

# SpecSolo®



Scalable soil carbon  
analytical platform by  
FT-NIRS & machine learning

# ANDRÉ MARCELO DE SOUZA

Analytical Chemistry, DSc.

Area of specialization: Multivariate  
Statistical Analysis (Chemometrics) and  
Instrumental Analysis.



# Market Challenges

Deadlines



Cost of Analysis



Waste Management



Skilled Labor



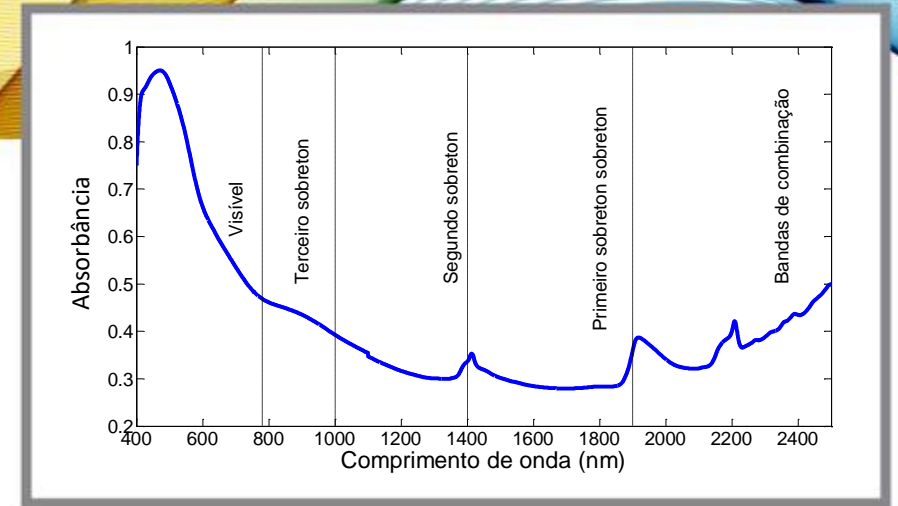
Quality





# Near Infrared Spectroscopy

12500 - 4000  $\text{cm}^{-1}$  ou 800 - 2500 nm);  
Overtones and combination bands  
C-H, N-H, O-H e S-H  
Wide and overlapping bands



## Vibrational Modes

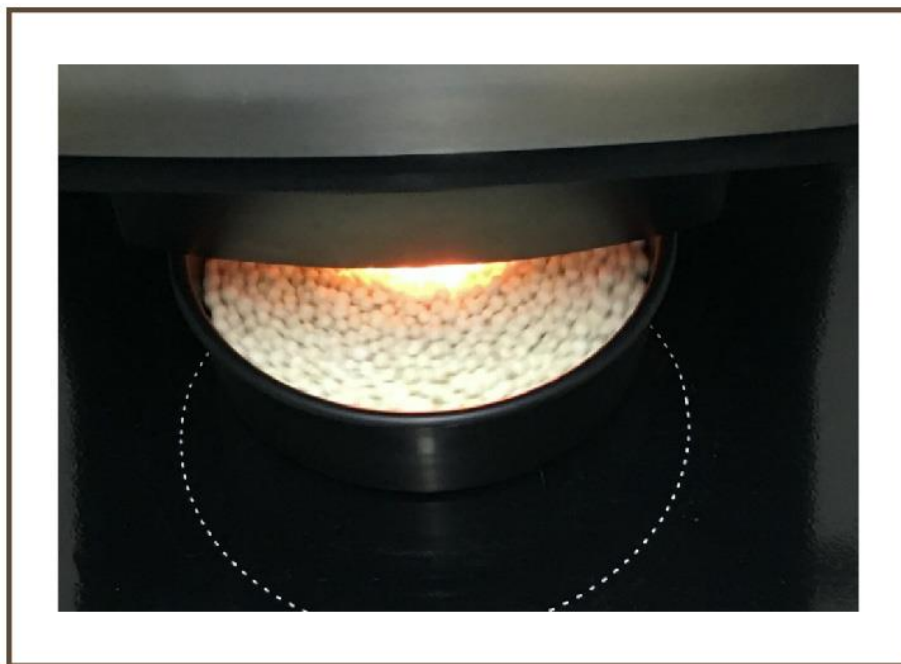




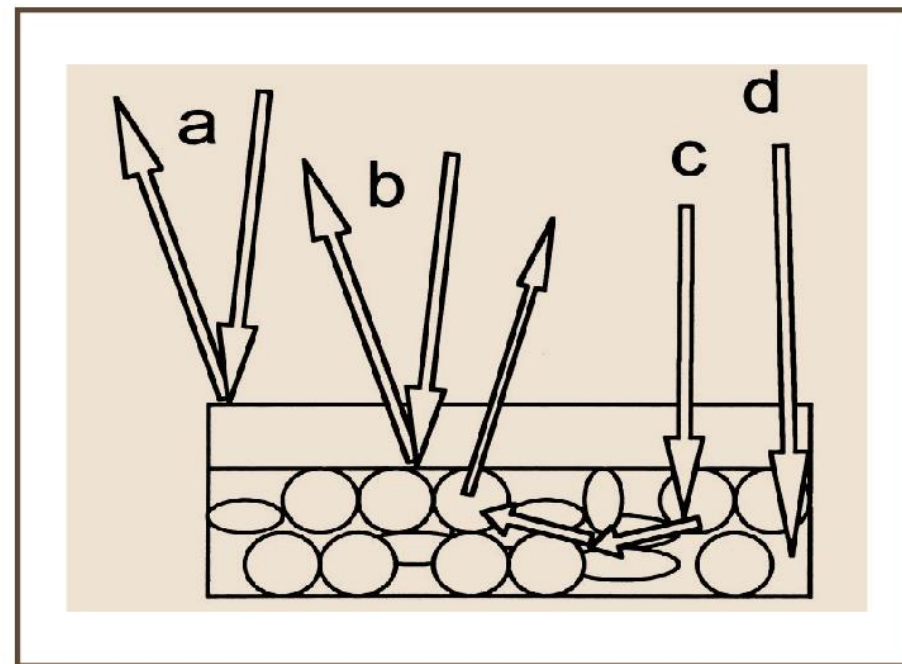
## ▶ Measures in NIR region

### Solids:

Diffuse reflectance measurements



- a. Reflection in the cell
- b. Specular reflectance in the sample
- c. Absorption and diffuse reflection in the sample
- d. Total absorption by the sample



## Innovation in soil analysis through spectral sensors



- 10 year Public-Private partnership with **Embrapa** (publisher of Official Methods for Soil Analysis in Brazil)
- Digital, scalable and precise soil analytical solution
- High analytical capacity - more than 6,000 samples/day
- Precise results - ISO 17025 accreditation
- No use of chemical reagents - no residues
- Ease of operation - dispense skilled labor
- Reduce operational cost



# SPECSOLO

ANALYTICAL PLATFORM



## SpecSolo-Scan

Innovation in soil analysis by spectral sensors, Big Data and Artificial Intelligence

## Lab.Online

Cloud-based LIMS solution for management of analytical routines and online results query

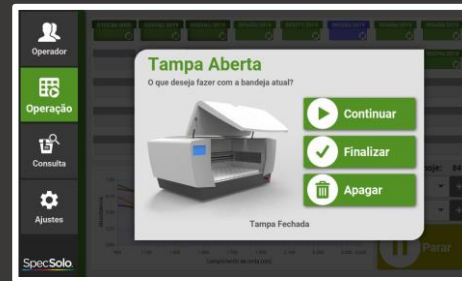
## SampSoil

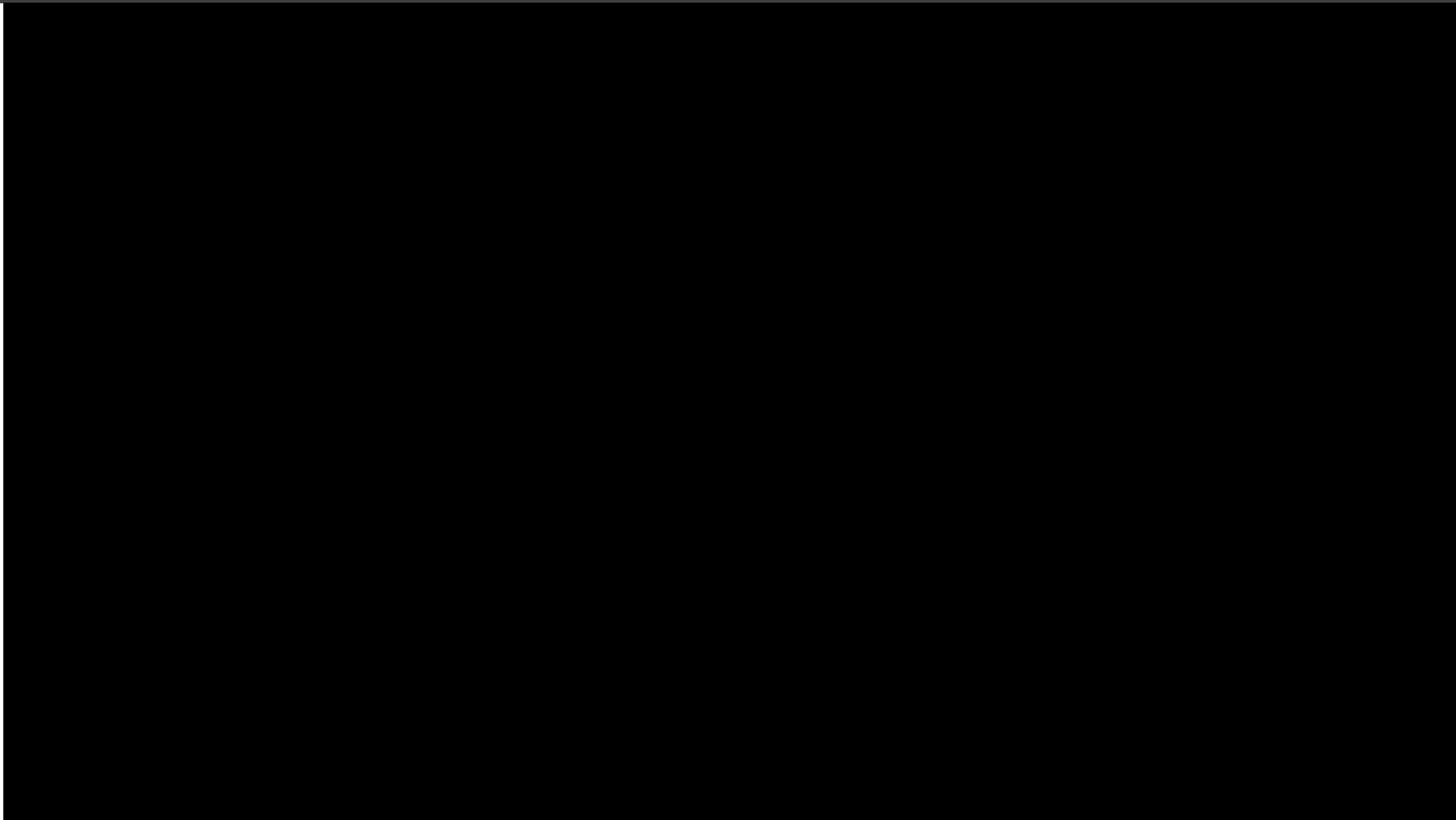
Online sampling planning and geo-located field collection

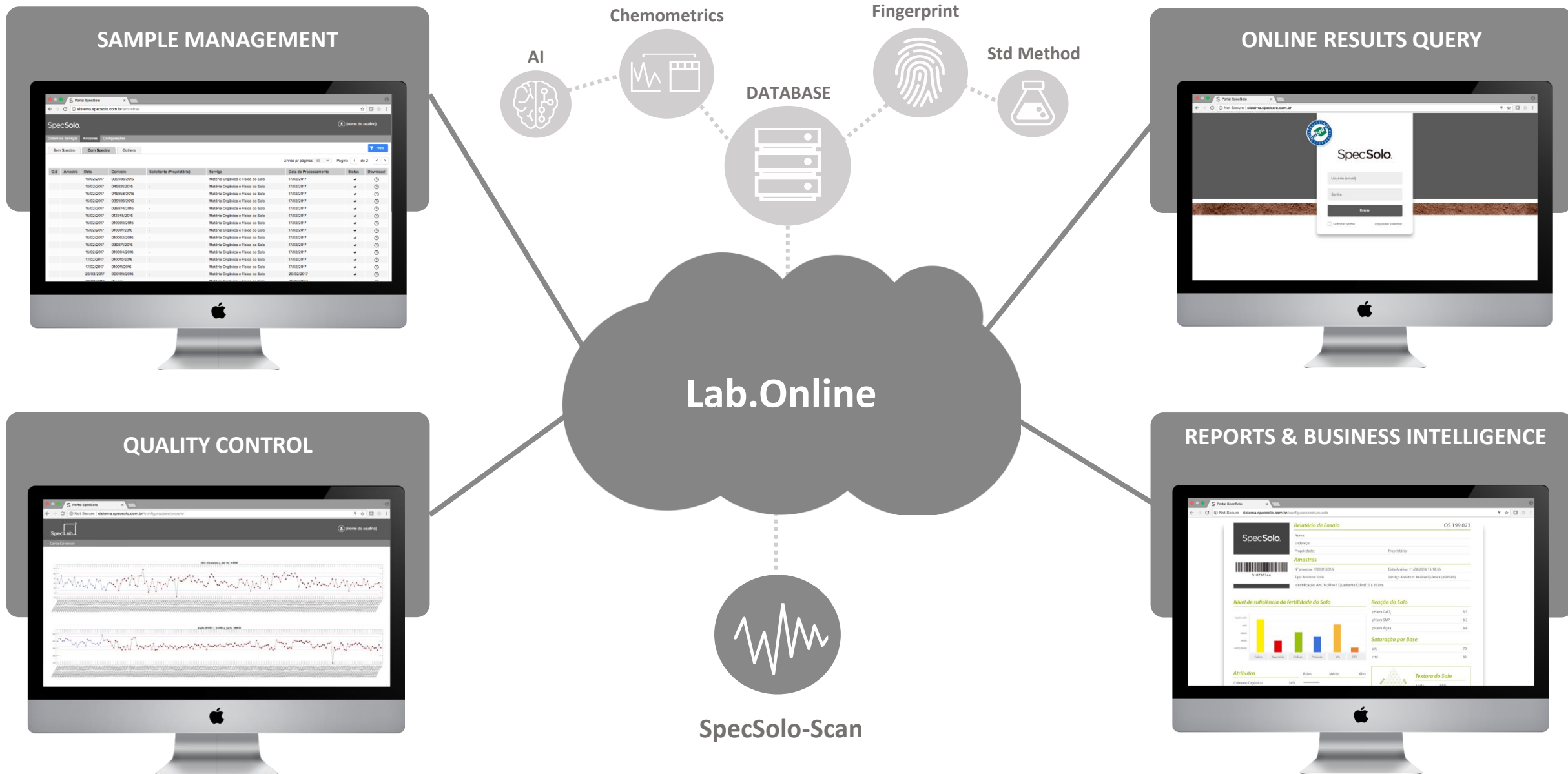




- Vis/FT-NIR spectrometer designed to **soil analysis**
- Analytical results calculated and published on **cloud**
- **Communication** - Wifi and Ethernet
- **Distance Sensor** - standardized soil spectrum collection
- **Barcode Scanner** - identification of the sample in the tray
- **Autosampler** with capacity for 40 samples
- **Control Chart** of control sample



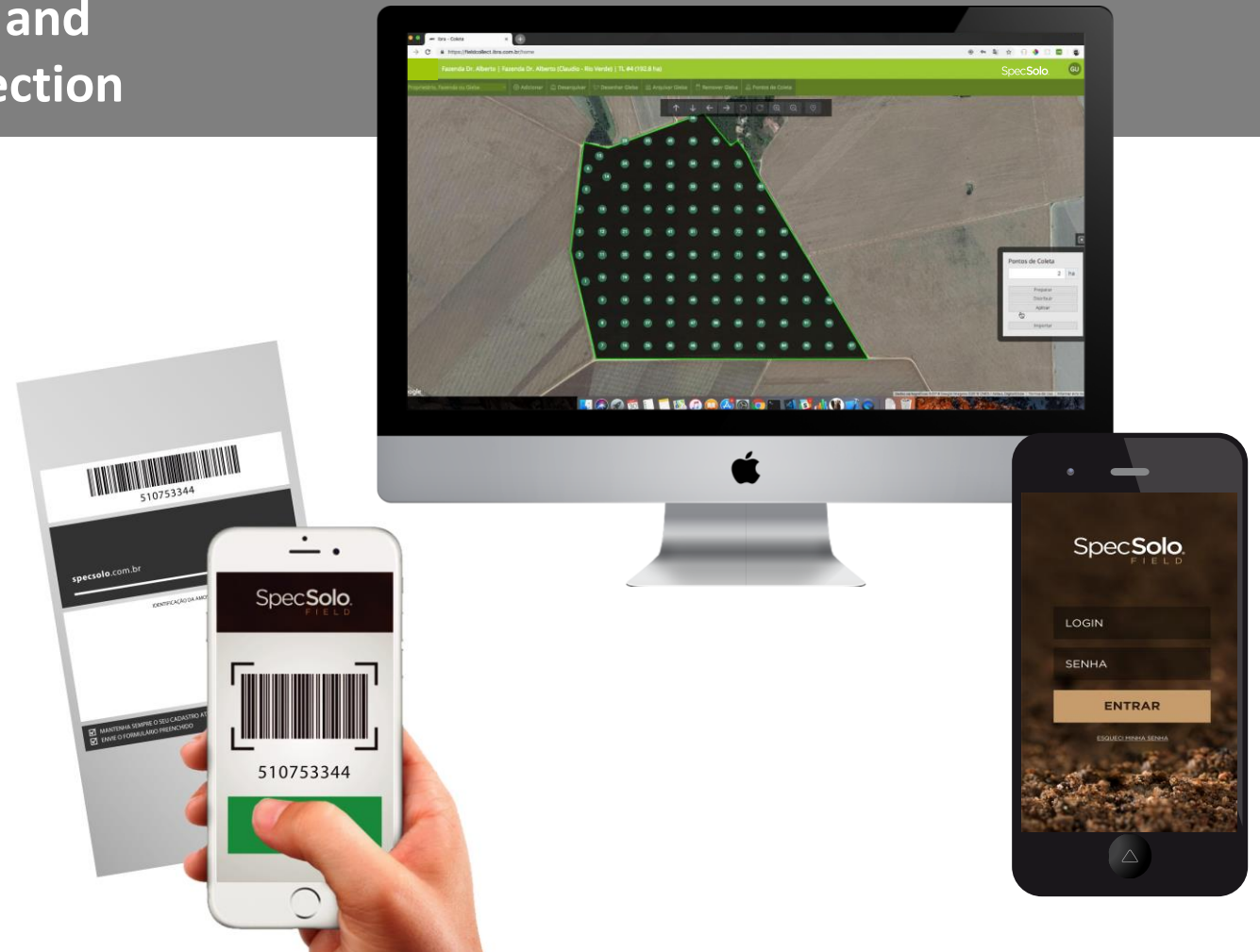




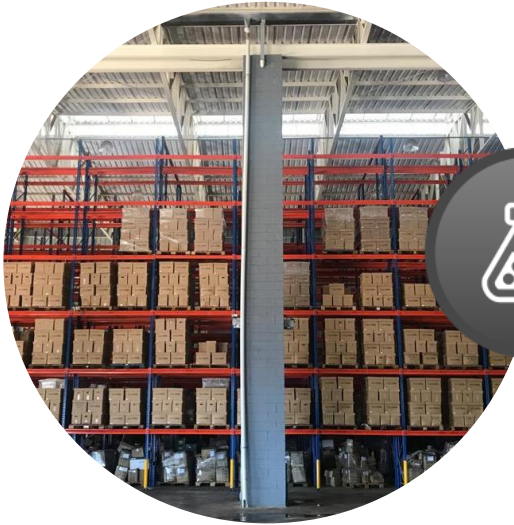


## Online Sampling Planning and App for Field Sample Collection

- ✓ Online system for georeferenced sampling planning through interactive maps
- ✓ Mobile App for in field sample collection and registration of coordinates through barcode scanning
- ✓ Exclusive sample bag and traceable with barcode







Soil Library  
**1 Million Samples**

analyzed by the reference method



Spectral Library  
**120.000**



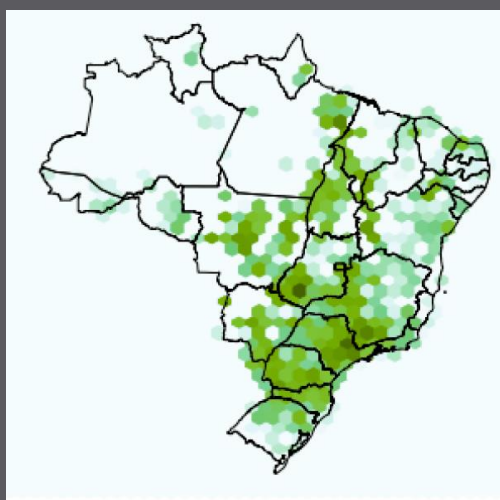
**Precise Results**

Analyzed in laboratory  
accredited ISO 17025

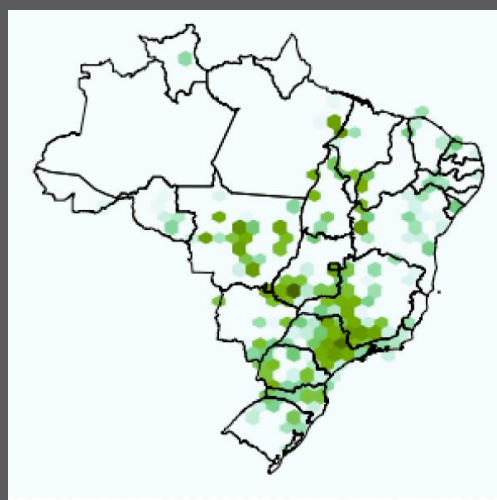




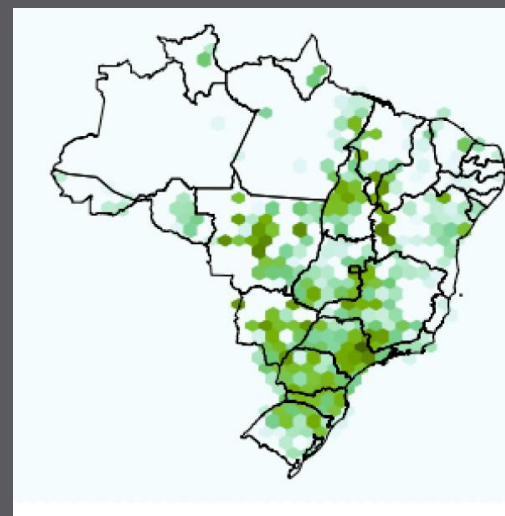
### O.M. – Soil Library



### O.M. - Spectral Database



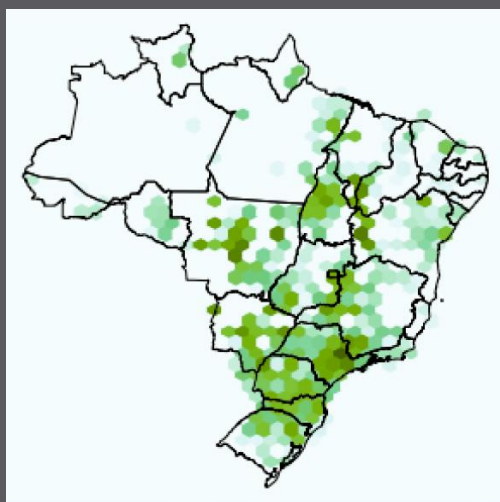
### Clay - Soil Library



### Clay – Spectral Database



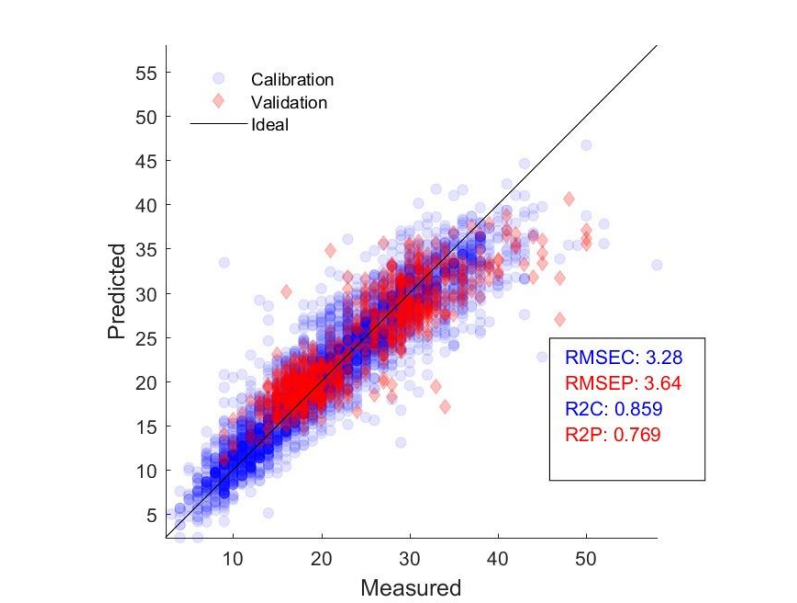
### Total Sand - Soil Library



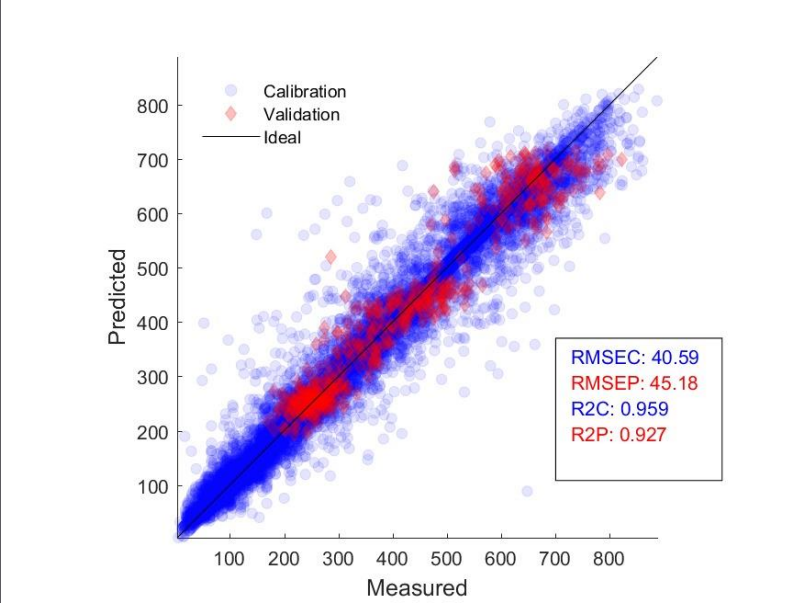
### Total Sand - Spectral Database



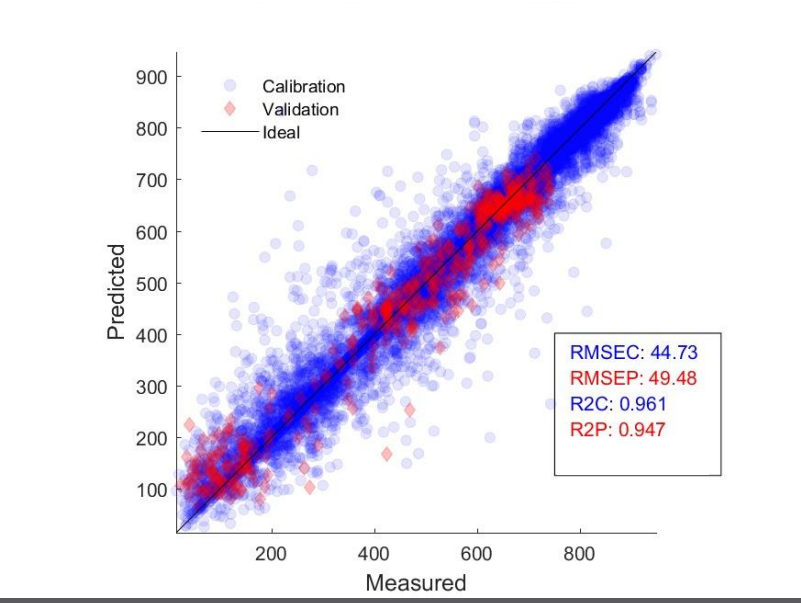
Soil Carbon



Clay



Total Sand



# Accreditation ISO 17025

**SpecSolo** method is accredited **ISO 17025** by INMETRO (Brazilian National Institute of Metrology, Quality and Technology) for analysis of **Soil Carbon** and **Texture** (clay, silt and sand), validating its **accuracy** and technical analytical competence.



ESCOPO DA ACREDITAÇÃO – ABNT NBR ISO/IEC 17025 - ENSAIO		
Norma de Origem: NIT-DICLA-016		Folha: 3
ACREDITAÇÃO Nº	TIPO DE INSTALAÇÃO	
CRL-0477	INSTALAÇÃO PERMANENTE	
ÁREA DE ATIVIDADE / PRODUTO	CLASSE DE ENSAIO / DESCRIÇÃO DO ENSAIO	NORMA E /OU PROCEDIMENTO
SOLO	Determinação do teor de matéria orgânica / carbono orgânico em Solo pelo método titulométrico LQ: 0,44%	Análises Químicas para Avaliação da Fertilidade do Solo – EMBRAPA 1998
	Determinação de matéria orgânica por Espectroscopia no Infravermelho Próximo (NIR) – Método Specsolo LQ: 4 g/dm <sup>3</sup>	ME SOLO 23 Rev.00
	Determinação de Granulometria por Espectroscopia no Infravermelho Próximo (NIR) – Método Specsolo	ME SOLO 23 Rev.00
	Argila: LQ: 5 g/Kg Silte: LQ: 2 g/Kg Areia Total: LQ: 6 g/Kg	



UNIVERSIDADE  
ESTADUAL DE  
CAMPINAS

*doutorado*

INSTITUTO DE QUÍMICA

UNICAMP

2014

ANDRÉ MARCELO DE SOUZA

EVALUATION OF THE POTENTIAL OF NEAR INFRARED SPECTROSCOPY AS A  
ROUTINE METHOD FOR THE DETERMINATION OF SOIL ORGANIC CARBON

PhD Thesis

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10/08/2017 870170057665  
17:31  
  
03.158.8.6.17.0707839.4

## Pedido nacional de Invenção, Modelo de Utilidade, Certificado de Adição de Invenção e entrada na fase nacional do PCT

Número do Processo: BR 10 2017 017235 0

### Dados do Depositante (71)

Depositante 1 de 2

Nome ou Razão Social: SPECLAB HOLDING S.A

Tipo de Pessoa: Pessoa Jurídica

CPF/CNPJ: 27310009000155

Nacionalidade: Brasileira

Qualificação Jurídica: Pessoa Jurídica

Endereço: Rua Ipê Branco, 214 - Sala 01 - Loteamento Industrial

Cidade: Sumaré

### Dados do Pedido

Natureza Patente: 10 - Patente de Invenção (PI)

Título da Invenção ou Modelo de Utilidade (54): ANÁLISE DE ATRIBUTOS QUÍMICOS E FÍSICOS DE FERTILIDADE DO SOLO POR ESPECTROSCOPIA VIS-NIR PARA USO EM ROTINA DE LARGA ESCALA

**Resumo:** O campo da invenção se volta ao agronegócio, e compreende o fornecimento de um novo método, ou seja, um processo, e respectivo sistema envolvendo produto (hardware + software) no sentido de aprimorar os procedimentos de análises químicas e físicas da fertilidade do solo em rotina de larga escala, mediante um pacote tecnológico dedicado à análise de solos, que combina:  
- o uso de um espectrofotômetro Vis-NIR, denominado SpecSolo-Scan com respectiva plataforma digital;  
- algoritmos quimiométricos de análise multivariada e;  
- um software integrado baseado em nuvem para produzir os resultados analíticos. Para aplicação em rotina da técnica de espectroscopia no infravermelho para determinação de atributos químicos e físicos do solo, é necessária a construção dos modelos de calibração para cada um dos atributos que será analisado no solo, associando o resultado da análise via úmida, realizado de acordo com os métodos de referências, com o espectrocorrespondente de cada amostra de solo, adquirida através de espectrofotômetro Vis-NIR da invenção, ou SpecSolo-Scan.

Figura a publicar: 1,2,3



**SPECIAL ISSUE:** Select proceedings III Indian Symposium on NIR Spectroscopy  
Study of ancient human bones/ Prediction of polyphenolics in sugarcane stems/ Honey botanical origin authentication/ Assessment of level before roasting



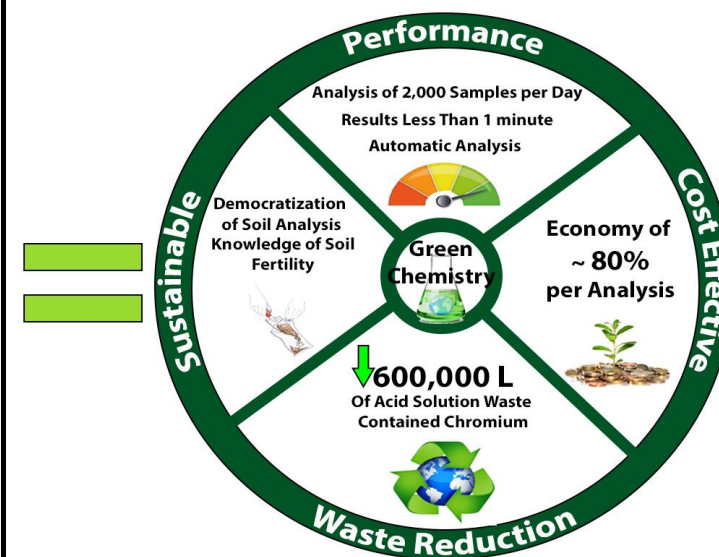
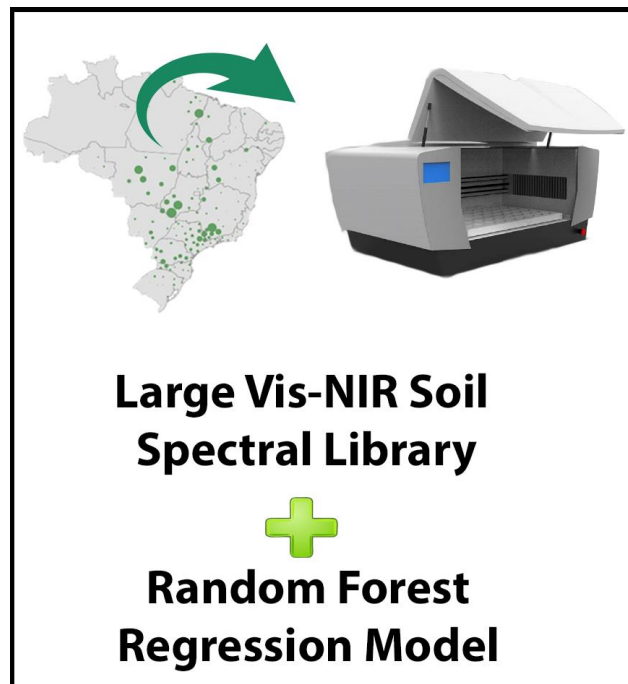
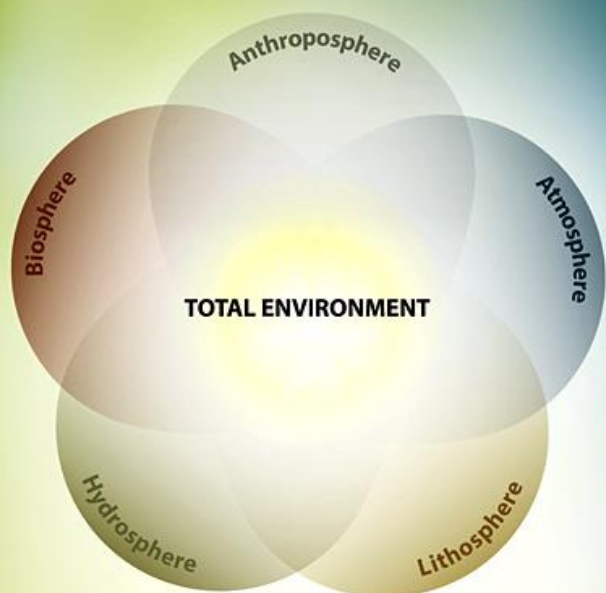
André Marcelo de Souza, Paulo Roberto Filgueiras, Maurício Rizzato Coelho, Ademir Fontana, Thayane Christine Barbosa Winkler, Patrícia Valderrama, Ronei Jesus Poppi, **Validation of the near infrared spectroscopy method for determining soil organic carbon by employing a proficiency assay for fertility laboratories.** | **Journal of Near Infrared Spectroscopy 24 (2016) 293-303.**





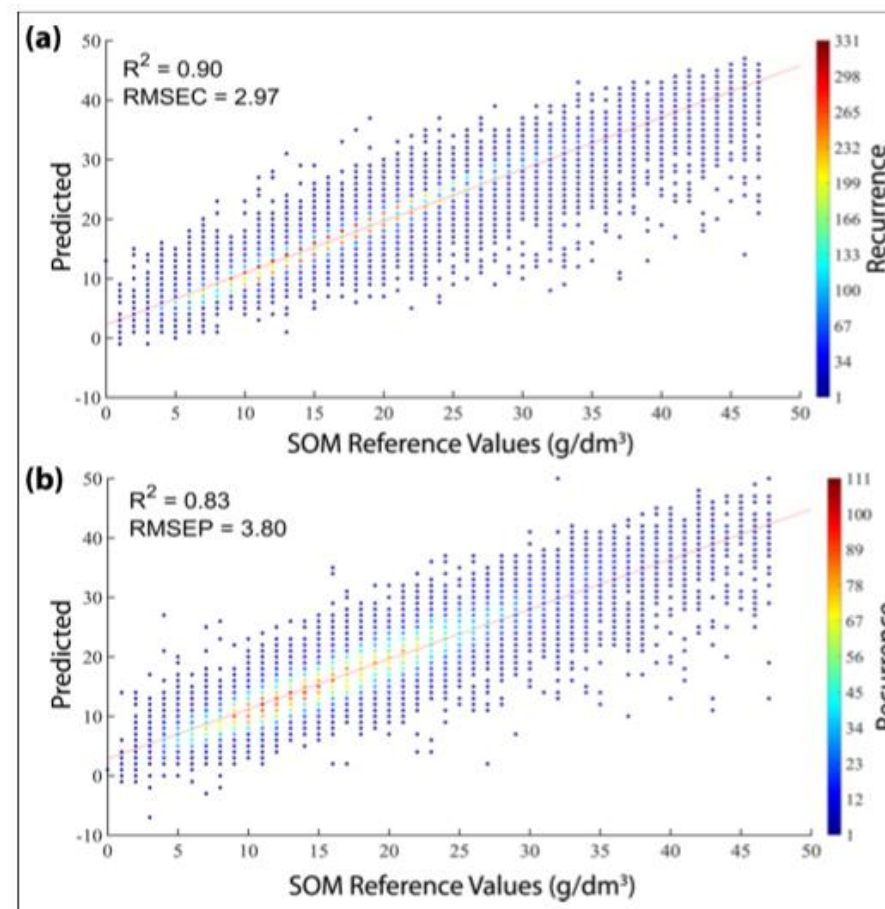
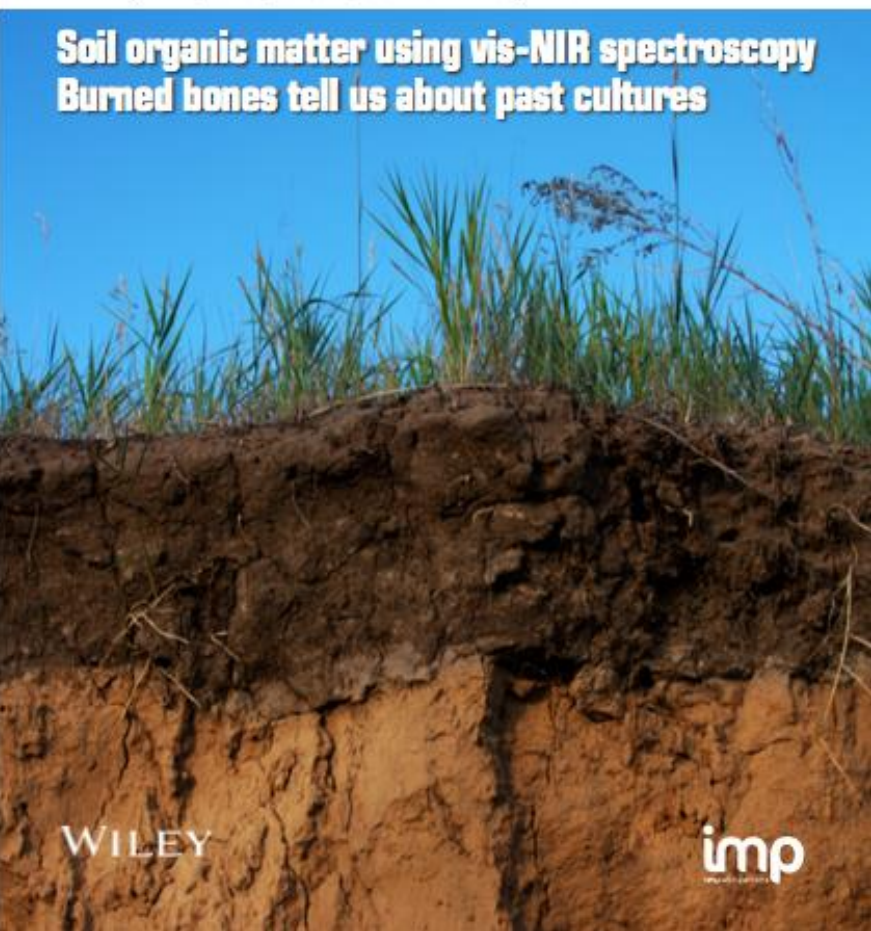
Published in 36 issues each year  
Volume 669 • 15 JUNE 2019 • ISSN 0048-9697

# Science OF THE Total Environment



Felipe B. de Santana, André M. de Souza, Ronei J. Poppi, Green methodology for soil organic matter analysis using a national near infrared spectral library in tandem with learning machine. | *Science of the Total Environment* 658 (2019) 895–900.

**Soil organic matter using vis-NIR spectroscopy**  
**Burned bones tell us about past cultures**



**Figure 3.** Plot of reference versus predicted values by SVM model in calibration (a) and validation (b) sets.

Felipe Bachion de Santana, Sandro Keiichi Otani, André Marcelo de Souza and Ronei Jesus Poppid, **Determination of soil organic matter using visible-near infrared spectroscopy and machine learning.** | **Spectroscopy Europe Vol. 31 NO. 4 (2019) 14-17.**



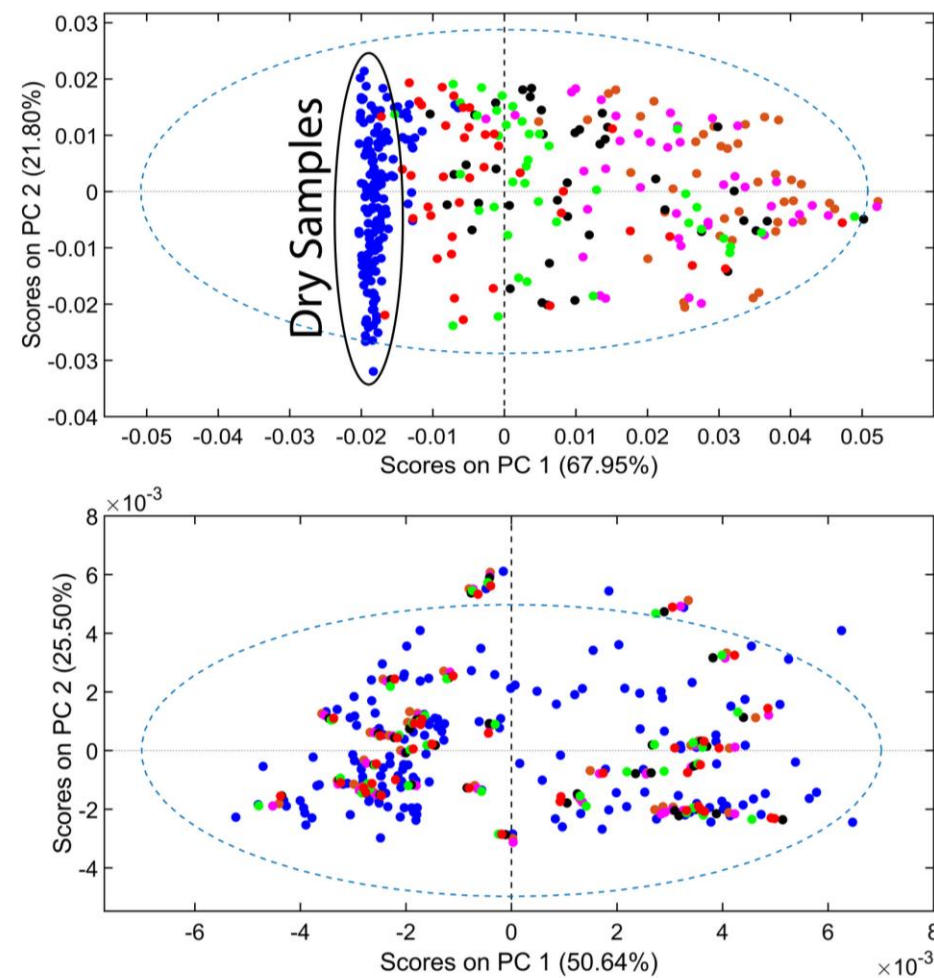


Volume 146, May 2019  
ISSN 0026-265X

# Microchemical JOURNAL

Devoted to the Application of  
Microtechniques in all branches  
of Chemistry

EDITOR-IN-CHIEF:  
MIGUEL DE LA GUARDIA



Felipe B. de Santana, Larissa O. de Giuseppea, André M. de Souza, Ronei J. Poppi, **Removing the moisture effect in soil organic matter determination using NIR spectroscopy and PLSR with external parameter orthogonalization.** | **Microchemical Journal 145 (2019) 1094–1101.**

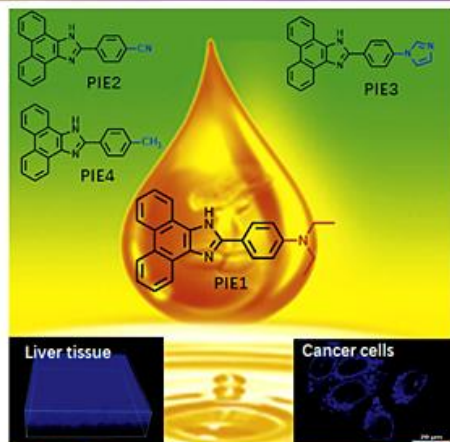


Volume 216, 5 June 2019

ISSN 1386-1425

# SPECTROCHIMICA ACTA

PART A: MOLECULAR AND BIOMOLECULAR SPECTROSCOPY



Novel two-photon fluorescent probe with high fluorescence quantum yields for tracking lipid droplets in biological systems  
Jie Niu, Yong Liu, Weishan Wang and Weiyang Lin

On-line Access via: [www.elsevier.com/locate/saa](http://www.elsevier.com/locate/saa)

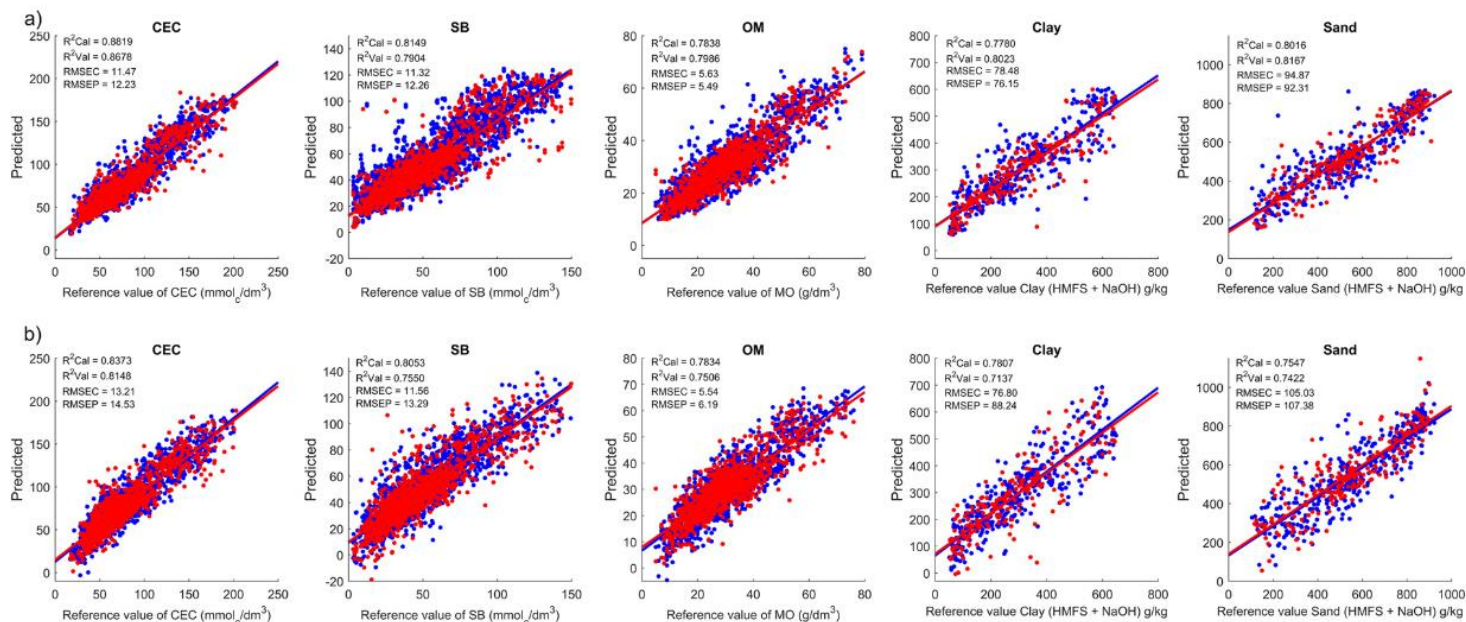


Fig. 7. Plot of reference values versus predict values from vis-NIR by random forest (a) and PLS (b) for CEC, SB, OM, clay and sand.

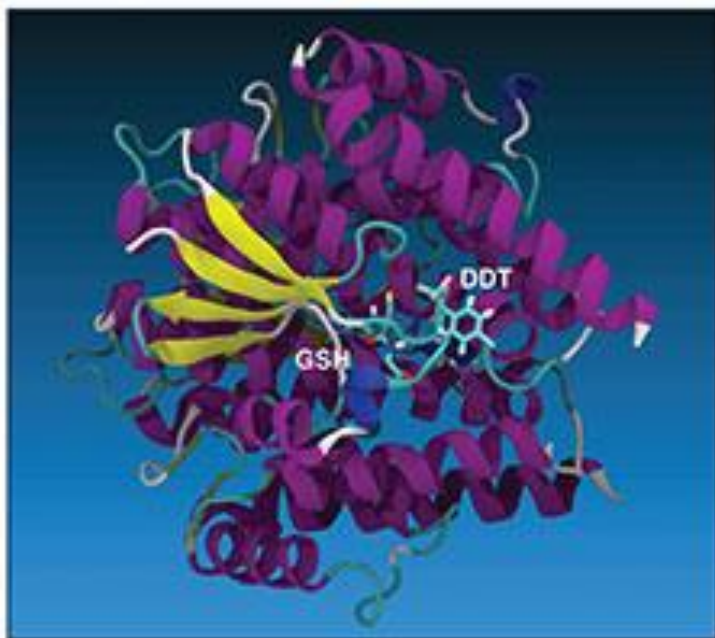
Felipe Bachion de Santana, André Marcelo de Souza, Ronei Jesus Poppi, Visible and near infrared spectroscopy coupled to random forest to quantify some soil quality parameters. | Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 191 (2018) 454–462.





# JBCS

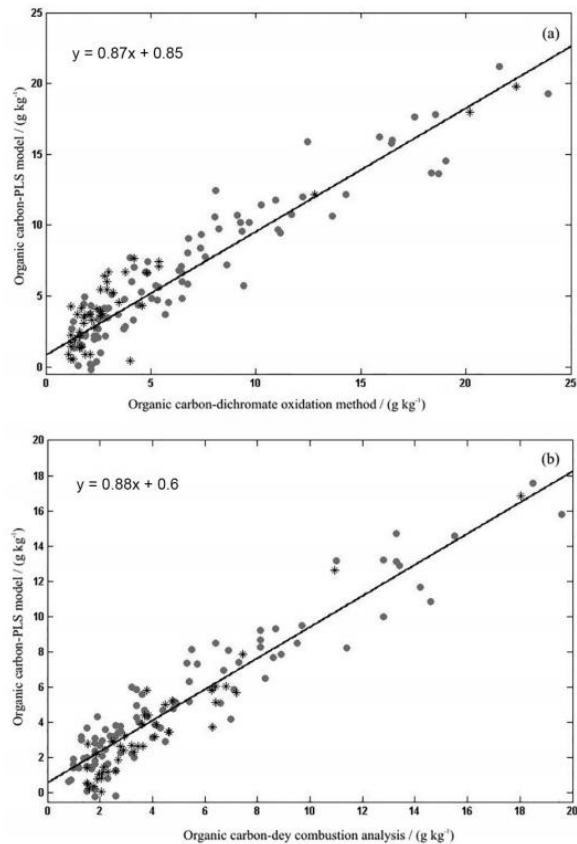
Vol. 27, No. 9  
September, 2016  
ISSN 0100-5003  
CODEN JBCH-DJ



Cover Picture

The Role of the Conformational Dynamics of Glutathione S-Transferase Epitope Class on Insecticide Resistance in *Anopheles gambiae*

Frederico J. S. Pinho, Rafael T. Mass, Maria Carolina F. Lima, Constança F. J. Aguiar and Theresia A. Soares



Karla K Beltrame, André M Souza, Maurício R Coelho, Thayane CB Winkler, Wyrllen E Souza, Patrícia Valderrama, **Soil organic carbon determination using NIRS: evaluation of dichromate oxidation and dry combustion analysis as reference methods in multivariate calibration.**  
 | **Journal of the Brazilian Chemical Society 27 (2016), 1527-1532.**

BrJAC

Brazilian Journal of Analytical Chemistry  
an International Scientific Journal

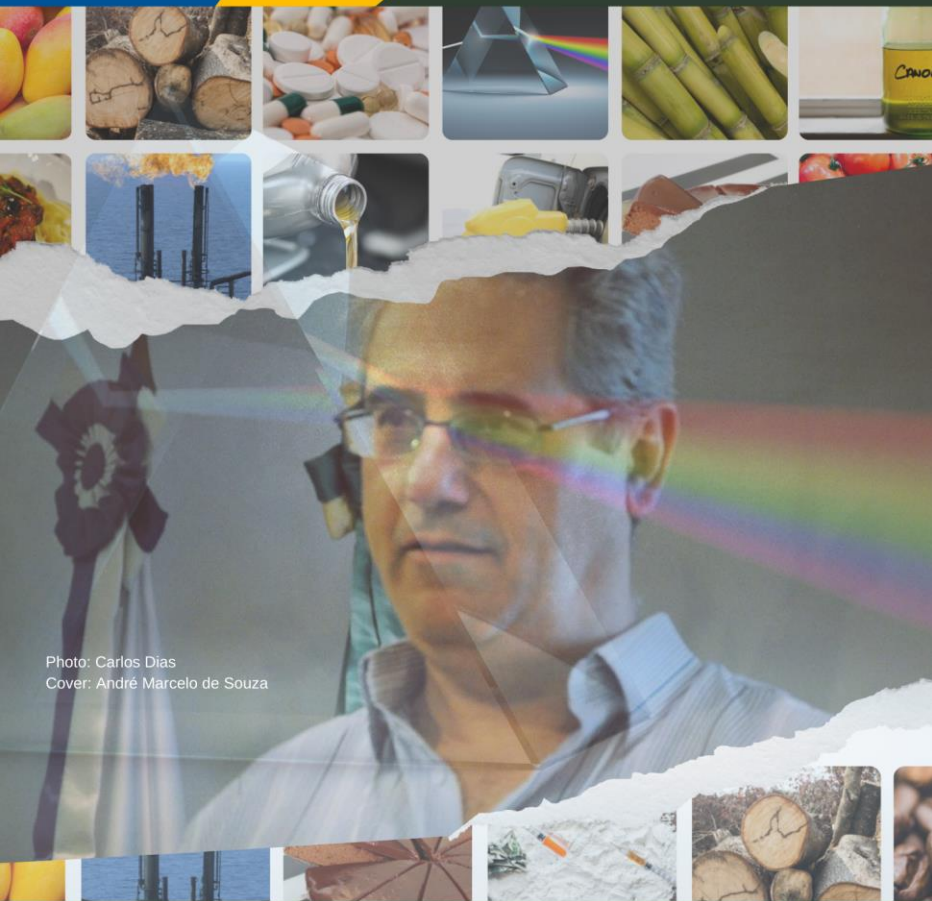


Photo: Carlos Dias  
Cover: André Marcelo de Souza

Special Issue dedicated to Prof. Ronei J. Poppi









July – September 2021 Volume 8 Number 32

Brazilian Journal of Analytical Chemistry  
2021, Volume 8, Issue 32, pp 78–90  
doi: 10.30744/brjac.2179-3425.AR-10-2021

BrJAC

ARTICLE

## Monitoring Mineral-Associated Organic Matter in Tropical Pastures using Near Infrared Spectroscopy

Felipe Bachion de Santana<sup>1</sup>, André Marcelo de Souza<sup>2\*</sup>, Fabiano de Carvalho Balieiro<sup>2</sup>, Mirelly Mioranza<sup>3</sup>, Renato Aragão Ribeiro Rodrigues<sup>2</sup>, Ronei Jesus Poppi<sup>1</sup>

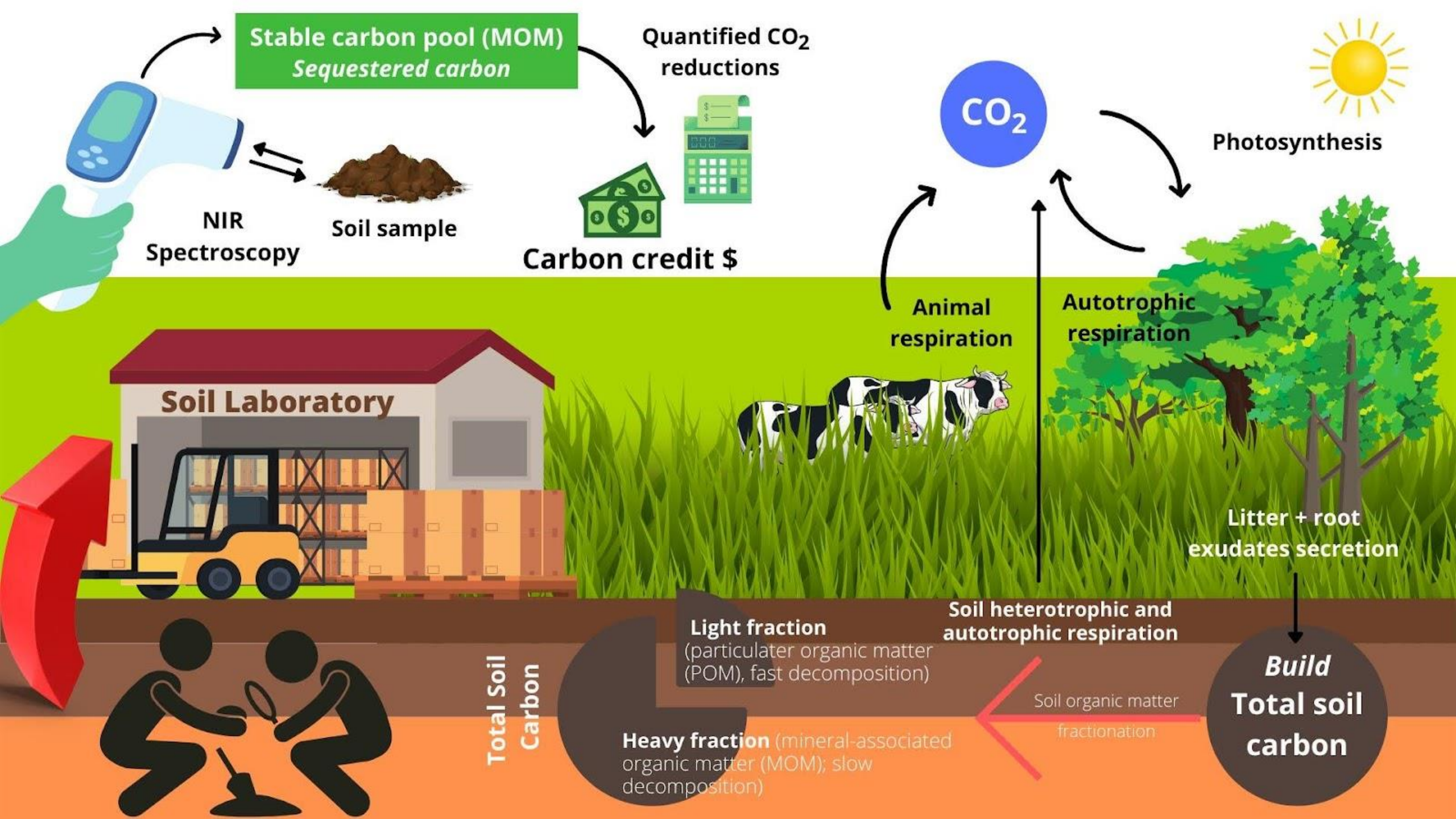
<sup>1</sup>Instituto de Química, Universidade Estadual de Campinas, Caixa Postal 6154, CEP 13084-971, Campinas, SP, Brazil

<sup>2</sup>Empresa Brasileira de Pesquisa Agropecuária (Embrapa Solos), R. Jardim Botânico, 1024, Rio de Janeiro, RJ, CEP 22460-000, Brazil

<sup>3</sup>Universidade Federal Fluminense, CEP 24020-141, Niterói, RJ, Brazil

† In memoriam (1961 – 2020)





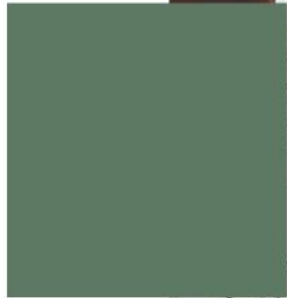






The background is a collage. On the right side, there is a 100 Euro banknote, showing the number '100' and the European Union flag. Below the banknote, a portion of a black computer keyboard is visible, with keys like 'Backspace', 'Cause Break', and 'Insert' clearly seen. A dark green rectangular box is overlaid on the left and center of the image, containing white text.

# AÇÕES DE TRANSFERÊNCIA E TECNOLOGIA DA SPECSOLO



# Capacitação

Treinamento Online na Plataforma e-Campo  
da Embrapa





**Curso de  
Capacitação**

# **Desenvolvimento e validação de métodos em espectroscopia no infravermelho próximo**

**e-Campo**

vitrine de capacitações on-line da Embrapa



**Inscrições Abertas**



**Até 30 de setembro de 2022**

**Embrapa**



Curso

# Conteúdo Programático

**Embrapa**  
Solos





Parte I

# Espectroscopia no Infravermelho Próximo

Fundamentos e Aplicações  
8 Módulos



Parte II



# Machine Learning em Python

Álgebra Linear em *Machine Learning*

21 Módulos



Parte III

# Análise Multivariada

Fundamentos e Aplicações  
12 Módulos





# Serviços

Prestação de Serviços de Análise de Carbono e Granulometria através da Tecnologia SpecSolo





**Scott Belsky**

**"IT'S NOT ABOUT  
IDEAS. IT'S ABOUT  
MAKING IDEAS  
HAPPEN"**

