EARTHOPTICS™

Mid-Infrared Spectroscopy: Faster, Reliable and Cost Effective Soil Carbon Analytics

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Executive Summary

The quantification of soil organic carbon (SOC) is crucial for verifying carbon credits and implementing climate-smart agriculture initiatives. While traditional dry combustion methods remain the gold standard for determining total carbon (TC), total inorganic carbon (TIC), and total organic carbon (TOC), their limited throughput and high operational costs present significant barriers to scaling carbon sequestration projects. This white paper presents Mid-Infrared (MIR) spectroscopy as a high-throughput alternative that can process large volumes of samples at **a reduced cost**, while still maintaining analytical accuracy sufficient for specific carbon projects.

EarthOptics has developed an automated MIR spectroscopy workflow utilizing the Bruker INVENIO platform, featuring HTS-XT high-throughput sampling and an LN_2-cooled MCT detector, in conjunction with proprietary sample preparation automation, to deliver cost-effective soil carbon analyses at scale. Calibrated against our NAPT-certified dry combustion reference data, MIR spectroscopy provides project developers and Scope 3 program managers with a practical and cost-effective pathway to comprehensive SOC determination, while also offering direct soil-texture measurements for model initiation.

With the transition of registries requiring equivalent soil mass (ESM), such as VM0026 to VM0042 standards, and the associated doubling of lab analytical costs using gold standard methods, **EarthOptics' MIR is the only commercial solution for adopting the new standard at no additional costs to the developer**.

1 - Technology Overview: Dry Combustion vs. MIR Spectroscopy

1.1 Dry Combustion Analysis (Reference Method)

Dry combustion analysis (DCA) is the internationally recognized reference method for determining soil carbon.

Principle: Complete oxidation of carbon to CO_2 at ~900–1000 °C with detection via non-dispersive infrared (NDIR) sensors or thermal conductivity detectors.

Process for TC/TIC/TOC determinations at EarthOptics:

- **Sample preparation:** Drying and grinding to <2mm; weigh 250–450 mg per crucible
- **Total Carbon (TC):** Direct combustion of the untreated sample
- **Total Inorganic Carbon (TIC):** Acidification to evolve CO_2 from carbonates with NDIR detection
- **Total Organic Carbon (TOC):** Calculated as TC - TIC

All fractions are analyzed on a Skalar Primacs ATC-100.

Advantages:

- Direct measurement with no calibration required
- NAPT certification available
- Accepted by all carbon credit registries
- Accuracy typically ±0.05% C for well-homogenized samples (lab/dataset dependent)

Limitations:

- Throughput: ~90 samples/day/instrument
- Labor intensive: ~15–20 minutes hands-on time per sample
- High consumable costs (oxygen, catalysts, combustion boats)
- Energy intensive: process combusts carbon, requiring a lot of energy and releasing CO_2

1.2 Mid-Infrared Spectroscopy

MIR spectroscopy leverages the fundamental molecular vibrations of soil components to predict carbon content through multivariate calibration models.

Principle: Soil organic matter exhibits characteristic absorption bands in the MIR region (4000–600 cm^{-1}), particularly: C-H stretching (2920–2850 cm^{-1}), C=O stretching (1740–1600 cm^{-1}), aromatic C=C (1600–1585 cm^{-1}), and C-O stretching/O-H bending (1450–1050 cm^{-1}).

Process summary (more details in Appendix B):

- Sample preparation: Drying and grinding to ‹2mm; load 100–150 mg per well; tamp flat (consistent surface height)
- Spectral acquisition: INVENIO + HTS-XT diffuse reflectance; 4 cm^{-1} resolution; 64 background / 32 sample scans
- Chemometric modeling: PLS/Cubist and related ML models trained against reference data set; applicability-domain checks

Advantages:

- Throughput: ›10x processing capacity when compared to DCA (with custom automation; scales with instruments/shifts)
- Minimal consumables: simultaneous multi-analyte prediction (TC, TIC, TOC, soil texture); non-destructive
- Environmentally friendly: No CO2 release, significantly lower energy consumption
- Cost reduction: Significantly reduced labor time per sample (with custom automation)

Limitations:

- Requires a robust, representative calibration dataset
- Model performance is dependent on sample representativeness, potential matrix effects in diverse soil types
- Regular model updating may be necessary
- Requires ≥10% of samples to be DCA processed in parallel to control for drift and be registry compliant.

2 - Scientific Foundation and Literature Review

2.1 Established Accuracy of MIR for Soil Carbon

Recent peer-reviewed studies demonstrate the viability of MIR spectroscopy for soil carbon analysis in a high-throughput, minimal preparation environment:

- Sanderman et al. (2023) evaluated large U.S. datasets and reported **strong relationships for TOC** (exact R^2/RMSE values vary with preprocessing/model; use local validation for program claims)
- Shi et al. (2024) showed **high agreement with dry combustion in agricultural soils** and found that regional models frequently outperform global models (results depend on soils and calibration design)
- Bachion de Santana & Daly (2022): Across 888 Irish soils, MIR/NIR models built on sieved ‹2 mm vs ball-milled (‹0.1 mm) showed no consistent accuracy advantage for milling across SVM/PLS/Cubist runs; VIP/MCC analyses indicated similar chemical information content—**supporting elimination of the milling step without degrading carbon predictions**
- Sanderman et al. (2023): Using 2,380 North American agricultural soils, **‹2 mm prep delivered nearly identical performance to fine-milled for TOC, clay, sand, pH, and BD** (best with SNV + memory-based learning), with minimal replicate variability and no texture-dependent bias; models built from the USDA NRCS mid-DRIFTS library likewise showed minimal differences between preps—endorsing routine ‹2 mm scanning under good SOP and QC.)

2.2 Soil Texture Determination

MIR captures texture-related features (e.g., phyllosilicate Si–O stretching 1100–900 cm^{-1}; Al–OH 915–830 cm^{-1}; Si–O–Si bending 540–400 cm^{-1}). Viscarra Rossel et al. (2023) reported high accuracy for clay/sand when calibrated against laser diffraction (texture performance is typically below carbon and soil-type dependent).

Our MIR analytic provides reliable %sand, %silt, and %clay readouts from each sample at no additional cost. This allows the project operator to use direct soil texture data instead of relying on granular SSURGO estimates to initialize carbon stock models, increasing accuracy and quality of the resulting credits.

2.3 Implications for Carbon Credit Projects

The literature shows MIR can deliver:

- High quality SOC/TOC measurements (errors near ~10% - External MIR-only tests report SOC RMSE = 0.10–0.33 % SOC across U.S. long-term sites and OC RMSE ≈ 9.3 g kg^{-1} in a national MIR library) (Sanderman et al. 2021; Baumann et al. 2021)
- Detection of management-induced carbon changes (Sanderman et al. 2021)

- High-quality texture predictions for carbon modeling initiation (Thomas et al. 2021; Rossel et al. 2006)
- Significant cost reductions vs. traditional analysis (Sanderman et al. 2020; Ramirez et al. 2022)

3 - EarthOptics MIR Implementation

3.1 Instrumentation

Bruker INVENIO FT-IR with HTS-XT (96-position), LN_2-cooled MCT detector; OPUS 8.x; LIMS integration; RockSolid™ interferometer for long-term stability. (Instrument can achieve finer resolution; routine measurements use 4 cm^{-1} per SOP.)

3.2 Automated Sample Preparation

Automation addresses sample preparation bottlenecks such as grinding to <2 mm, consistent analysis plate dispense and tamping, and barcode tracking throughout the sample lifecycle. EarthOptics has developed and implemented several proprietary, custom automation solutions that not only resolve bottlenecks but also eliminate operator bias, resulting in increased quality and consistency.

3.3 Calibration Strategy

- **Operational default (scientific literature-derived models).** We deploy the Open Soil Spectral Library (OSSL) Cubist models—**mir_cubist_ossl_na_v1.2** (broad North America training set) and **mir_cubist_kssl_na_v1.2** (USDA KSSL–based, U.S.-optimized). These are pre-trained MIR→property regressors that provide immediate TC/TIC/TOC and texture predictions while any project-specific localized model is being built. We select the model (or blend) that performs best on early verification samples and monitor bias/precision in production.
- **Project-tailored calibration.** When local reference data are available—either from client archives or newly analyzed samples—we adapt the model to the project. Typical workflow:
    1. Compile paired spectra and laboratory references (DCA for TC/TIC/TOC; hydrometer/laser for texture) with QC;
    2. Confirm coverage across soils, texture classes, and the project's TOC range;
    3. Screen spectral outliers and domain mismatch (e.g., leverage/Mahalanobis, SNR/baseline checks);
    4. Fit/evaluate candidate updates (e.g., Cubist/PLS, or a simple slope/intercept correction) using grouped cross-validation by site/field and, where counts permit, a small independent holdout;
    5. Report R^2, RMSE, MAE, and Bias, and adopt the simplest adjustment that meets targets.

- **Rolling updates and verification.** We routinely incorporate a verification subset of dry-combustion samples from each monitoring round to refresh the calibration and track drift; model versions, change logs, and performance dashboards are maintained.
- **Routing rules.** Samples flagged as out-of-domain or failing QC are routed to DCA; program settings define thresholds and escalation.

3.4 Quality Assurance Protocol

- Daily instrument checks with certified reference materials; ≥2 certified reference materials (CRM) per 96-well plate
- Duplicates: ≥2 duplicates per 96-well plate (carbon relative percent difference (RPD) <15%, texture RPD <20%)
- Control charts for standards; signal-to-noise ratio (SNR) > 500:1 @ 2000 cm^{-1}, baseline drift <2%, resolution verification 4.0 ± 0.1 cm^{-1}
- Routine manufacturer maintenance

3.5 Error and Bias Quantification and Reporting

We report the observed mean differences between the MIR and DCA processed sample subsets as bias (calculated as mean[MIR - DCA]), expressed in the same units as the original measurements (%C for carbon analytes). To assess the magnitude of errors independent of their direction, we calculate the Mean Absolute Error (MAE), which represents the average absolute deviation between methods. Additionally, we compute the Root Mean Squared Error (RMSE), which is the square root of the mean squared deviation between methods and summarizes overall predictive dispersion; RMSE is reported in the same units as the original measurements. These metrics collectively characterize both systematic differences (bias) and overall prediction accuracy (MAE, RMSE) between the spectroscopic and reference methods.

4 - Preliminary Validation Study

4.1 Study Design

We validated MIR predictions with dry-combustion measurements for TC, TIC, and TOC. Each point represents a unique agricultural or rangeland soil sample (or mean value if replicated). Summary statistics were calculated after excluding the outer ~1% of points identified by residual and stabilized percentage-error thresholds. Bias is defined as the mean (MIR - Lab). Full criteria for replicate handling, outlier identification, denominator flooring for percentage errors, and metric formulas are provided in Appendix B.2 – Analysis SOP.

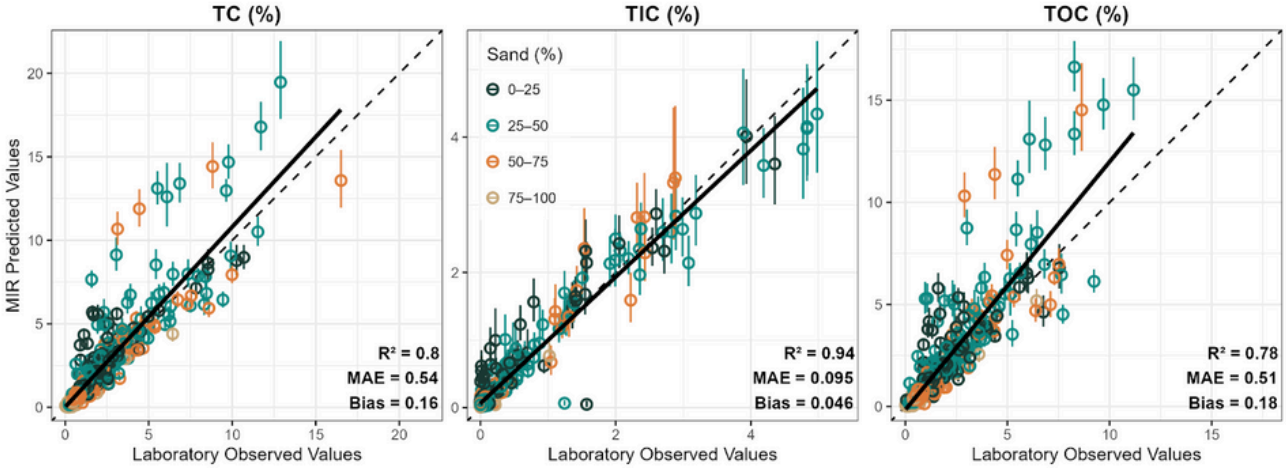

Figure 1 – MIR vs. dry-combustion for TC, TIC, TOC on common scales; dashed 1:1 reference, black OLS fit, hollow markers color-binned by MIR-predicted sand, vertical bars show prediction bounds. Statistics (R^2, MAE, Bias) are computed after excluding extreme outliers (Table 1 & Appendix B).

4.2 Results and Discussion

Carbon analytes, as determined by the interpretation of MIR spectra, show agreement with the gold-standard reference. These results indicate MIR provides decision-grade accuracy for high-throughput carbon monitoring. The small positive biases observed for the carbon analytes are consistent and can be addressed, where required, with a simple linear post-hoc adjustment using a project-specific reference set. Texture behavior is summarized below and discussed further in Appendix A: Texture Results.

Analyte	R^2	RMSE	MAE	Bias	Mean	n	excl
TC	0.80	1.2	0.54	0.16	1.85	560	9
TIC	0.94	0.19	0.095	0.046	0.28	560	9
TOC	0.78	1.1	0.51	0.18	1.56	560	9
Sand 2000–50 µm	0.77	14.0	11.0	-5.9	46.0	84	2
Silt 50–2 µm	0.76	9.8	8.6	1.2	34.0	83	3
Clay 2–0 µm	0.70	7.7	6.1	2.8	19.1	83	3

Table 1 – Summary metrics for all analytes (post outlier exclusion; Bias = mean[MIR − Lab]). Carbon metrics in %C; texture metrics in percentage points (%)

5 - Implementation Recommendations

5.1 Optimal Use Cases for MIR Spectroscopy

Large-scale carbon credit projects (>1,000 ha); Scope 3 supply chain monitoring with high sample volumes; temporal monitoring with baseline data; projects with relatively homogeneous or stratifiable soil types; rapid screening before verification sampling.

5.2 Scenarios Requiring Dry Combustion

Regulatory compliance sampling, carbon credit verification audits (recommended at 10–20% of samples); highly heterogeneous or unusual soils; calibration development and updating; dispute resolution or third-party verification.

6 - Conclusions and Path Forward

Mid-infrared spectroscopy represents a novel approach to soil carbon analysis, addressing the scaling challenges faced by carbon projects. While MIR maintains slightly lower intrinsic accuracy than dry combustion, it enables high-throughput, cost-effective monitoring, which is essential for large-scale sequestration initiatives. EarthOptics' implementation provides project developers with a practical solution that balances analytical quality with economic feasibility. The substantial cost reduction and order-of-magnitude increase in analytical capacity enable more comprehensive spatial and temporal monitoring, improving project outcomes and credit value.

Key Takeaways for Project Developers:

- Cost savings of 50% ($100,000+ for projects >300,000 acres)
- Comparable quality of core analytics (TC, TIC, TOC) with free direct soil texture data
- A hybrid approach with partial selective dry combustion maintains verification standards
- Rapid turnaround enables adaptive management decisions

7 - References

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8 - Appendices

8.1 Appendix A: Texture Results and Discussion

MIR texture predictions track laboratory references with moderate agreement: Sand R^2=0.77, Silt R^2=0.76, Clay R^2=0.70 (n≈83–84 each). Errors are larger than for carbon (Table 1): MAE ≈ 11% for Sand, 8.6% for Silt, and 6.1% for Clay. Directionally, the models tend to underestimate Sand (Bias −5.9%) and slightly overestimate Clay (+2.8%) and Silt (+1.2%). These patterns are typical of MIR texture modeling and reflect both spectral–mineralogical sensitivity and differences between hydrometer/laser references and the MIR proxy.

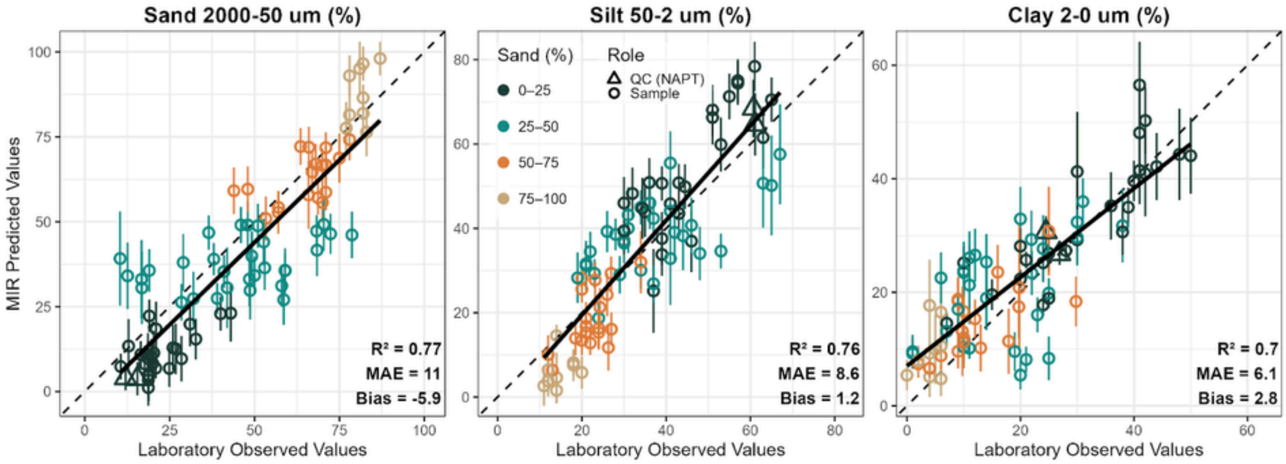


Figure A1 – MIR vs. hydrometer for Sand, Silt, and Clay on standard scales; dashed 1:1 reference, black OLS fit, hollow markers color-binned by MIR-predicted sand, vertical bars show prediction bounds. Statistics (R^2, MAE, Bias) are computed after excluding extreme outliers (Appendix 2).

8.2 Appendix B: Standard Operating Procedures

Appendix B.1 – Laboratory SOP (MIR sample prep & acquisition)

Scope. Sample preparation and spectral acquisition for predicting soil carbon and texture.

Materials & equipment

- Bruker INVENIO FT-IR with HTS-XT (96-position) autosampler and LN_2-cooled MCT detector
- OPUS 8.1 software
- 96-well aluminum plates; tamping tool; balance

Sample preparation

- Air- or oven-dry soils; grind and sieve to < 2 mm
- Load ~100–150 mg per well; tamp flat to a consistent surface height

Spectral acquisition

- Spectral range 4000–600 cm^{-1}; resolution 4 cm^{-1}
- 64 background scans; 32 sample scans per well
- Retain plate ID, well ID, run timestamp, operator, and instrument in LIMS

Plate QC & acceptance

- ≥2 CRMs and ≥2 within-plate duplicates per 96-well plate
- Acceptance targets: carbon RPD <15%, texture RPD <20%; SNR >500:1 @ 2000 cm^{-1}; baseline drift <2%; resolution 4.0 ± 0.1 cm^{-1}
- Investigate, document, and re-acquire any plate-failing targets

Traceability

- Maintain complete LIMS linkage: sample → well → spectrum → prediction; archive raw OPUS data and processed exports

Appendix B.2 – Analysis SOP (prediction, QC, and reporting)

Scope. Data ingestion, model prediction, aggregation, outlier handling, metrics, and reporting.

Data ingest

- Import OPUS/CSV exports and bind with plate metadata
- Map analytes to reporting names: TC, TIC, TOC, Sand (2000–50 µm), Silt (50–2 µm), Clay (2–0 µm)
- Convert $CaCO_3$ → TIC using 12.011/100.09 when required

Models & prediction

- Use OSSL Cubist models mir_cubist_ossl_na_v1.2 (default) and/or mir_cubist_kssl_na_v1.2
- Emit point predictions with 95% uncertainty bounds and model-applicability flags

Aggregation & references

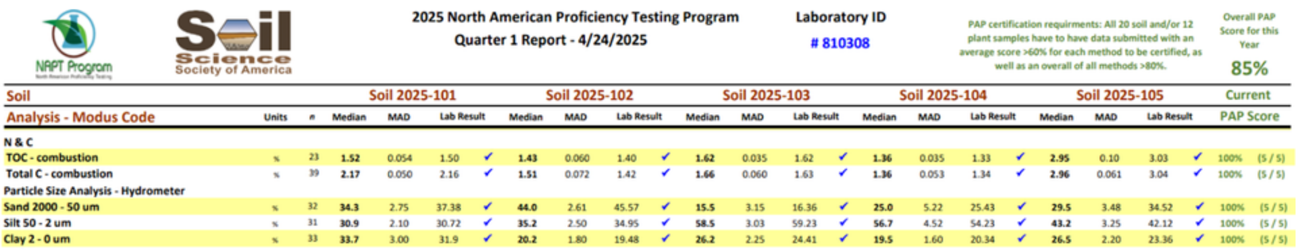
- Average replicate wells to the sample level before statistics/plots
- QC: join NAPT medians/MADs by analyte. Samples: join laboratory observations (EO LIMS or partner lab). Compute TOC = TC − TIC with propagated SD when needed

Outlier handling (applies to correlation panels and metrics)

- Why: Trim only extreme mismatches so a few bad pairs (e.g., mislabels or spurious predictions) don't skew correlation and error metrics
- How: For each analyte, compute residuals $r = \text{MIR} - \text{Lab}$ and absolute percent error $\text{APE} = |r|/\max(|\text{Lab}|, 1\times10^{-6})$. Flag an observation as an outlier if r lies below the 0.5th or above the 99.5th percentile or if APE exceeds the 99.5th percentile for that analyte. Exclude flagged points from summaries and trend fits; record counts excluded (excl)

8.3 Appendix C: Certification Documentation

Soil PAP
NAPT
naptprogram.org
Approved for
2025



NAPT Program

Soil Science Society of America

2025 North American Proficiency Testing Program
Quarter 1 Report - 4/24/2025

Laboratory ID
810308

PAP certification requirments: All 20 soil and/or 12 plant samples have to have data submitted with an average score >60% for each method to be certified, as well as an overall of all methods >80%.

Overall PAP Score for this Year
85%

Soil			Soil 2025-101				Soil 2025-102				Soil 2025-103				Soil 2025-104				Soil 2025-105				Current	
Analysis - Modus Code	Units	n	Median	MAD	Lab Result		Median	MAD	Lab Result		Median	MAD	Lab Result		Median	MAD	Lab Result		Median	MAD	Lab Result		PAP Score	
N & C																								
TOC - combustion	%	23	**1.52**	0.054	1.50	✓	**1.43**	0.060	1.40	✓	**1.62**	0.035	1.62	✓	**1.36**	0.035	1.33	✓	**2.95**	0.10	3.03	✓	100%	(5 / 5)
Total C - combustion	%	39	**2.17**	0.050	2.16	✓	**1.51**	0.072	1.42	✓	**1.66**	0.060	1.63	✓	**1.36**	0.053	1.34	✓	**2.96**	0.061	3.04	✓	100%	(5 / 5)
Particle Size Analysis - Hydrometer																								
Sand 2000 - 50 um	%	32	**34.3**	2.75	37.38	✓	**44.0**	2.61	45.57	✓	**15.5**	3.15	16.36	✓	**25.0**	5.22	25.43	✓	**29.5**	3.48	34.52	✓	100%	(5 / 5)
Silt 50 - 2 um	%	31	**30.9**	2.10	30.72	✓	**35.2**	2.50	34.95	✓	**58.5**	3.03	59.23	✓	**56.7**	4.52	54.23	✓	**43.2**	3.25	42.12	✓	100%	(5 / 5)
Clay 2 - 0 um	%	33	**33.7**	3.00	31.9	✓	**20.2**	1.80	19.48	✓	**26.2**	2.25	24.41	✓	**19.5**	1.60	20.34	✓	**26.5**	2.20	23.36	✓	100%	(5 / 5)

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About EarthOptics

Headquartered in Minneapolis, Minnesota, EarthOptics harnesses advances in soil-sensing technologies, genomics, and data science to provide farmers and ranchers with deep, actionable insights into their soil's chemical, physical, and biological properties. By blending cutting-edge laboratory analysis with industry-leading field-based sensors, we deliver powerful predictive insights that enable producers to optimize input use, improve soil health, increase yields, and unlock new opportunities in sustainable agriculture.

EarthOptics is also the leading carbon measurement company in the U.S., supporting the growth of carbon markets with accurate, verifiable soil data. The company has offices in Raleigh, North Carolina; Emeryville, California; Blacksburg, Virginia; and Fayetteville, Arkansas, with laboratories in Emeryville, California, and Memphis, Tennessee. Learn more at www.EarthOptics.com.