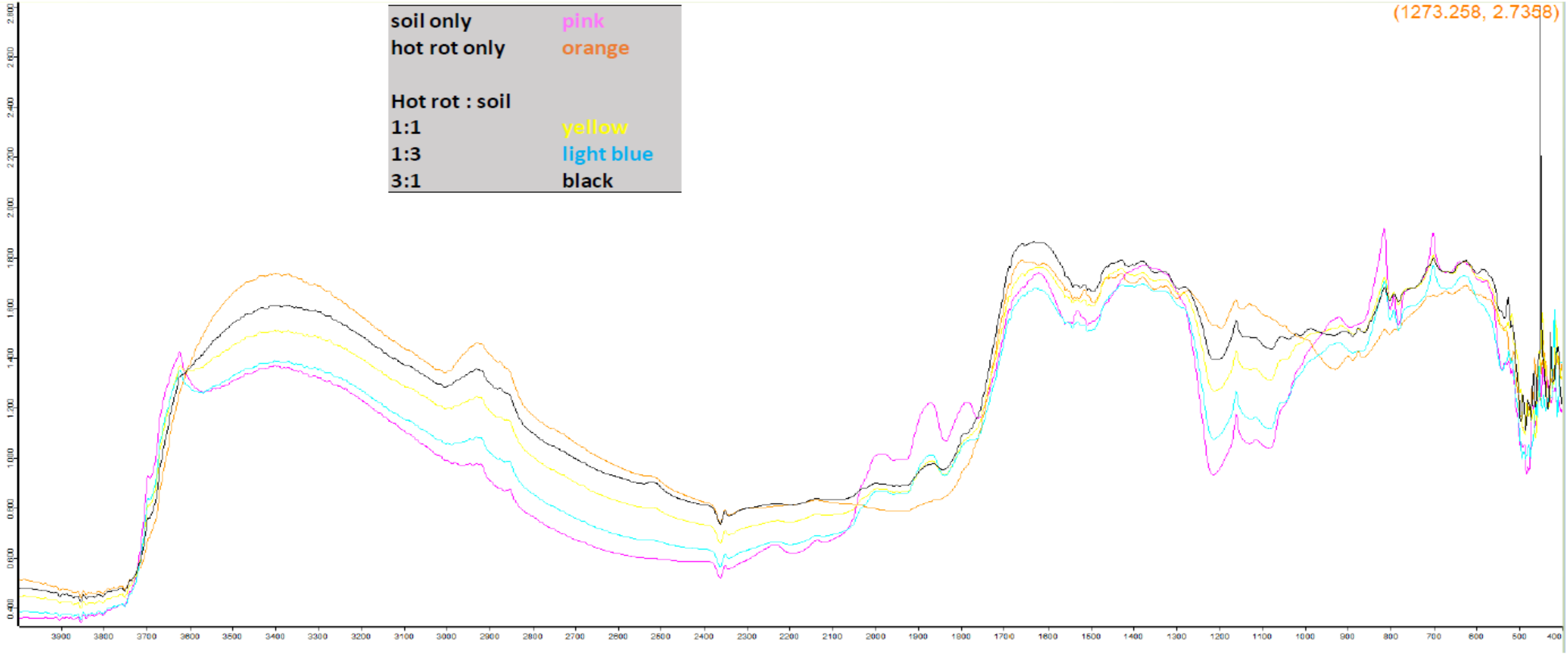


https://soilmir.wisc.edu/about/soil-mir-spectra/

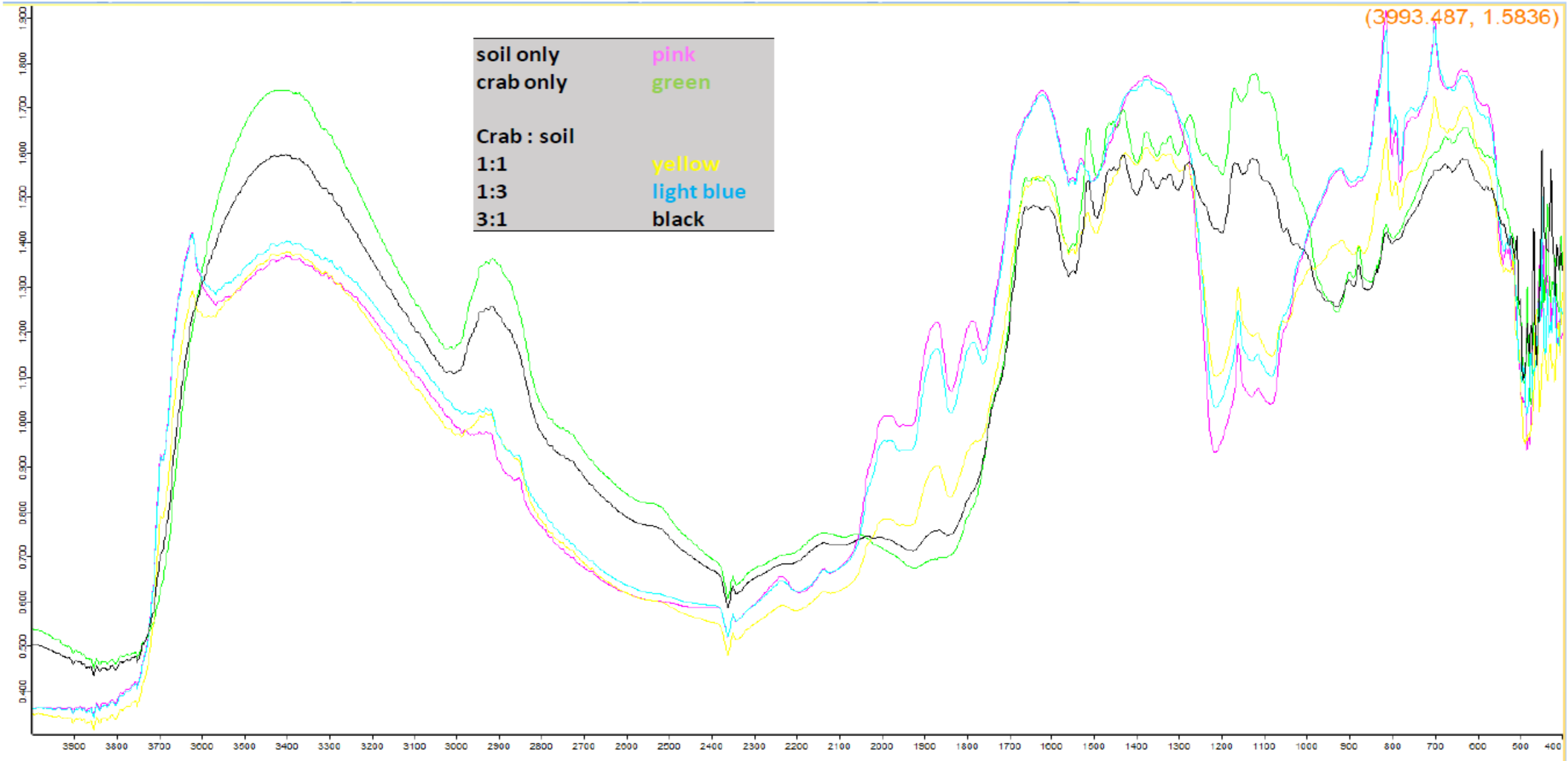


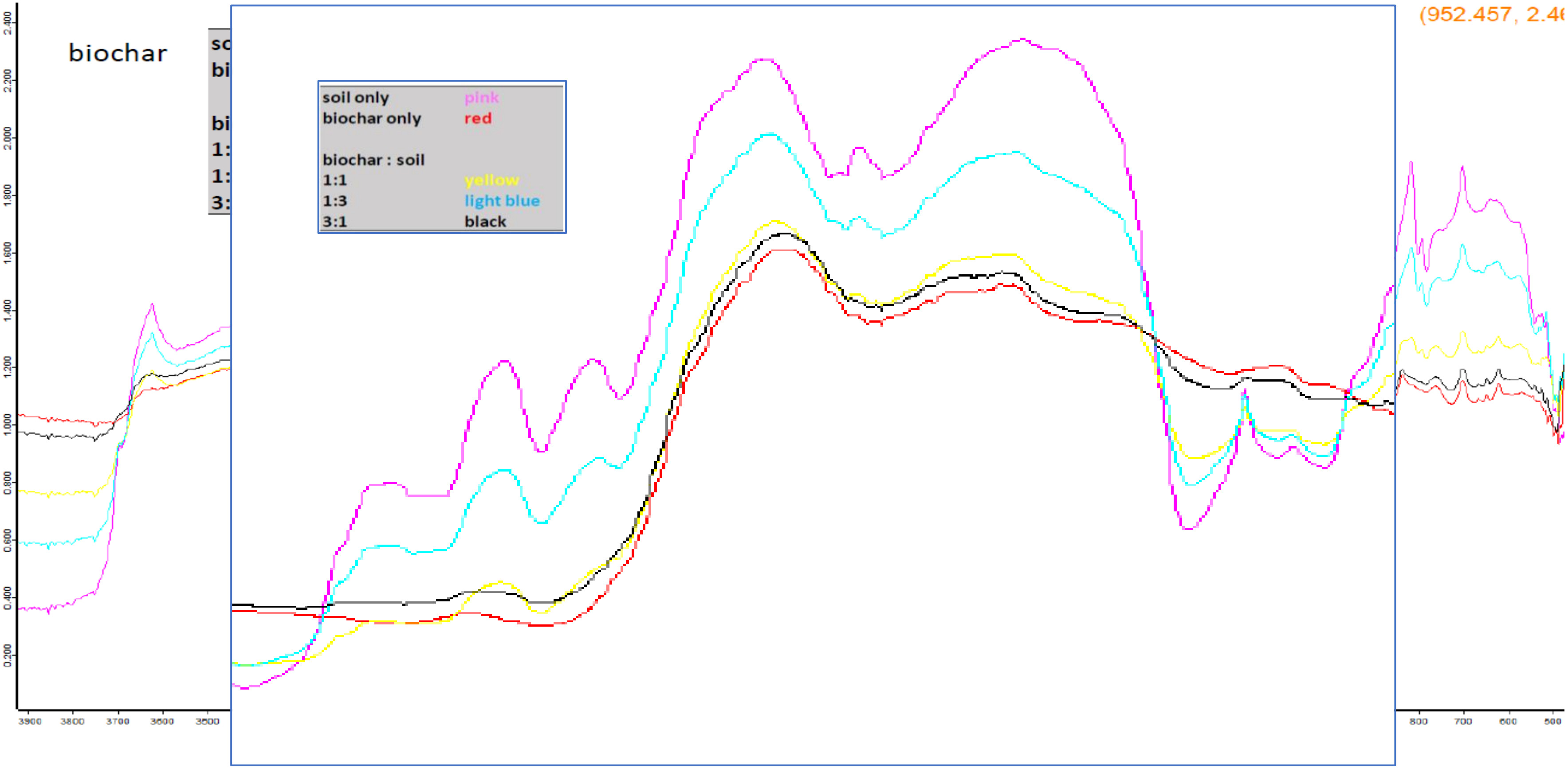

soil only pink
biochar only red
Hot rot only orange
Crab compost green
(671.451, 2.4367)
2.400
2.200
2.000
1.800
1.600
1.400
1.200
1.000
0.800
0.600
0.400
0.200
3900 3800 3700 3600 3500 3400 3300 3200 3100 3000 2900 2800 2700 2600 2500 2400 2300 2200 2100 2000 1900 1800 1700 1600 1500 1400 1300 1200 1100 1000 900 800 700 600 500 400

In-Vessel Compost of Animal Manure and Bedding using HotRot System



Crab compost




biochar
soil only pink
biochar only red
biochar : soil
1:1 yellow
1:3 light blue
3:1 black
(952.457, 2.4
2.400
2.200
2.000
1.800
1.600
1.400
1.200
1.000
0.800
0.600
0.400
0.200
3900
3800
3700
3600
3500
800
700
600
500

Summary

- To date, overall performance of the MIR spectroscopy models for various soil health parameters followed the order:
  TOC > TN > OM > Clay > pH > CEC

- Models in this study were only regionally validated. Further study needs to be conducted to develop globally robust MIR models that account for variability across regions.

Acknowledgements

net-zero atlantic

irda

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NOVA SCOTIA Natural Resources and Renewables

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  - Dr. Brandon Heung
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  - Jill Pyke
  - Jessica Lloyd
  - Zheya Lin