Assessing the differences of two vineyards soils' by NIR spectroscopy and chemometrics

Sandia Machado[1], Luisa Barreiros[1,2], António R. Graça[3], Manuel Madeira[4], Ricardo N.M.J. Páscoa[1*], Marcela Segundo[1], João A. Lopes[5]

[1] LAQV/REQUIMTE, Department of Chemical Sciences, Laboratory of Applied Chemistry, Faculty of Pharmacy, University of Porto, Rua de Jorge Viterbo Ferreira n º 228, 4050-313, Porto, Portugal

[2] Escola Superior de Saúde, Instituto Politécnico do Porto, Rua Dr. António Bernardino de Almeida 400, 4200-072 Porto, Portugal

[3] Departamento de Investigação e Desenvolvimento, SOGRAPE Vinhos S.A., Aldeia Nova, 4430-852, Avintes, Portugal

[4] Forest Research Centre (CEF), School of Agriculture (ISA), University of Lisbon (ULisboa), Tapada da Ajuda, 1399-017 Lisboa, Portugal

[5] Research Institute for Medicines (iMed-ULisboa), Faculty of Pharmacy, University of Lisbon, Av. Prof. Gama Pinto, 1649-003, Lisboa, Portugal

OBJECTIVES:

Soil analysis by NIR spectroscopy

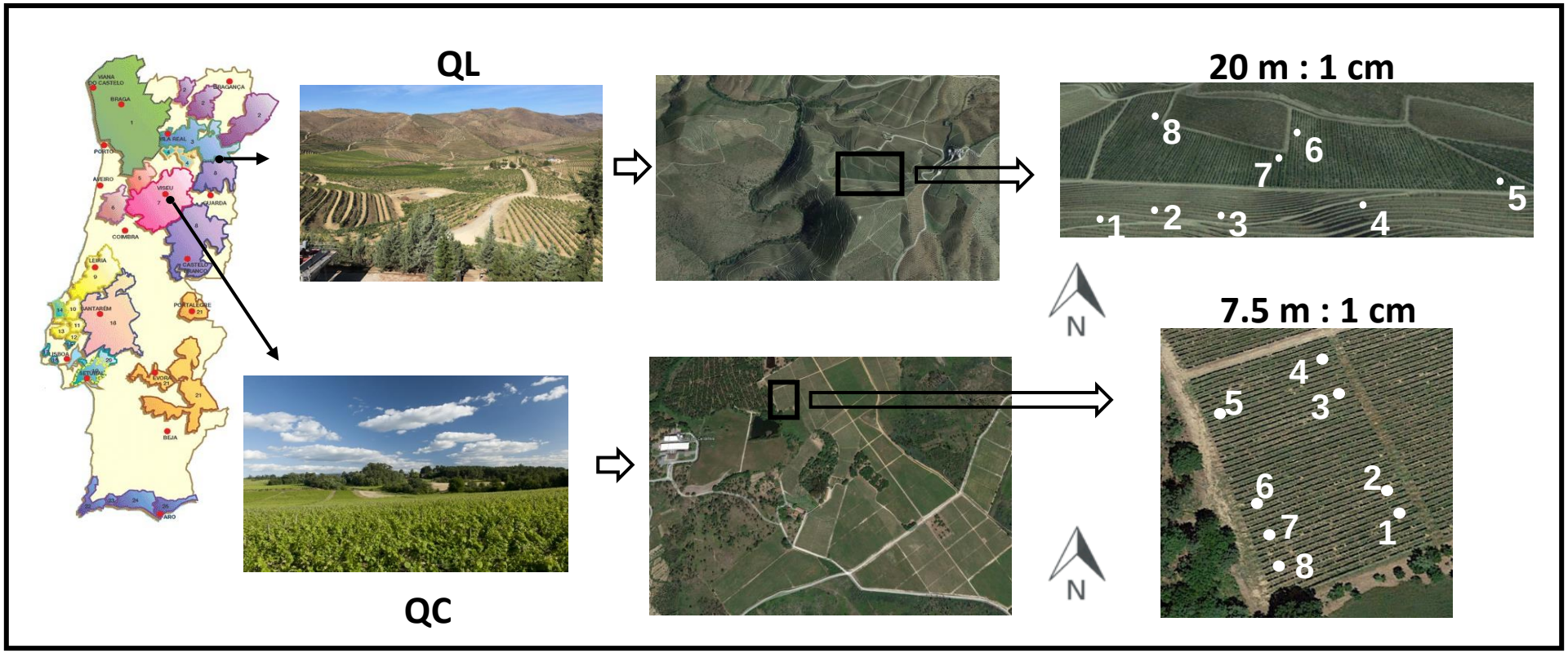
Qualitative approach

- ✓ Formation of clusters;
- ✓ Outlier screening;
- ✓ Discrimination of soil types;

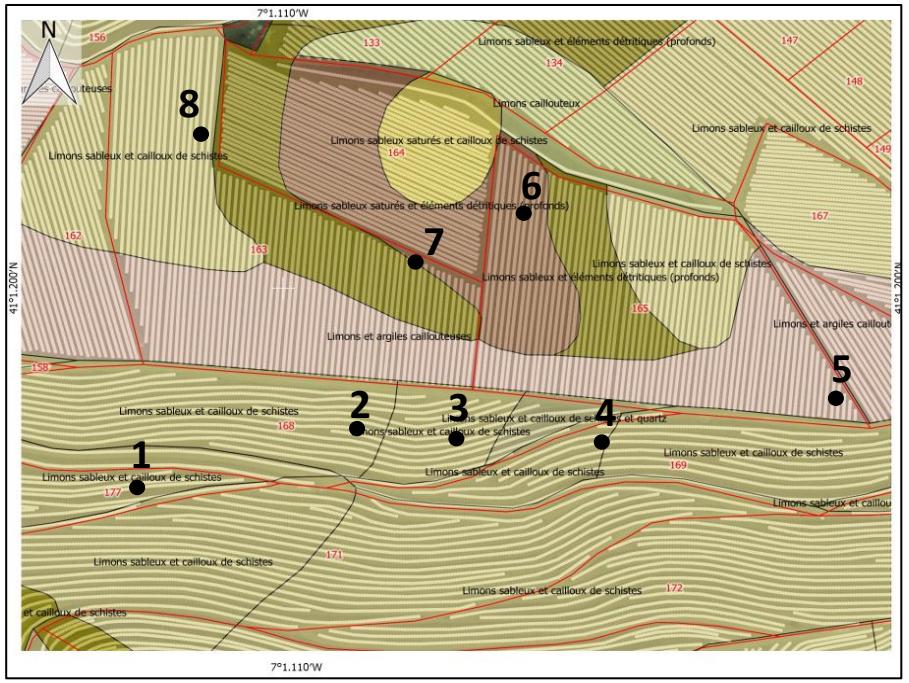
Quantitative approach

- ✓ Calibration models for pH(H_2O), pH(KCl), C_{org}, N, C/N, Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, SB, Al^{3+}, CEC, ECEC, GSB, GSA, P, K;

Sampling spots



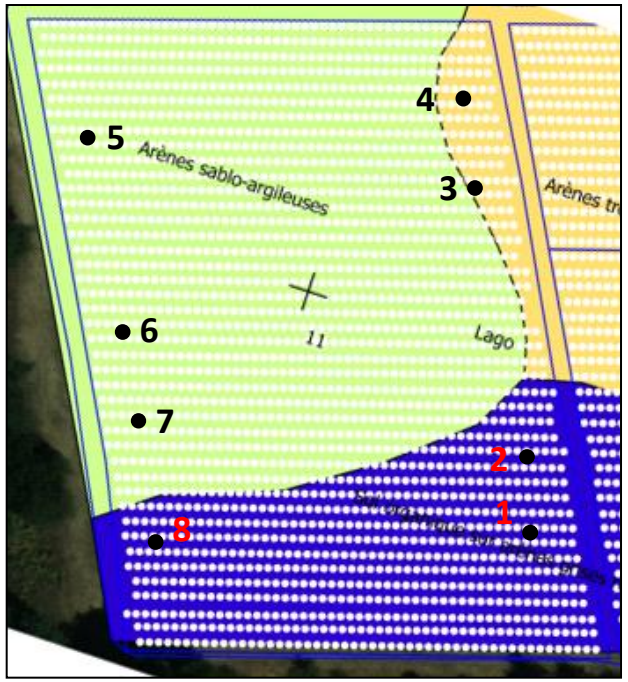
Pedology soil map for QL



Legend: 1,2,3,4,8- Limons sableux et cailloux de schistes; 5- Limons et argiles cullouteuses; 6- Limons sableux saturès et éléments détrifiques; 7- Limons sableux et éléments détrifiques;

N

Pedology soil map for QC



Legend: 1,2- Sol organique sur arènes grises remaniées; 3,4- Arènes très sableuses; 5,6,7- Arènes sablo-argileuses; 8- Sol organique sur arènes grises remaniées;

Soil's collection

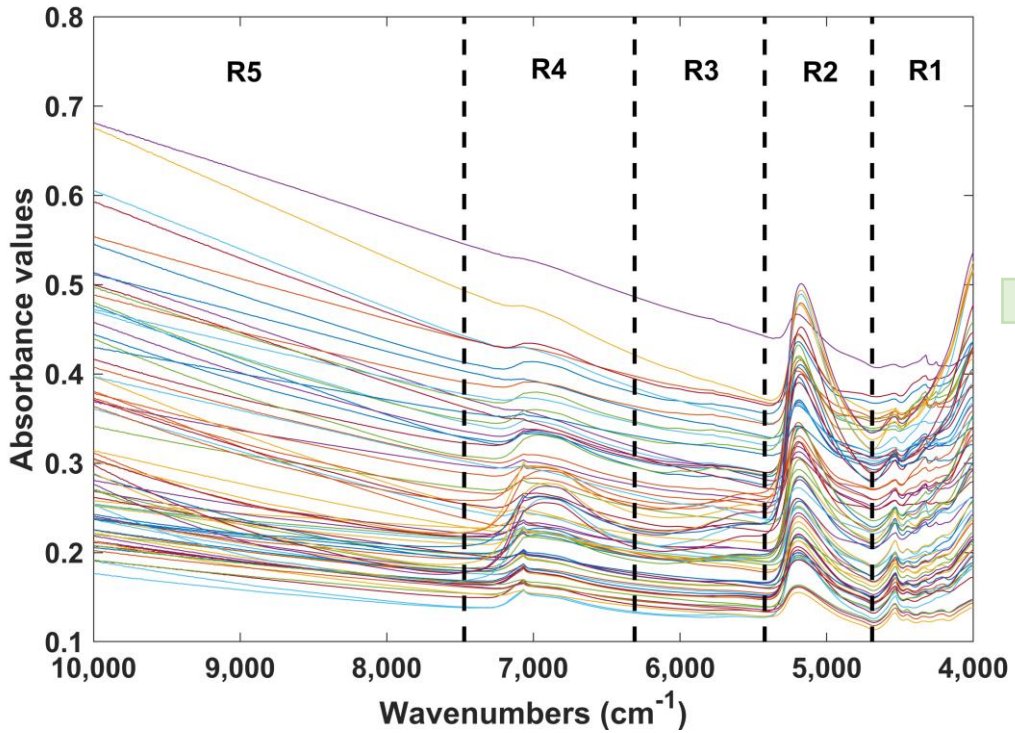
Spectral acquisition

NIR instrument

FTLA 2000, ABB
(diffuse reflectance mode)

Data analysis

NIR soil's spectra



Chemometric analysis:

- Qualitative approach

Principal component analysis (PCA)

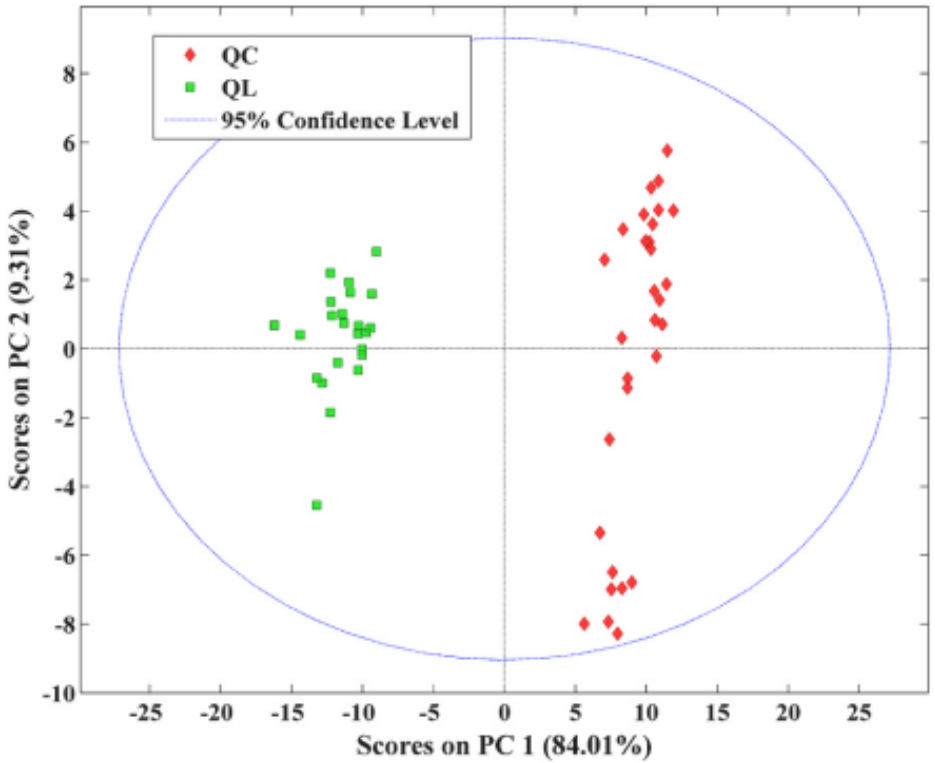
Partial least squares – discriminant analysis (PLS-DA)

- Quantitative approach

Partial least squares (PLS)

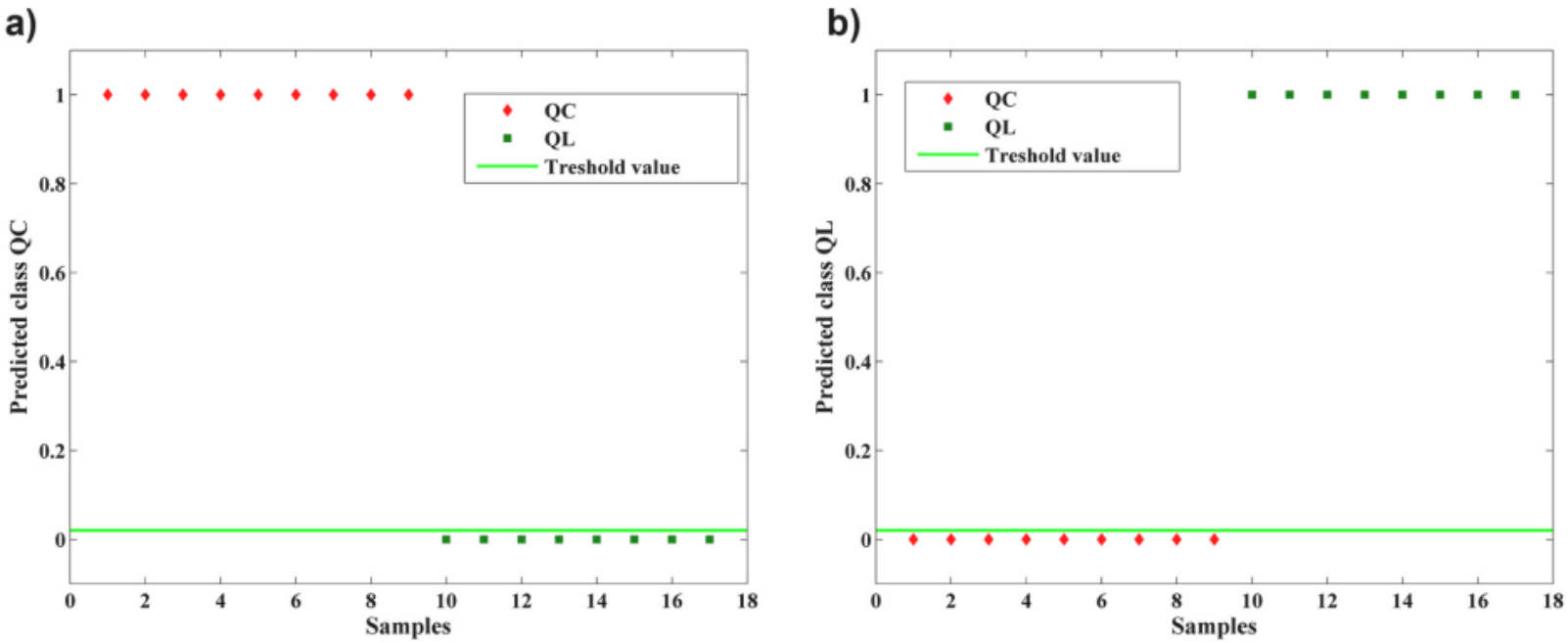
rnpascoa@ff.up.pt

PCA: Scores plot



Score plot of the first two principal components using NIR soils ' spectra (spectra were pre- processed with Savitzky-Golay (using 15 points filter width, second polynomial order and first derivative) followed by SNV and then mean centered).

PLSDA: Confusion matrices



Class predictions for the 2 LV PLS-DA model calibrated from the soils NIR spectra for QC (a) and QL (b).

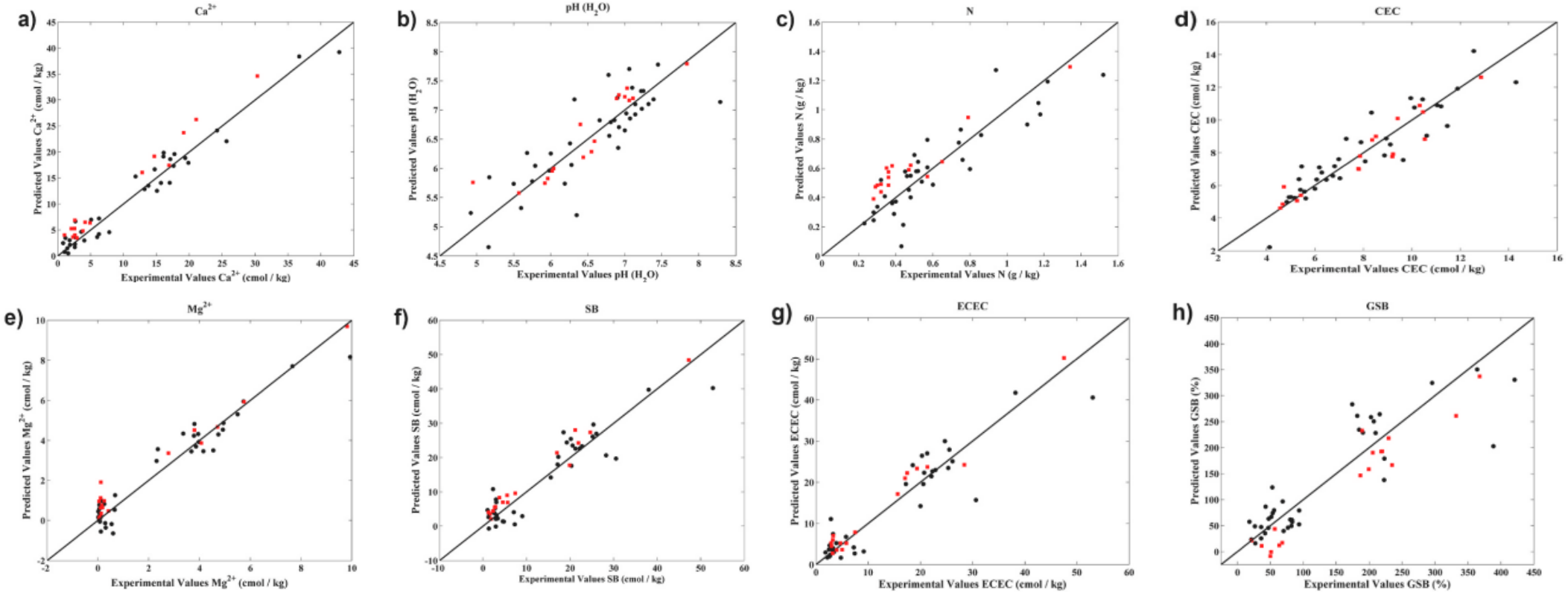
100% of correct predictions

PLS: calibration models

PLS calibration models results for the different soils parameters using the entire NIR spectra pre-processed with Savitzky-Golay (using 15 points filter widt, second polynomial order and first derivative by SNV and then mean centered

Parameters	LV	RMSEC	RMSECV	RMSEP	R_C^2	R_P^2	RER
pH -H_2O	8	0.19	0.44	0.27	0.94	0.85	11
pH - KCl	6	0.30	0.50	0.25	0.73	0.78	7
Corg	6	1.50	2.20	1.70	0.86	0.84	9
Cn*H*	6	0.79	1.30	1.50	0.85	0.27	4
N	6	0.09	0.14	0.10	0.91	0.90	13
C/N	3	3.70	4.50	2.80	0.42	0.55	6
Ca^{2+}	8	1.40	3.50	1.70	0.98	0.98	17
Mg^{2+}	5	0.42	0.64	0.52	0.97	0.97	19
Na^{+}	2	0.12	0.13	0.09	0.37	0.46	5
K^{+}	6	0.06	0.09	0.08	0.75	0.56	5
SB	5	2.20	4.40	3.00	0.97	0.95	16
Al^{3+}	6	0.20	0.34	0.21	0.55	0.69	7
CEC	5	0.65	1.00	0.77	0.94	0.89	11
ECEC	7	1.80	4.50	2.40	0.98	0.97	19
GSB	7	19.00	52.00	27.00	0.97	0.93	13
GSA	6	8.70	13.00	11.00	0.68	0.49	5
P	4	13.00	18.00	14.00	0.19	0.07	4
K	5	27.00	38.00	31.00	0.61	0.36	5

PLS: calibration models



Experimental values versus the cross-validation (●) and prediction (■) model estimated for Ca^{2+} (a), pH(H2O) (b), N (c), CEC (d), Mg^{2+} (e), SB (f), ECEC (g) and GSB (h).

Conclusions:

- ✓ The developed methodology demonstrated its suitability for the qualitative analysis of soil.
- ✓ Although not accurate for several soil parameters, it was accurate for 6 soil parameters (Ca^{2+}, pH(H2O) (b), N (c), CEC (d), Mg^{2+} (e), SB (f), ECEC (g) and GSB (h).)
- ✓ The developed methodology is much more rapid, cost-effective, less-laborious and environmentally friendly that the reference procedures.

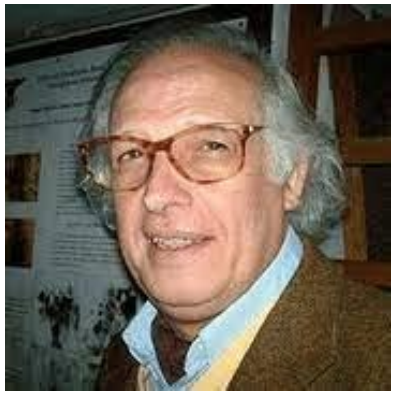
Thanks for your attention!

Sandia Machado

Luisa Barreiros

António R. Graça

Manuel Madeira



Ricardo N. M. J. Páscoa

Marcela Segundo

João A. Lopes

rnpascoa@ff.up.pt