6th Bioanalytical School

Quimiometria de Imagens Empregando Celulares

Chemometrics of Images Employing Cell Phones

Prof. Dr. Marco F. Ferrão

IQ - UFRGS - BRASIL

Image Analysis

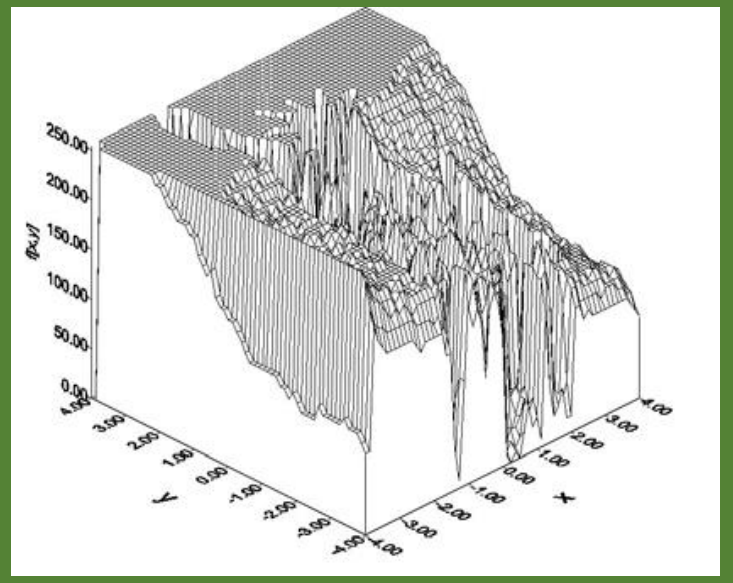


Image $f\ [x, y]$ (a) and spatial function of two coordinates $f\ [x, y]$ (b).

$[x, y]$ – pixel

$f[x, y]$ – imagem em preto e branco

$f[x, y, t_n]$ – filme monocromático;

$f[x, y, \lambda_n]$ – imagem multiespectral.

$f[x, y, z]$ – holograma monocromático;

$f[x, y, t_n, \lambda_m]$ – filme colorido;

$f[x, y, z, t_n, \lambda_m]$ – realidade.

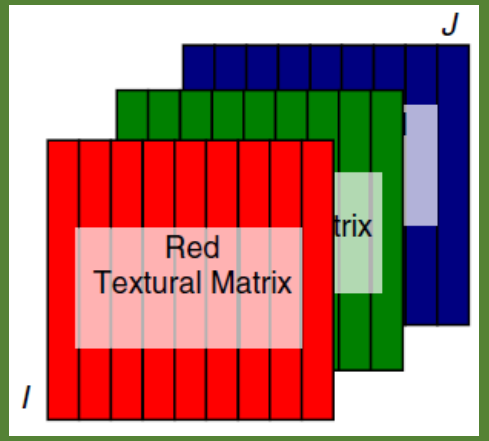
Image Analysis

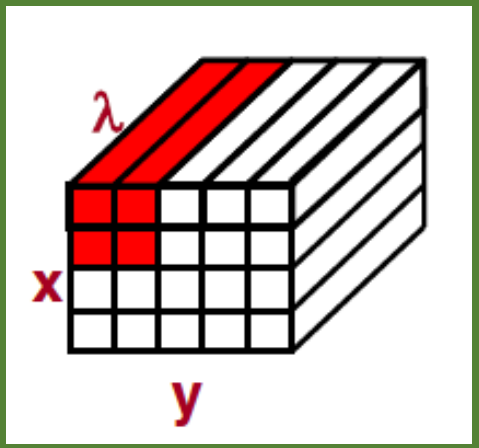
Dimensão Espectral $[\lambda]$

Monocromática (escala de cinza $[\lambda = 1]$

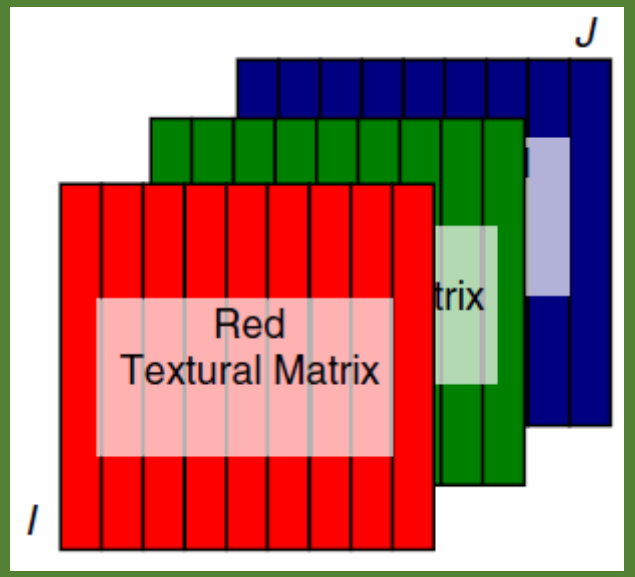
Multiespectral $[\lambda > 1]$
- RGB
- HSV

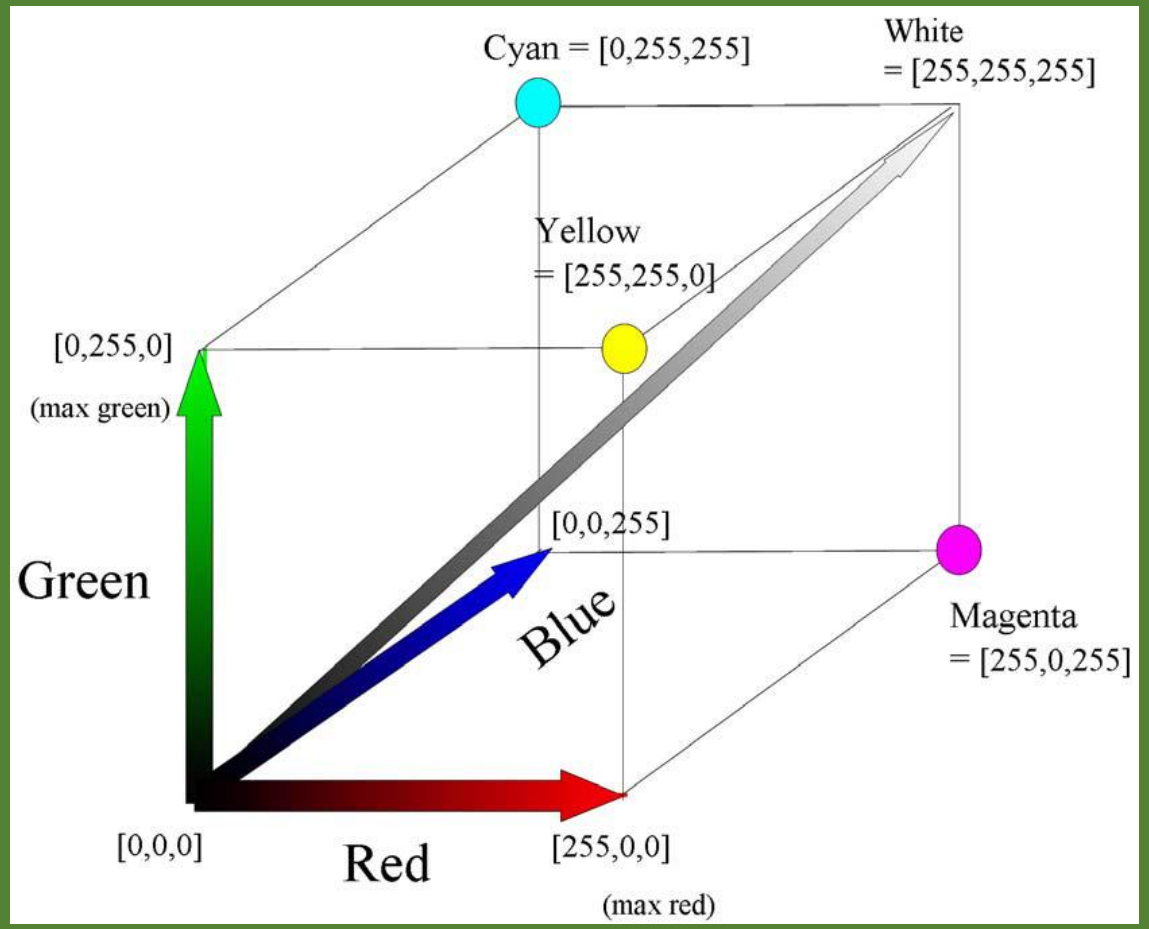
Hiperespectral $[\lambda \gg 1]$
- NIR
- RAMAN





Vermelho, Verde e Azul (RGB)





Cartesian coordinates for the RGB color system.

low Cost Equipment

Scanner

Digital Cameras

WebCam

Smartphone

Colorimetric determination of ascorbic acid based on its interfering effect in the enzymatic analysis of glucose: An approach using smartphone image analysis

Mayra S. Coutinho, Camilo L. M. Morais, Ana C. O. Neves, Fabrício G. Menezes and Kássio M. G. Lima

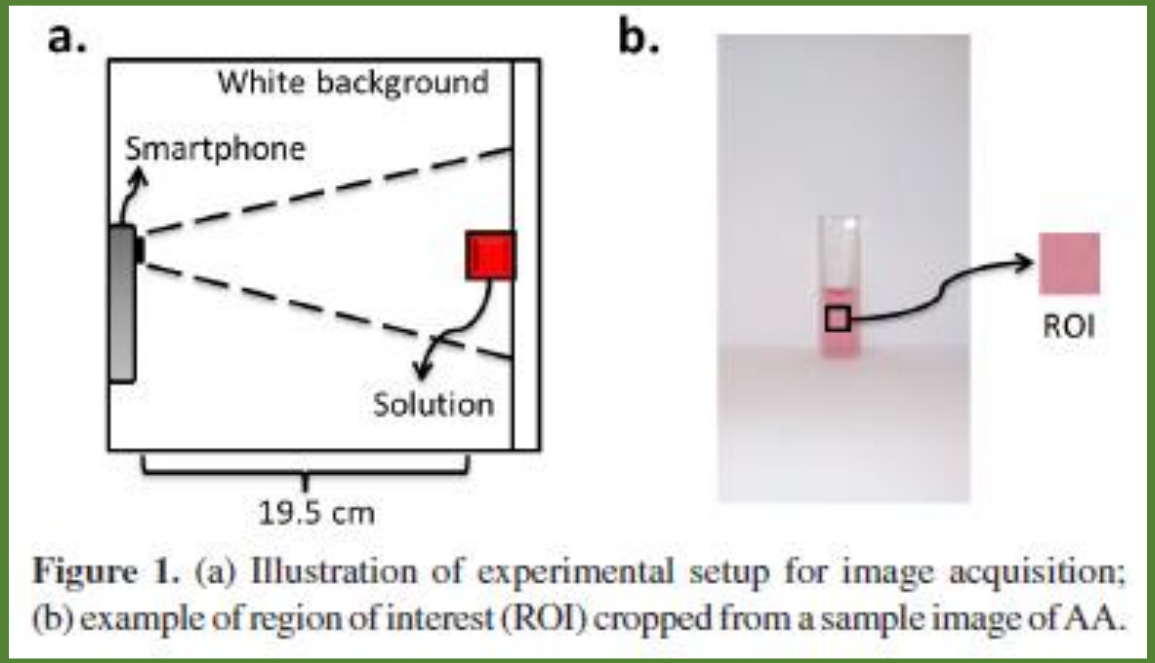
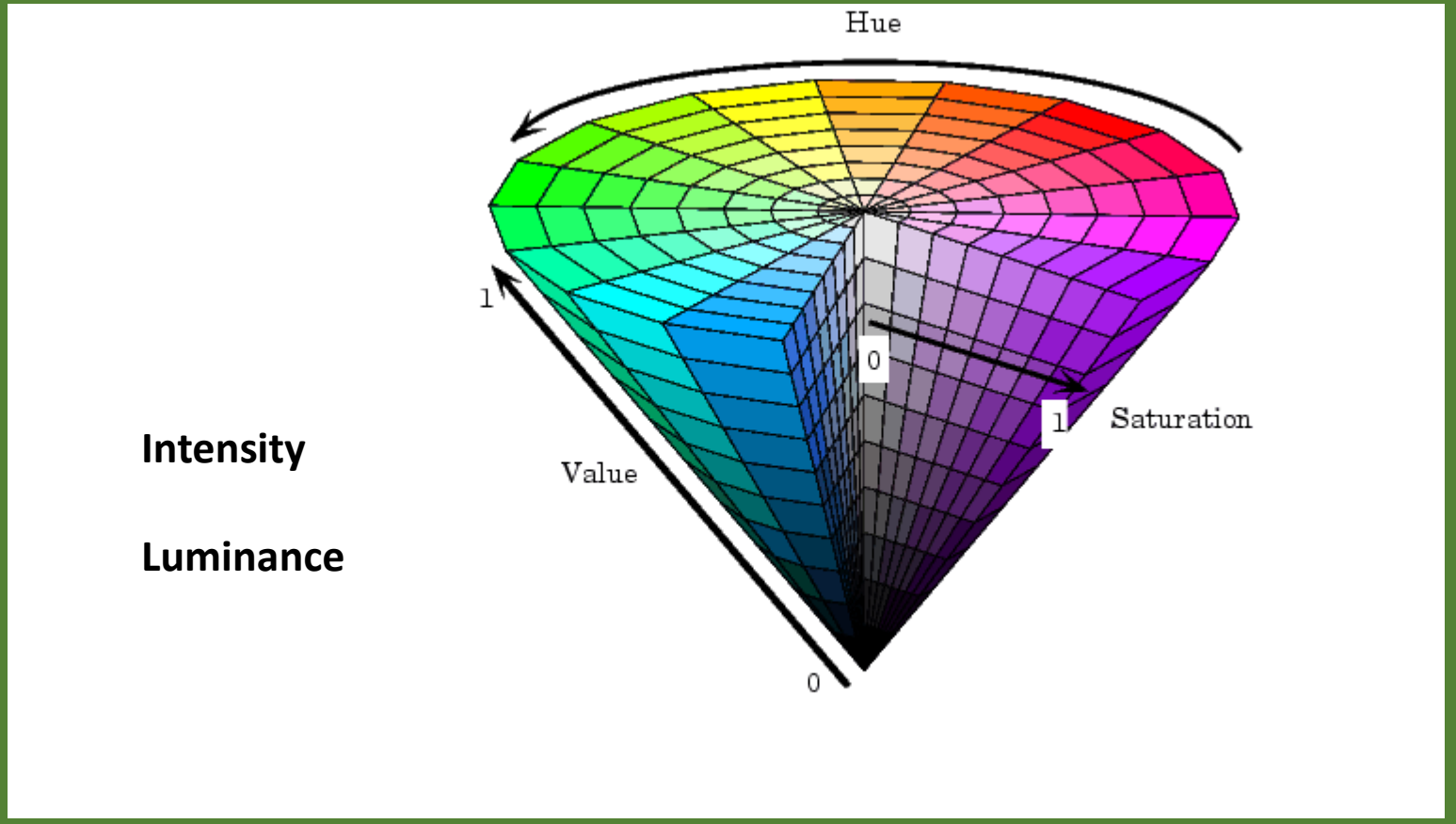


Figure 1. (a) Illustration of experimental setup for image acquisition; (b) example of region of interest (ROI) cropped from a sample image of AA.

Image Analysis (H S V) I and L



Intensity

Luminance

A Fast and Inexpensive Chemometric-Assisted Method to Identify Adulteration in Acai (Euterpe oleracea) Using Digital Images

Alisson Araújo & Weverton Marinho & Adriano de Araújo Gomes

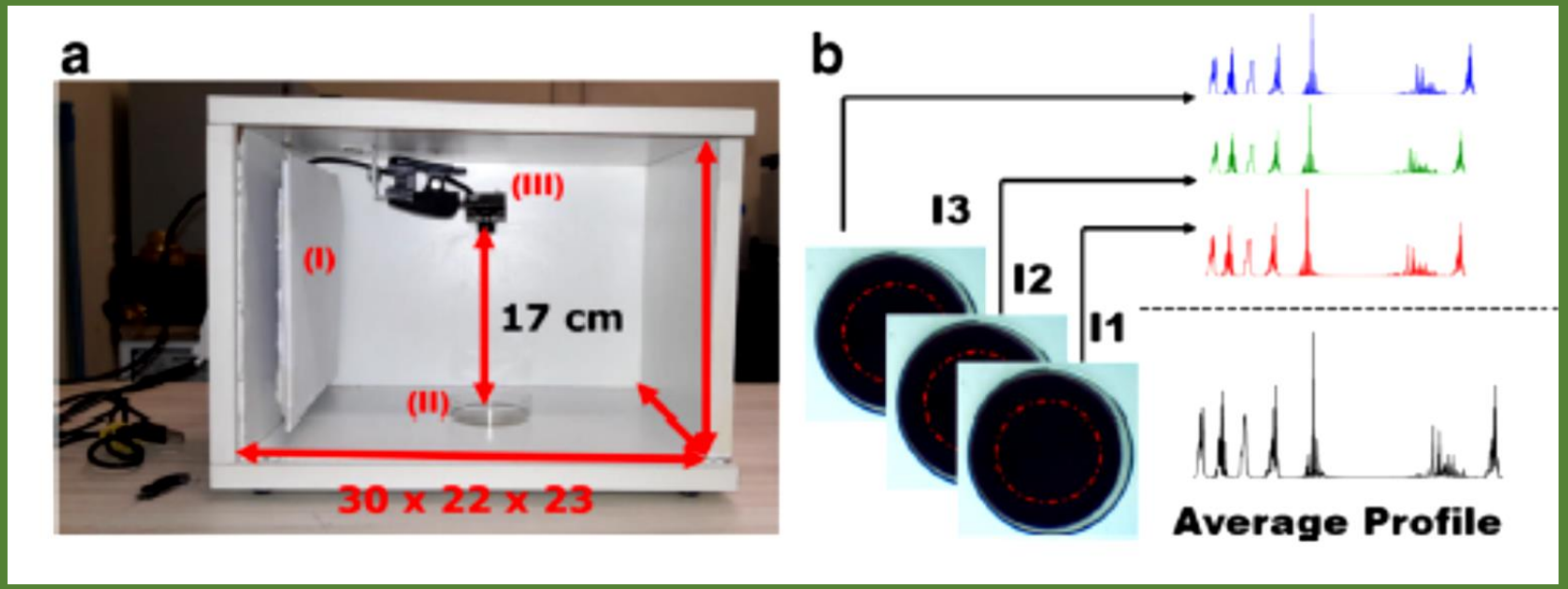
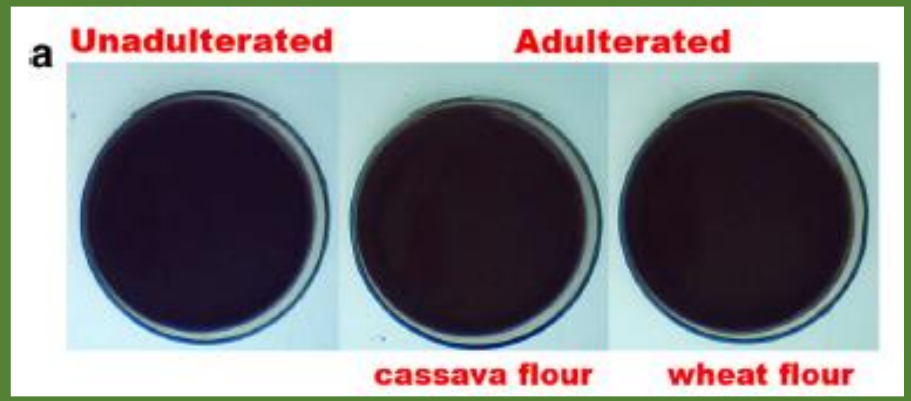


Fig. 1 **a** Digital imaging acquisition system. **b** Working region definition



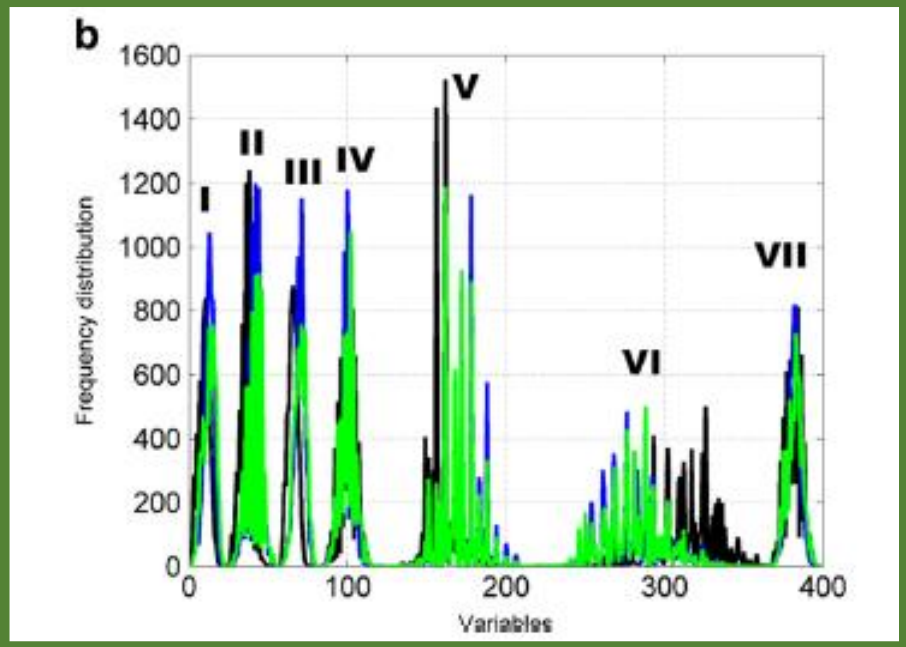
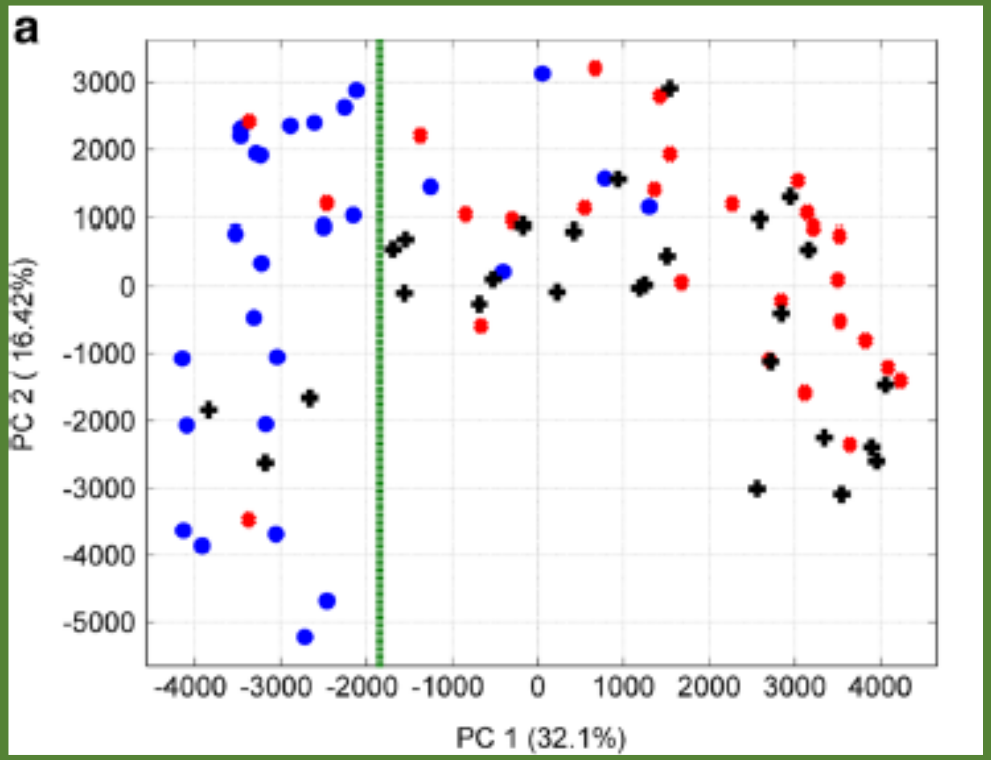


Fig. 2 Typical digital images (**a**) recorded for acai samples and average histogram profiles (**b**) for unadulterated samples (black line), samples adulterated with wheat (blue line), and samples adulterated with cassava (green line). Roman numerals indicate color channel (I: grayscale, II: red, III: green, IV: blue, V: hue, VI: saturation, and VII: intensity)



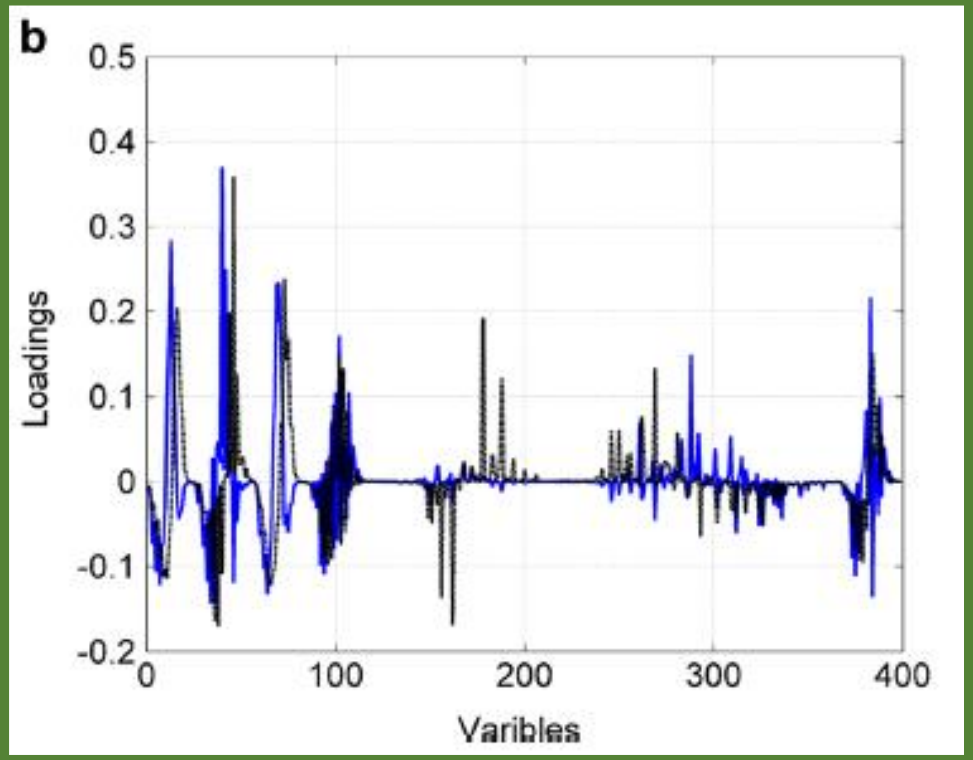
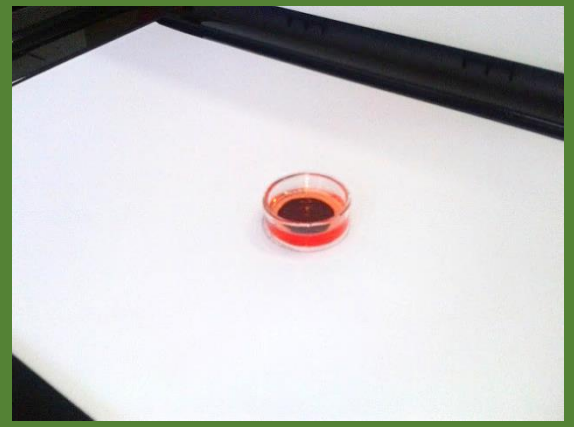
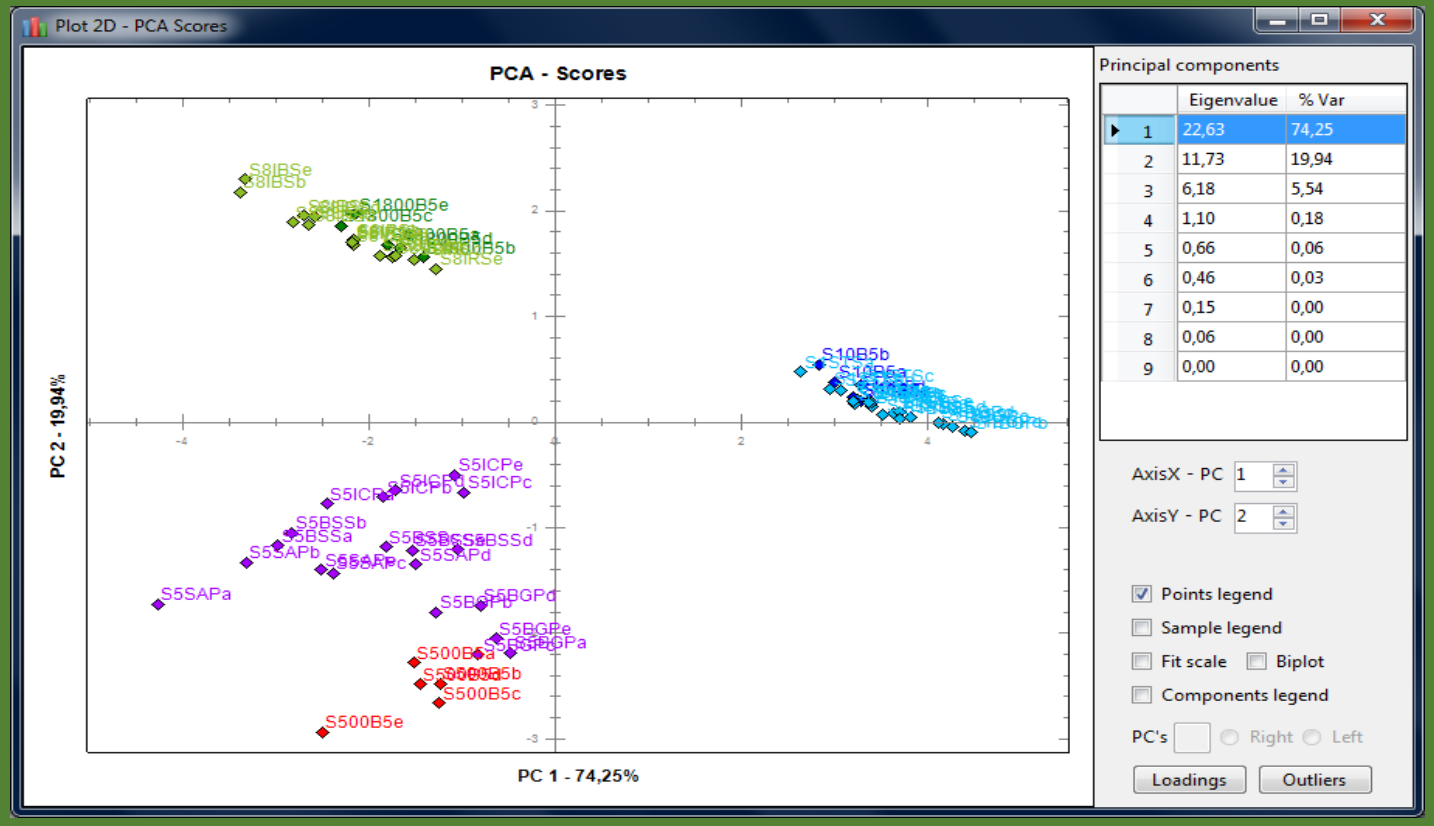


Fig. 3 PCA results. **a** Score plot, unadulterated samples (blue ball), samples adulterated with wheat (red ×), and samples adulterated with cassava (black cross). **b** Loading plot (PC1 blue solid line and PC2 black dotted line)

ChemoStat

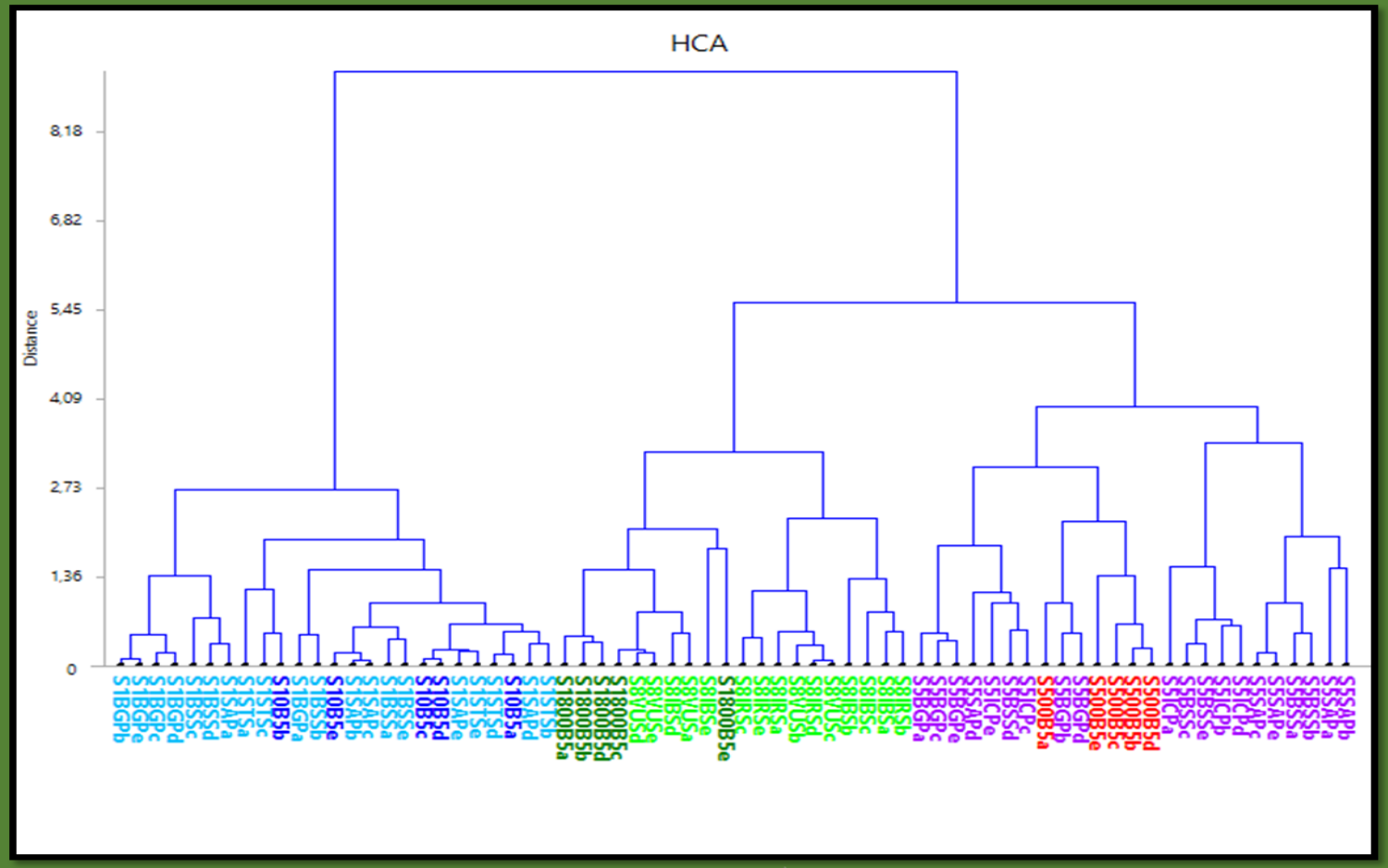


Diesel

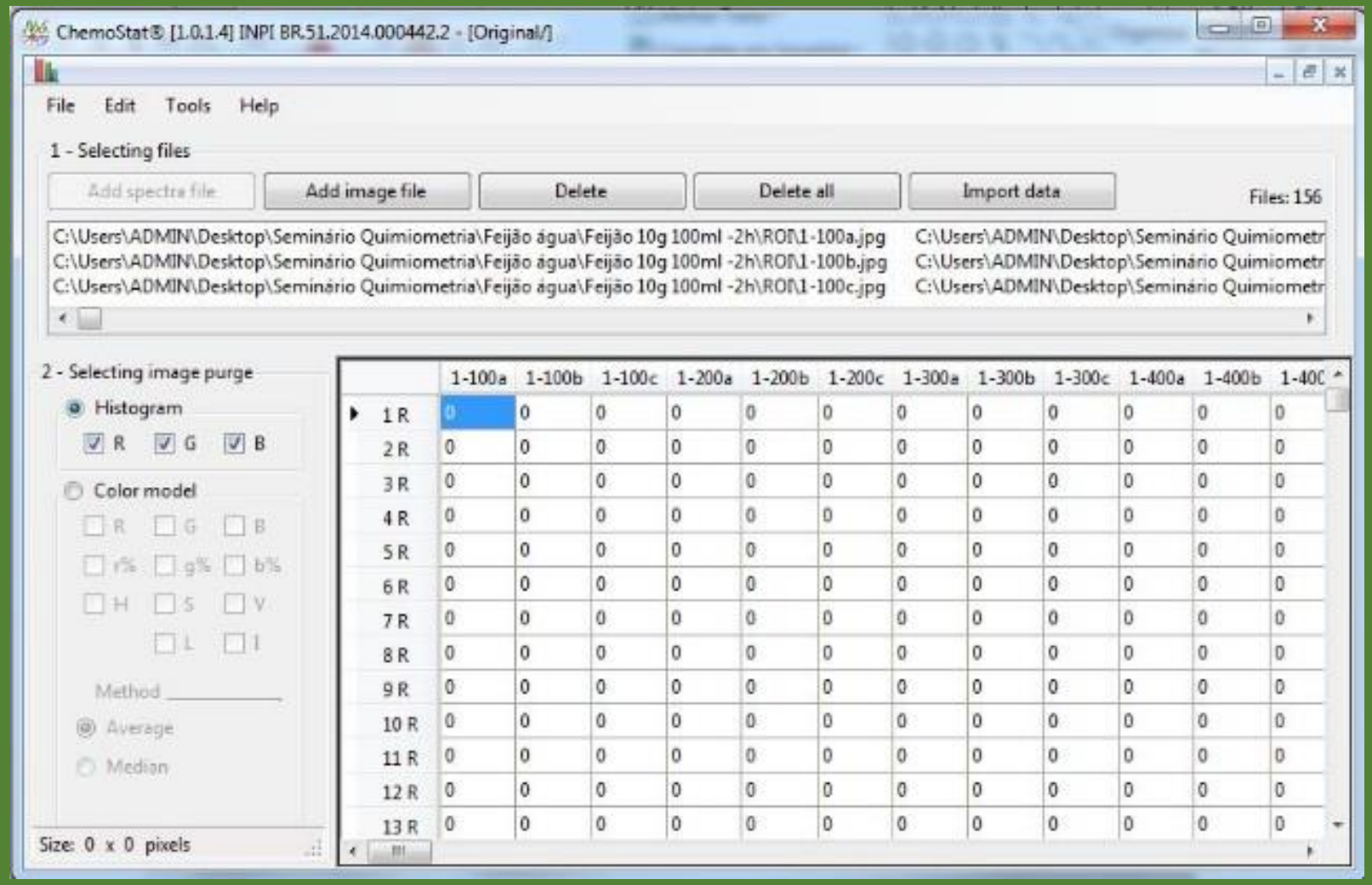


CHEMOSTAT: EXPLORATORY MULTIVARIATE DATA ANALYSIS SOFTWARE. Química Nova 2015

Image Analysis



ChemoStat ®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File
Edit
Tools
Help
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Add spectra file
Add image file
Delete
Delete all
Import data
Files: 156
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C:\Users\ADMIN\Desktop\Seminário Quimiometria\Feijão água\Feijão 10g 100ml -2h\ROI\1-100b.jpg
C:\Users\ADMIN\Desktop\Seminário Quimiometria\Feijão água\Feijão 10g 100ml -2h\ROI\1-100c.jpg
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Histogram
R
G
B
Color model
Method
Average
Median
Size: 0 x 0 pixels
1-100a
1-100b
1-100c
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1-200b
1-200c
1-300a
1-300b
1-300c
1-400a
1-400b
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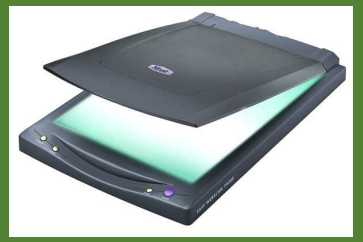
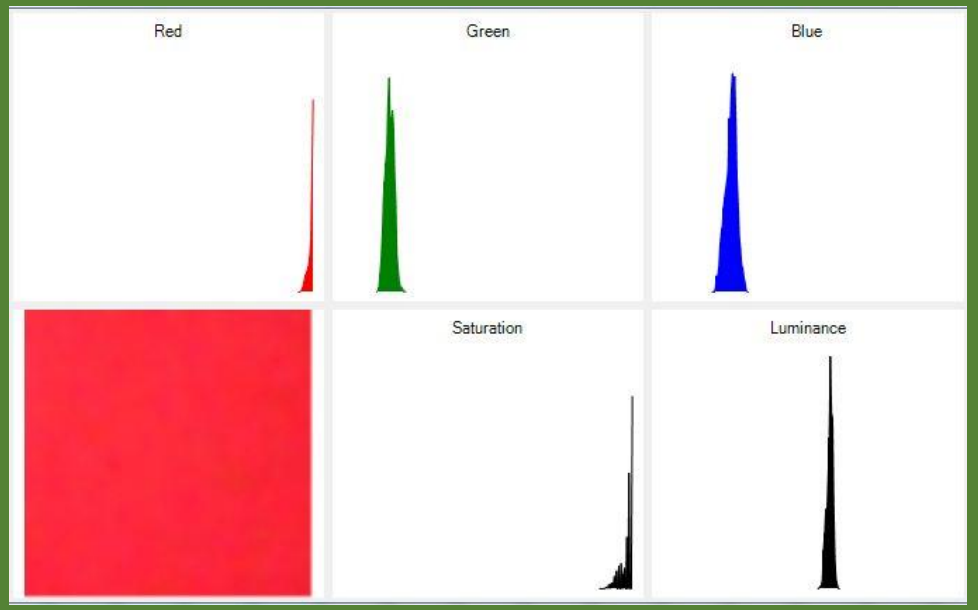
3 R
4 R
5 R
6 R
7 R
8 R
9 R
10 R
11 R
12 R
13 R

ChemoStat ®




SONY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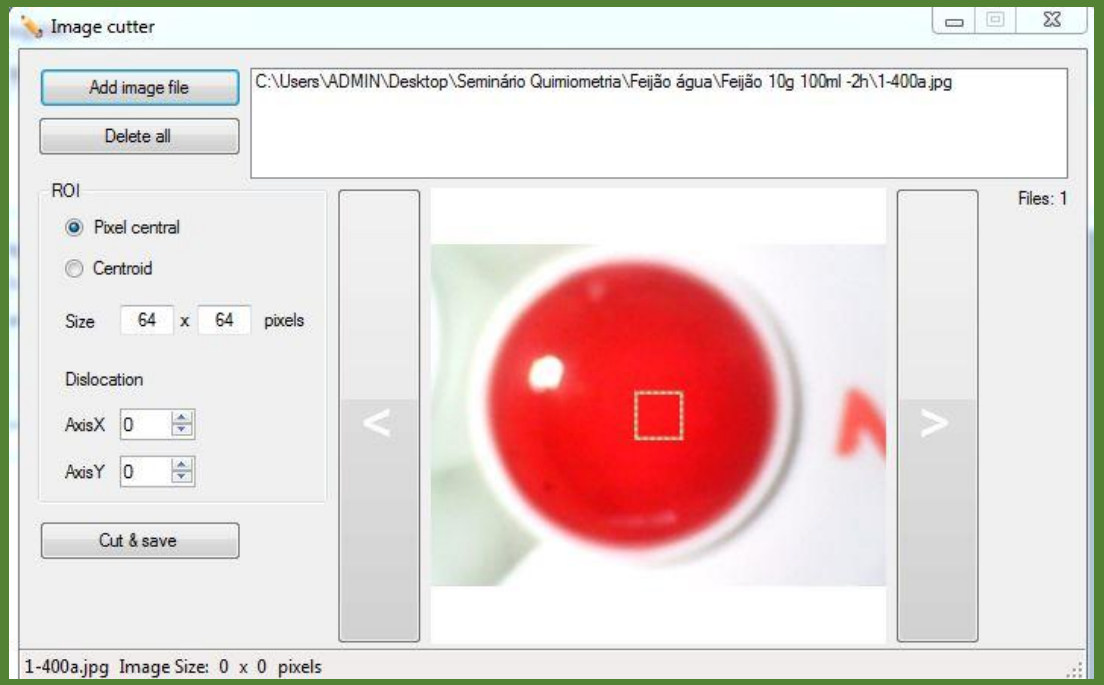
Green
Blue
Saturation
Luminance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Centroid
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Dislocation
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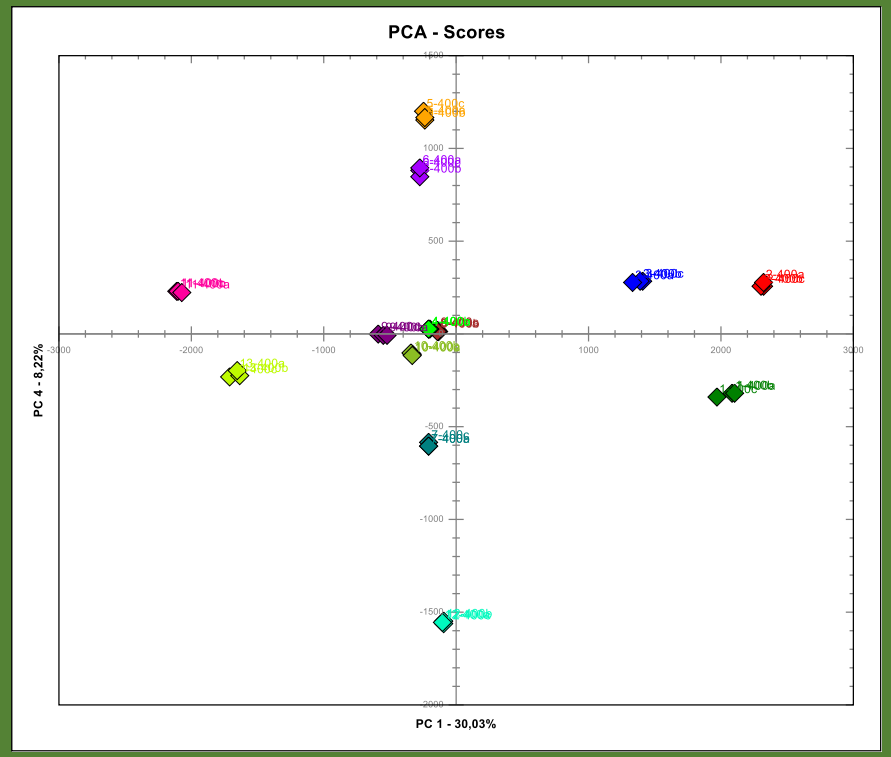
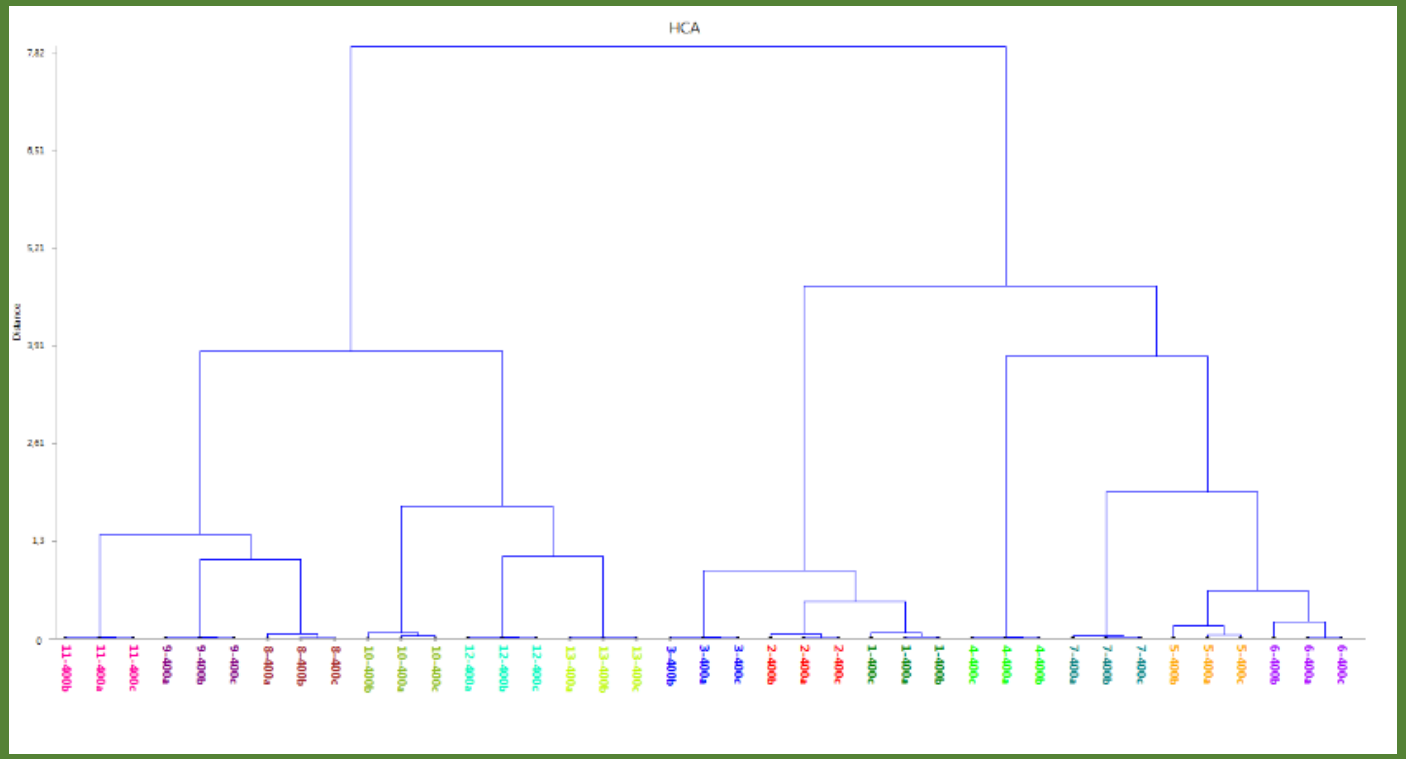
Image Analysis

ChemoStat ®

PCA





Dendrogram

RVq | Revista Virtual de Química

ISSN 1984-6835

Artigo

Uma Proposta Didática no Ensino de Análise Exploratória de Dados com Imagens de MDF (*Medium-Density Fiberboard*)

Böck, F. C.;* Assmann, D.; Helfer, G. A.; Costa, A. B.

Rev. Virtual Quim., **2015**, *7* (6), 2475-2486. Data de publicação na Web: 23 de setembro de 2015

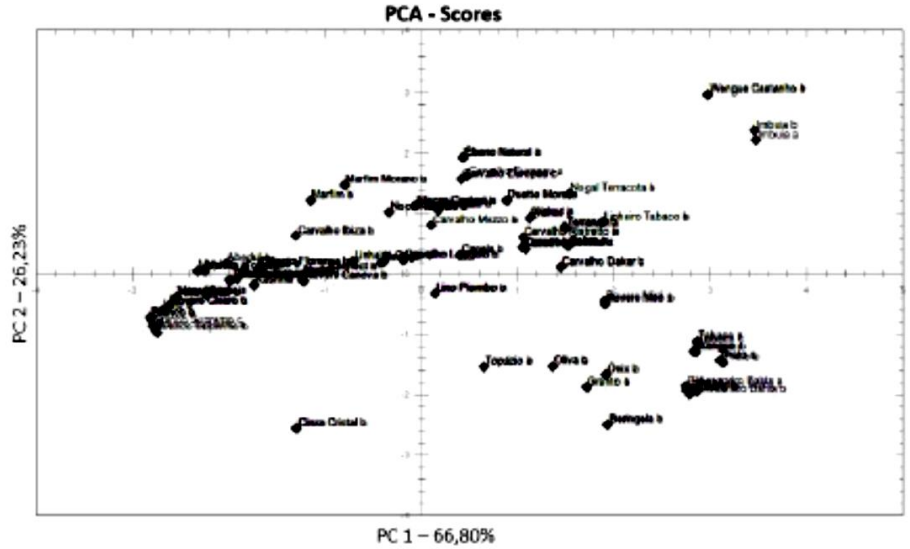


Figura 4. Gráfico de *scores* PC1 x PC2

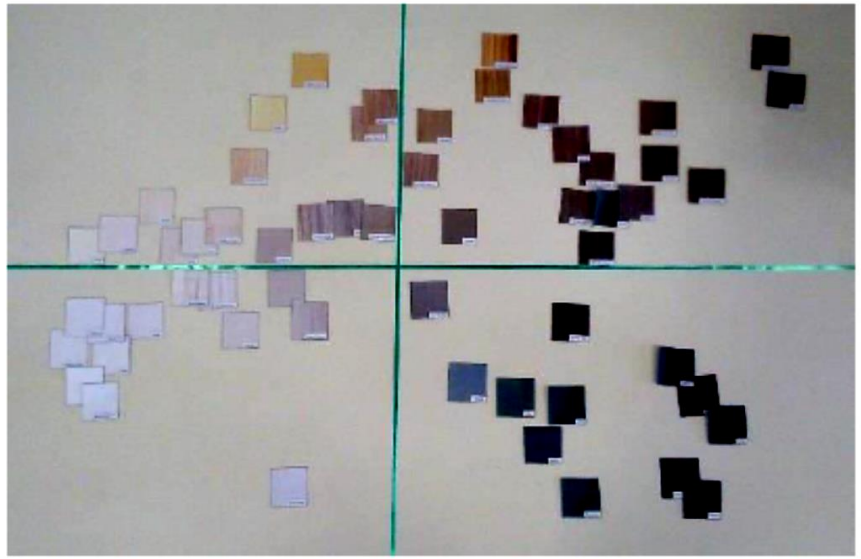
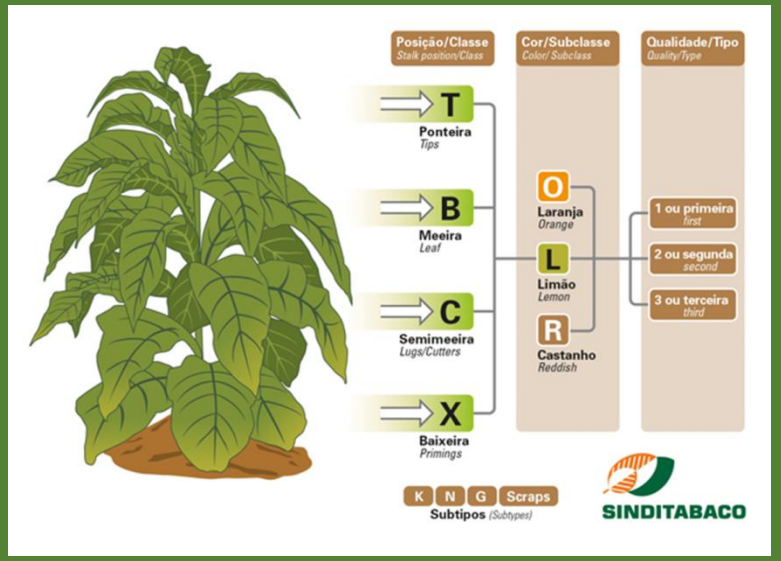


Figura 5. Representação com imagens do gráfico de *scores* da PC1 x PC2

Classificação de tabaco (*Nicotiana Tabacum*) no processo industrial por análise multivariada de imagens

Marcel R. Martins; Adriano C. Freitas; Gilson A. Helfer; Aline Teichmann, Julia F. Radtke, Adilson B. Costa



METODOLOGIA

SONY CYBER SHOT W830

CCD (*charge-coupled device*)

Distância: 1 m

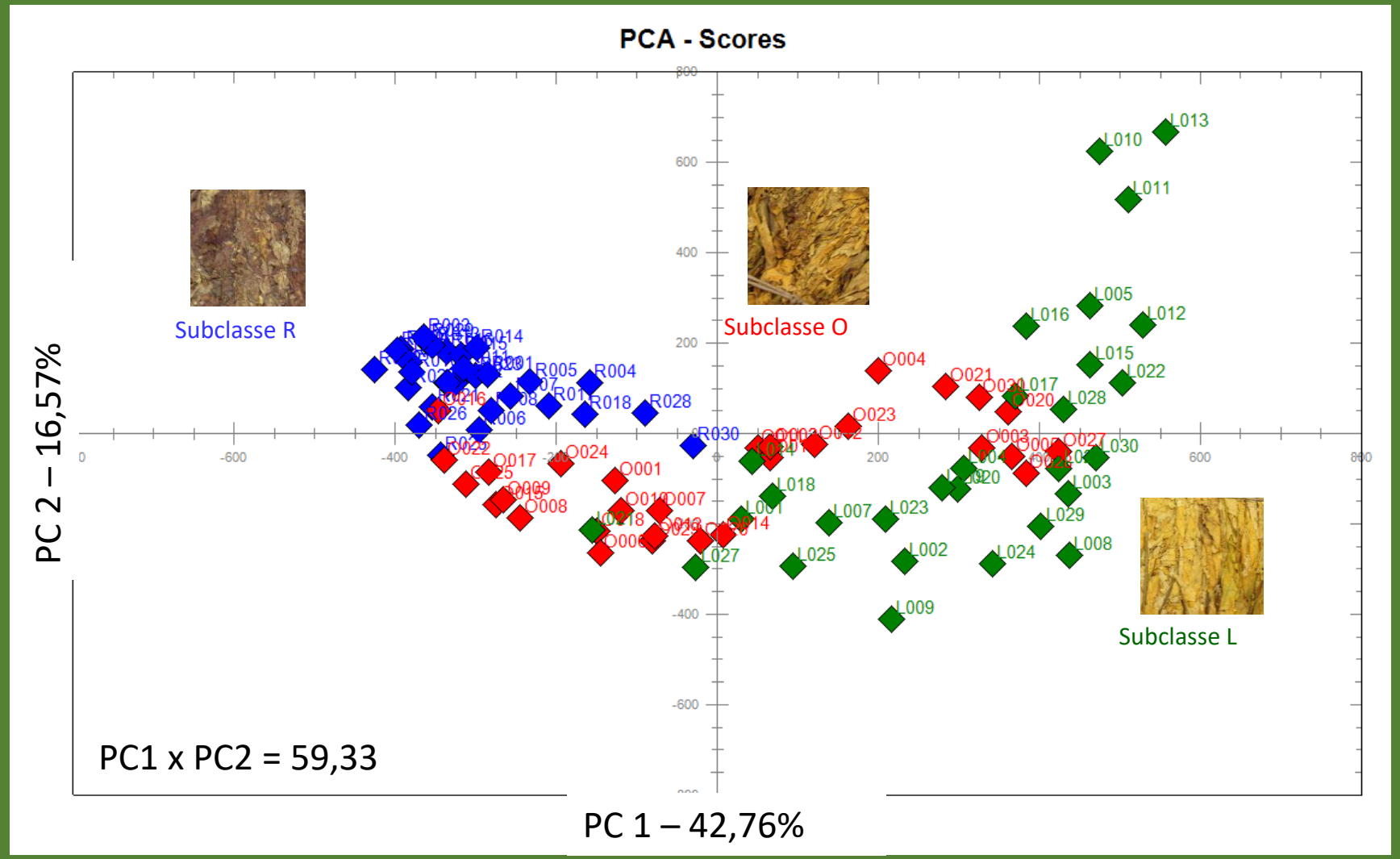
90 amostras de referência

Subclasse L	Subclasse O	Subclasse R
30	30	30

15 amostras para predição

Subclasse L	Subclasse O	Subclasse R
5	5	5

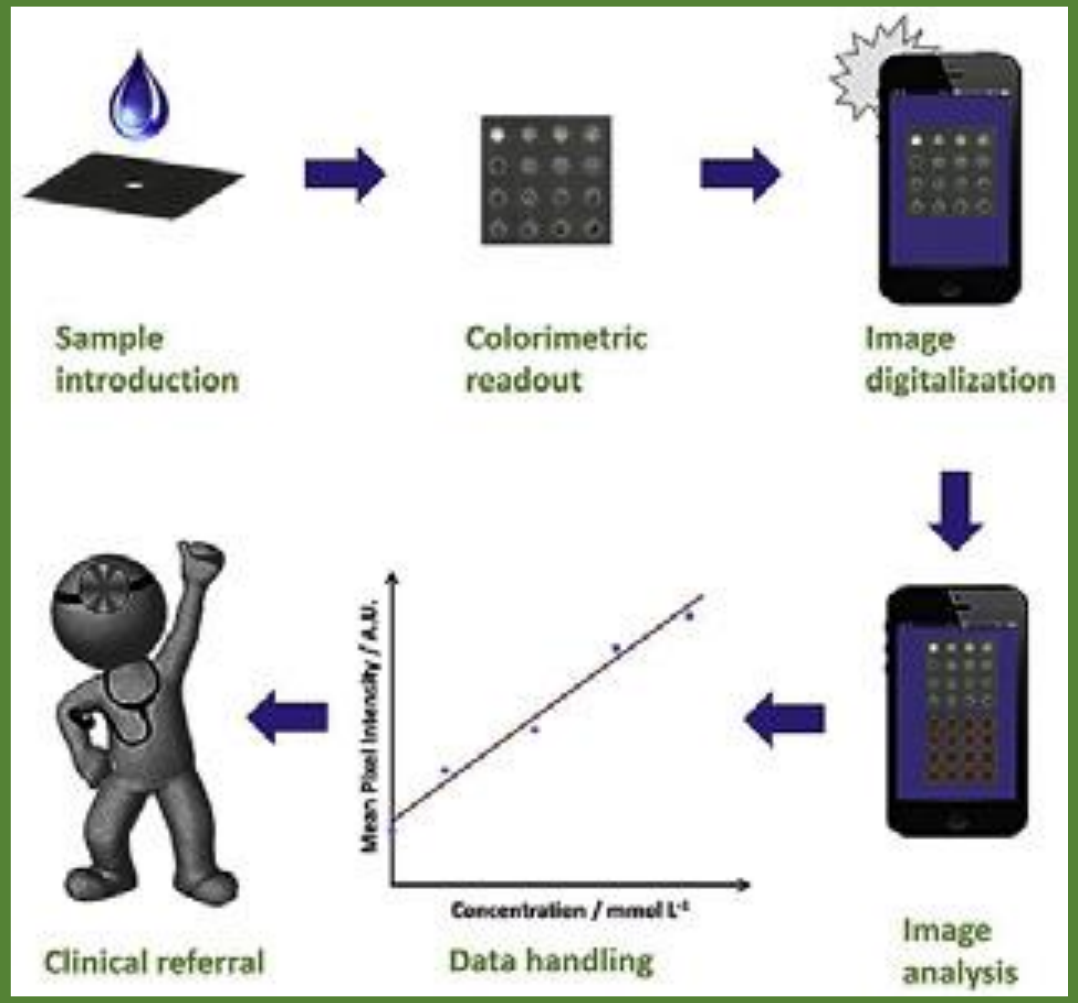
RESULTADOS


PCA - Scores
Subclasse R
Subclasse O
Subclasse L
PC 2 – 16,57%
PC 1 – 42,76%
PC1 x PC2 = 59,33

Technical aspects and challenges of colorimetric detection with microfluidic paper-based analytical devices (mPADs) - A REVIEW

G. G. Morbioli, T. Mazzu-Nascimento, A. M. Stockton, E. Carrilho

Analytica Chimica Acta 970 (2017) 1-22



A SPOT TEST FOR IODINE VALUE DETERMINATION IN BIODIESEL BASED ON DIGITAL IMAGES EXPLOITING A SMARTPHONE

Samara Soares, Manoel J.A. Lima, Fábio R.P. Rocha

Microchemical Journal 133 (2017) 195–199

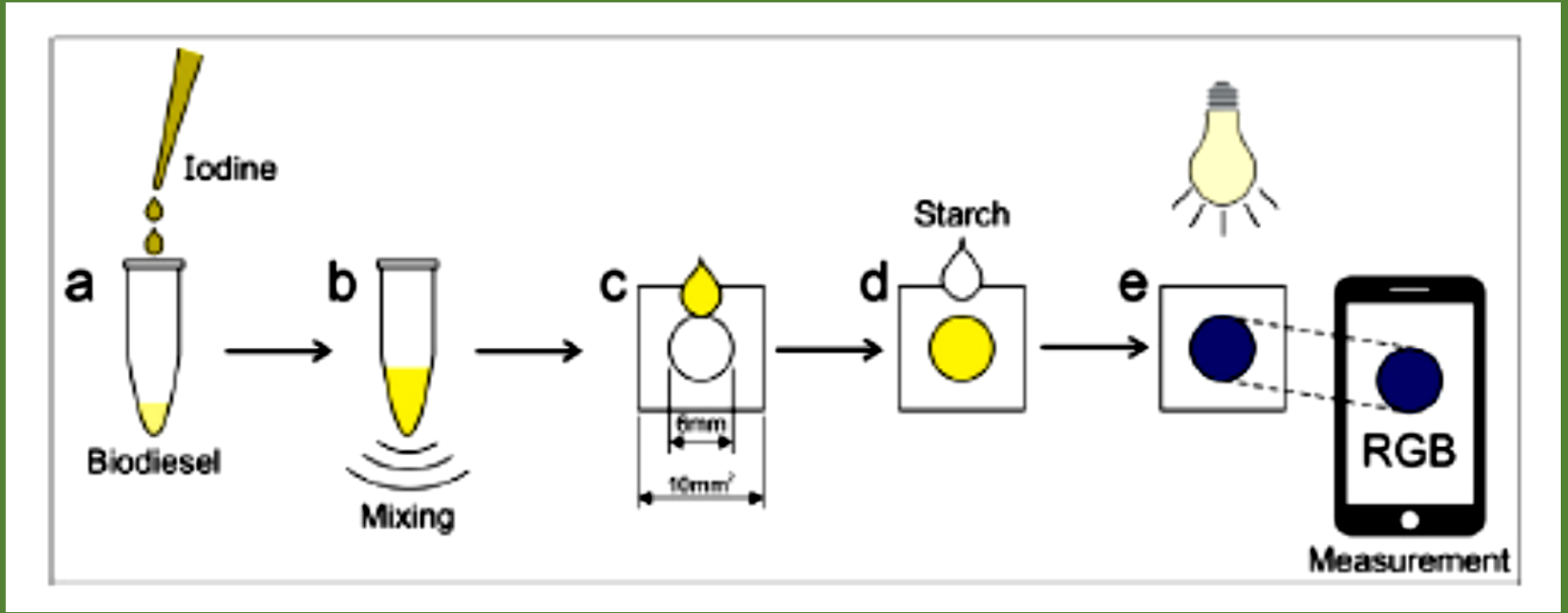
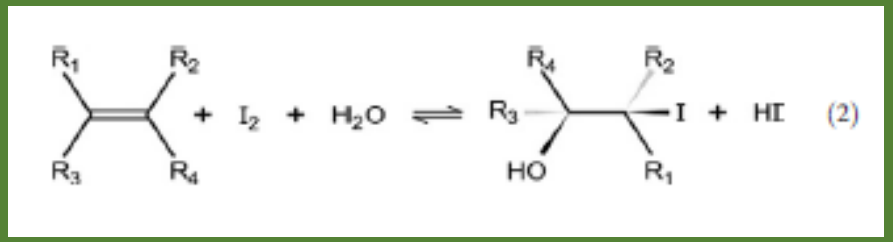


Fig. 1. Schematic diagram of the colorimetric spot test. (a) Reaction of biodiesel with iodine; (b) Mixing and subsequent reaction time; (c) Transfer of 5 μL of the mixture to the paper; (d) Addition of 5 μL of starch (1% m/v) and (e) acquisition of the RGB value by employing the software PhotoMetrix® 1.11.



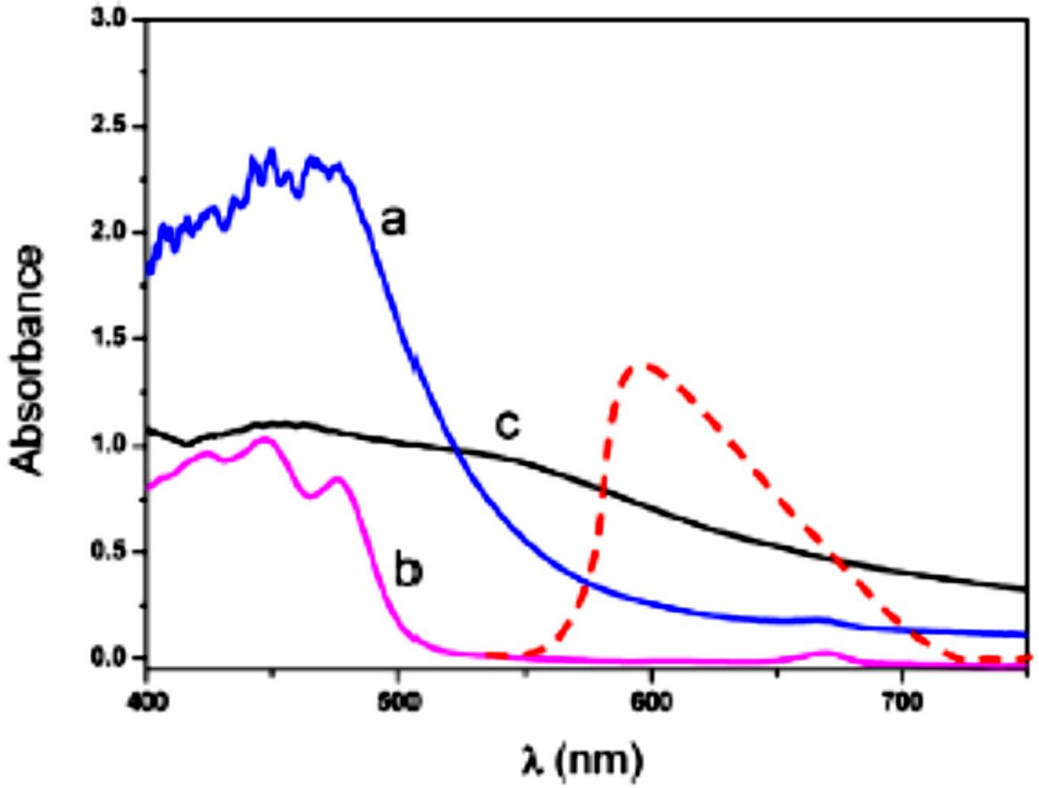


Fig. 2. Absorption spectra of a biodiesel-hexane 1:1 (v/v) mixture with (a) and without (b) 8 mmol L^{-1} iodine; (*c*) biodiesel-hexane 1:1 (v/v) mixture + 8 mmol L^{-1} iodine + starch (measurement in the aqueous phase). Dashed lines correspond to the spectral region covered by the red channel of the CMOS sensor.

Table 1
Iodine values in biodiesel (mean ± standard deviation, n = 3) determined by the proposed and reference procedures. Values between parenthesis refer to volumetric proportions of the raw material.

Sample	Iodine value (g I_2/100 g of biodiesel)	
	Proposed procedure	Reference procedure [13]
Soybean oil (100)	110 ± 7	106 ± 2
Soybean oil/animal fat (90/10)	113 ± 5	98 ± 6
Soybean oil/animal fat (90/10)	103 ± 3	106 ± 2
Soybean oil/animal fat (90/10)	116 ± 6	106 ± 1
Soybean oil/cottonseed oil (90/10)	95 ± 8	104 ± 1
Soybean oil/animal fat (70/30)	99 ± 5	101 ± 2

PORTABLE AND LOW-COST COLORIMETRIC OFFICE PAPER-BASED DEVICE FOR PHENACETIN DETECTION IN SEIZED COCAINE SAMPLES

Gabriela O. da Silva, William R. de Araujo, Thiago R.L.C. Paixão

Talanta 176 (2018) 674–678

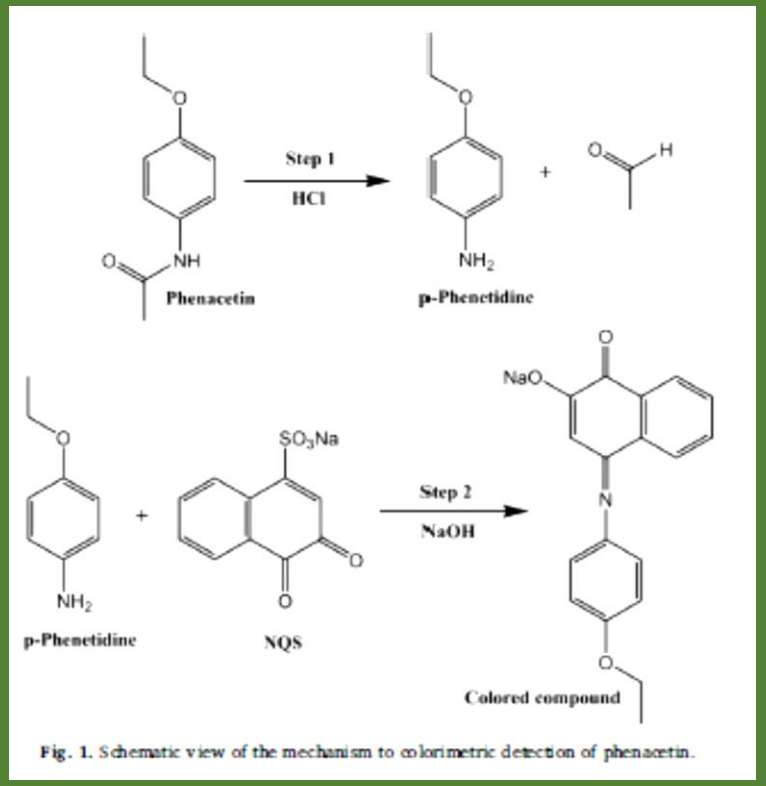


Fig. 1. Schematic view of the mechanism to colorimetric detection of phenacetin.

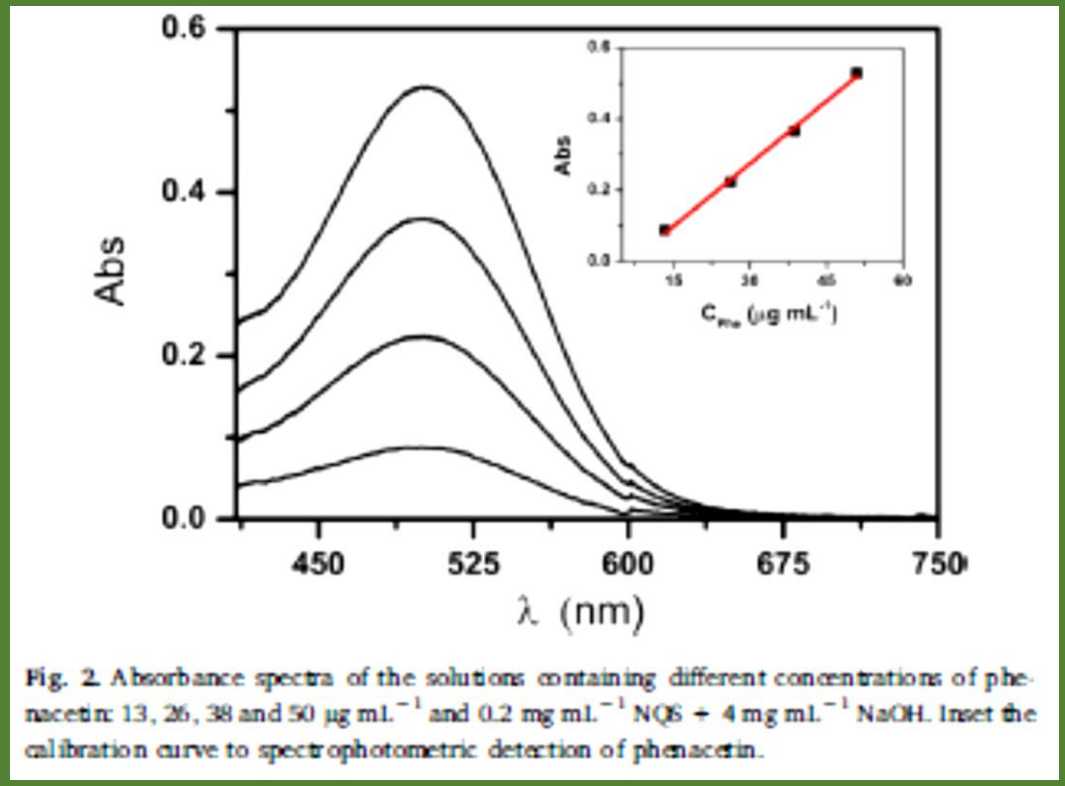
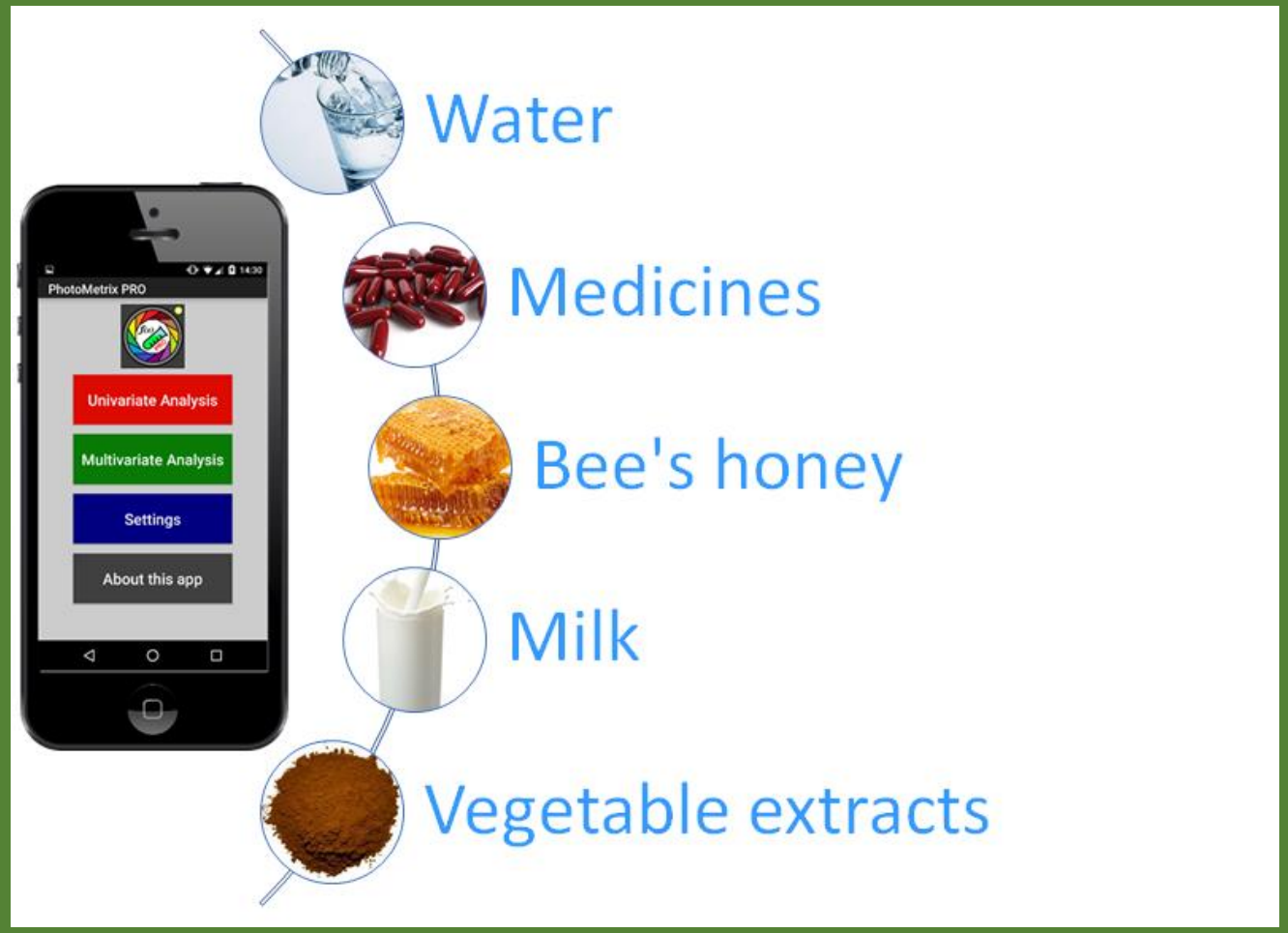


Fig. 2. Absorbance spectra of the solutions containing different concentrations of phenacetin: 13, 26, 38 and 50 μg mL^{-1} and 0.2 mg mL^{-1} NQS + 4 mg mL^{-1} NaOH. Inset the calibration curve to spectrophotometric detection of phenacetin.

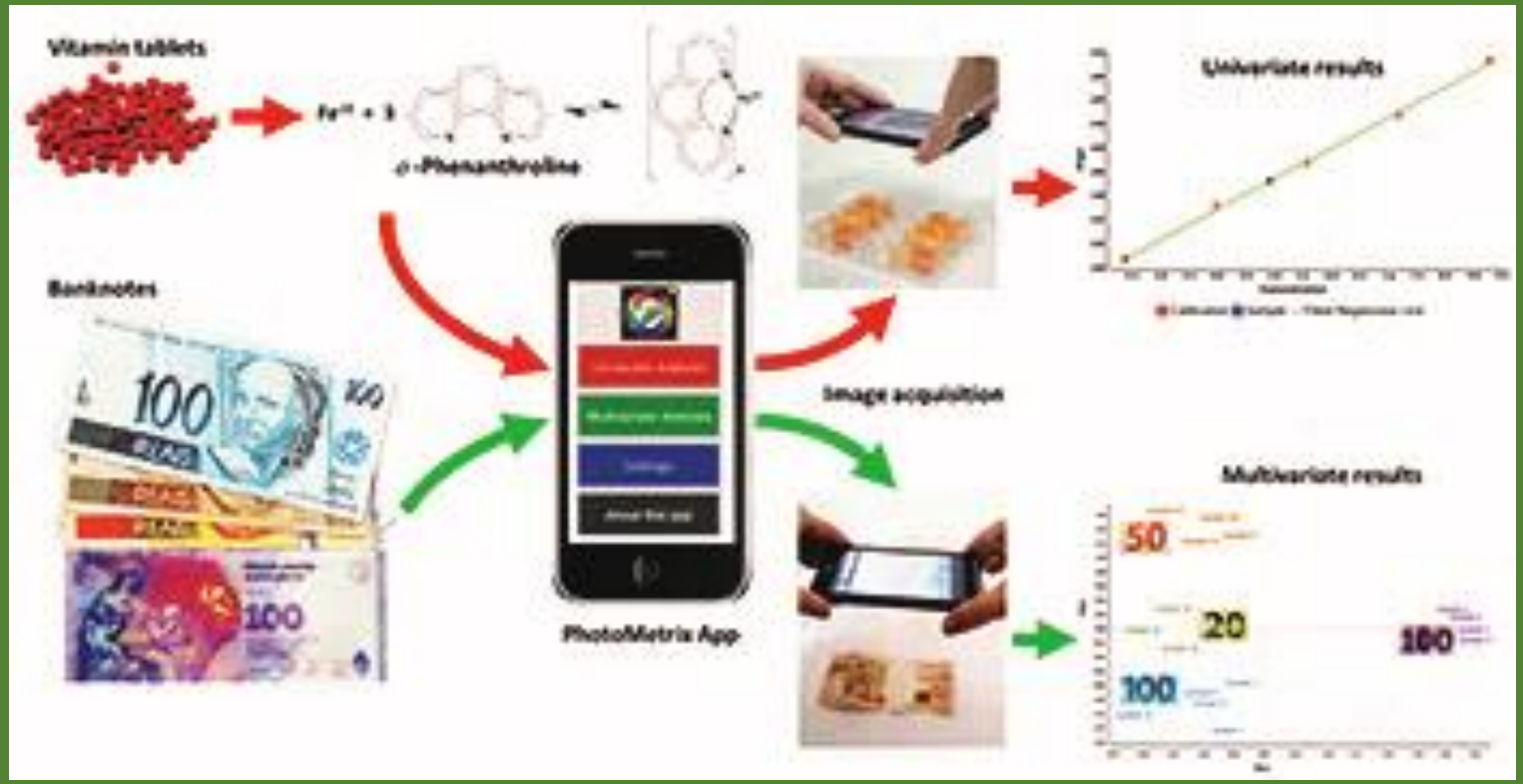
PhotoMetrix : A Mobile Application for Analytical Chemistry



PhotoMetrix

http://dx.doi.org/10.5935/0103-5053.20160182

J. Braz. Chem. Soc., Vol. 28, No. 2, 328-335, 2017.
Printed in Brazil - ©2017 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00



PhotoMetrix

http://dx.doi.org/10.5935/0103-5053.20160182

J. Braz. Chem. Soc., Vol. 28, No. 2, 328-335, 2017.
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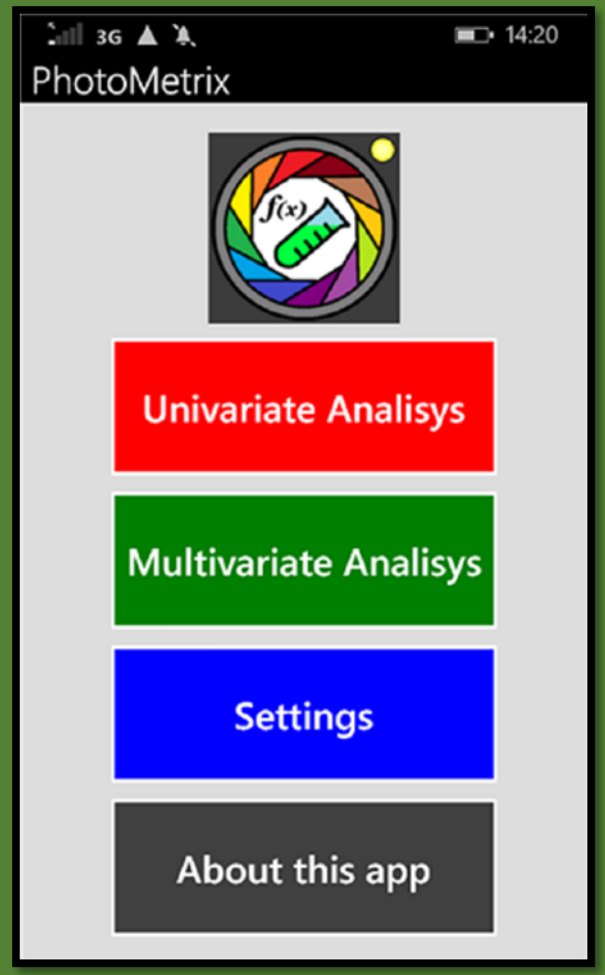
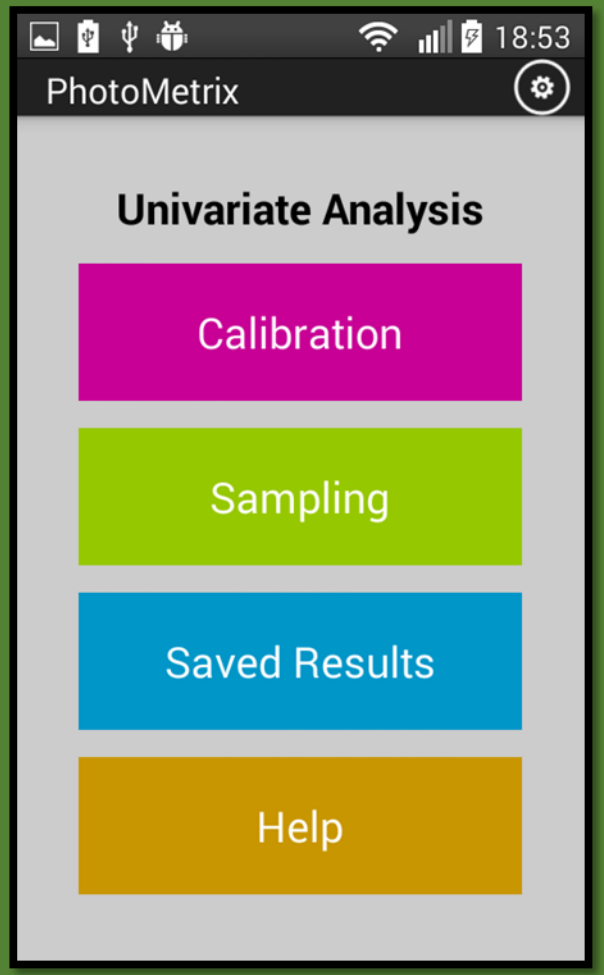
0103 - 5053 $6.00+0.00





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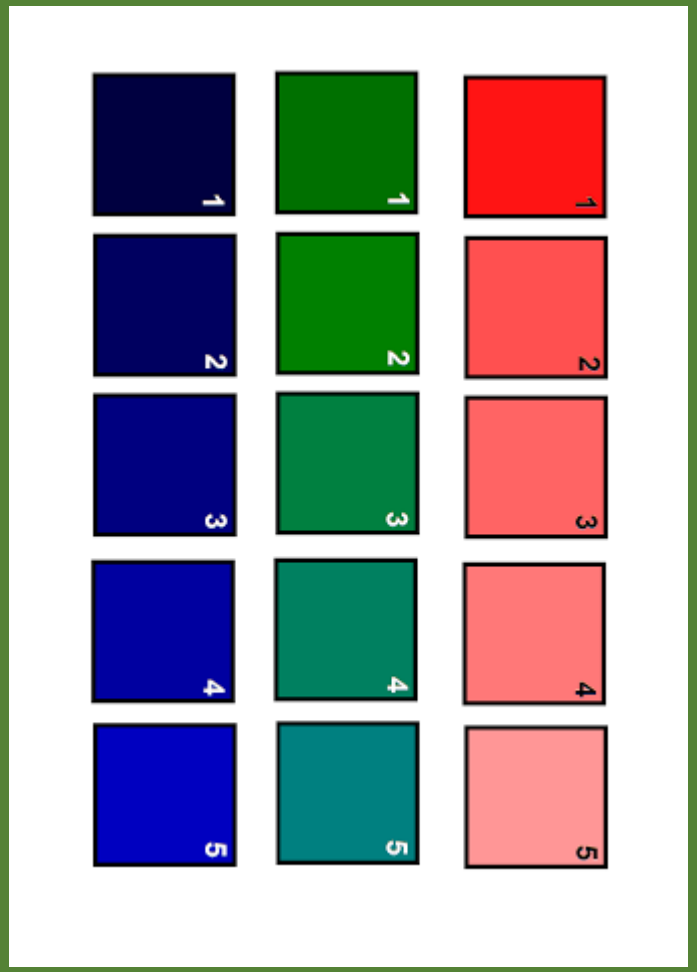
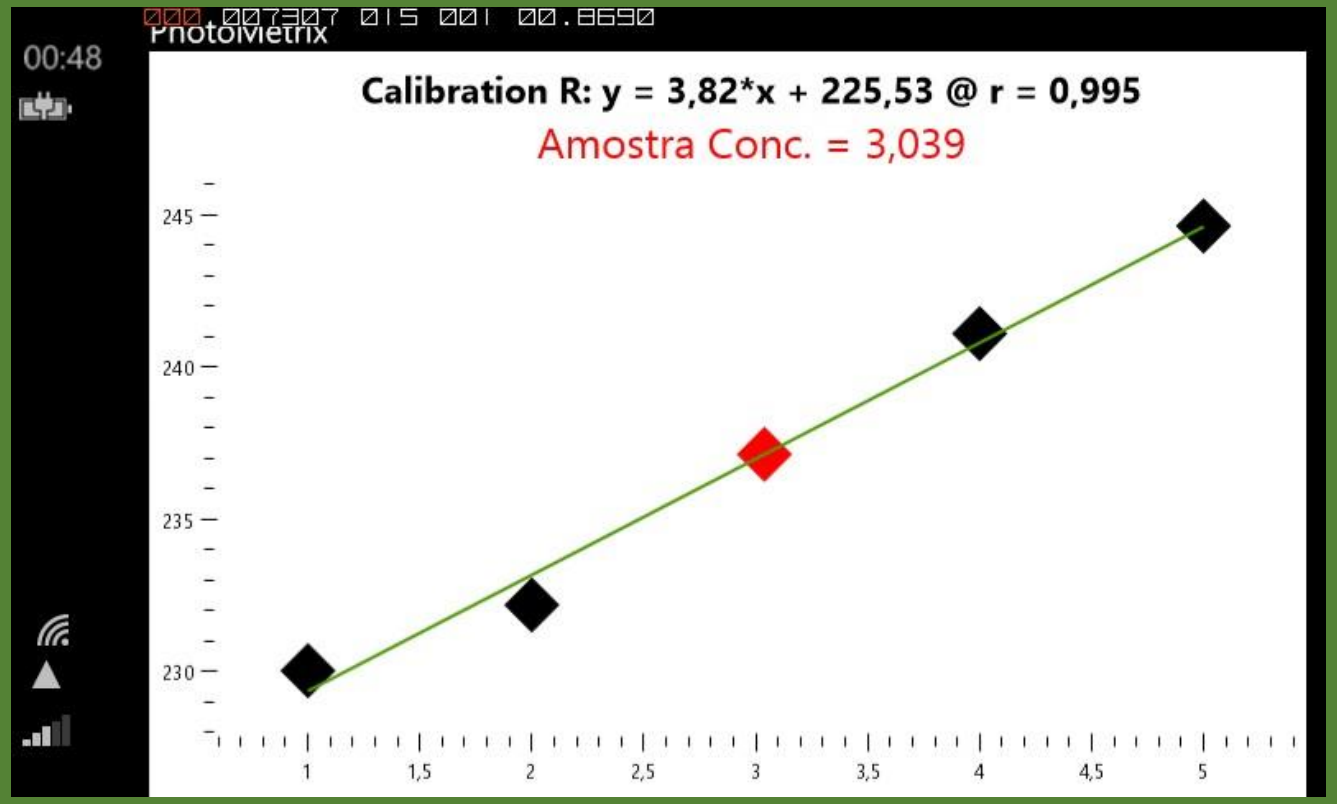
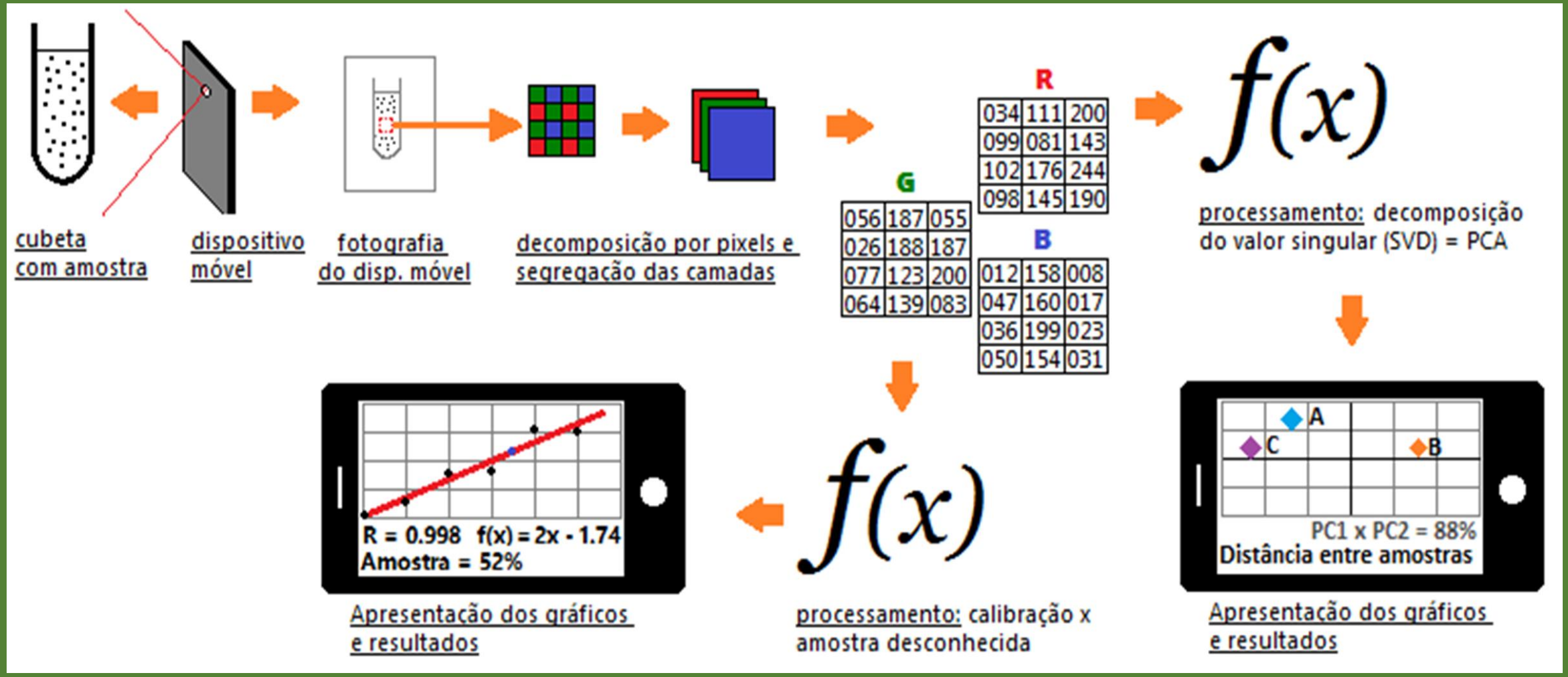


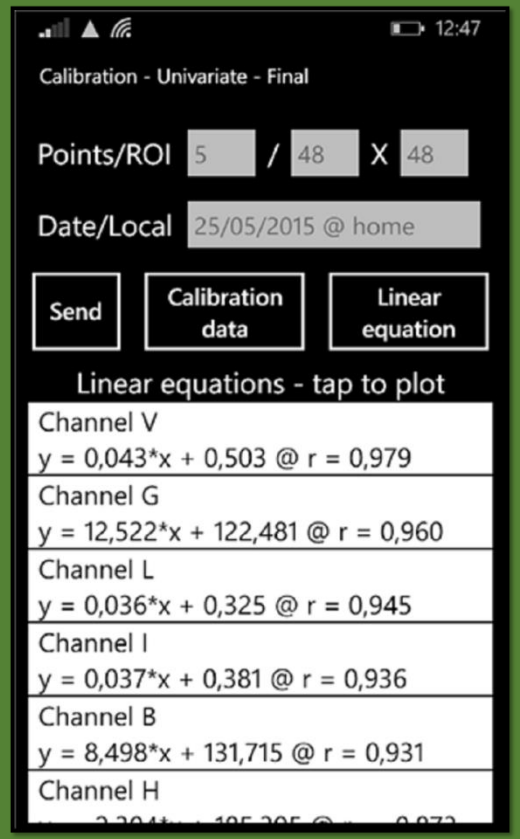


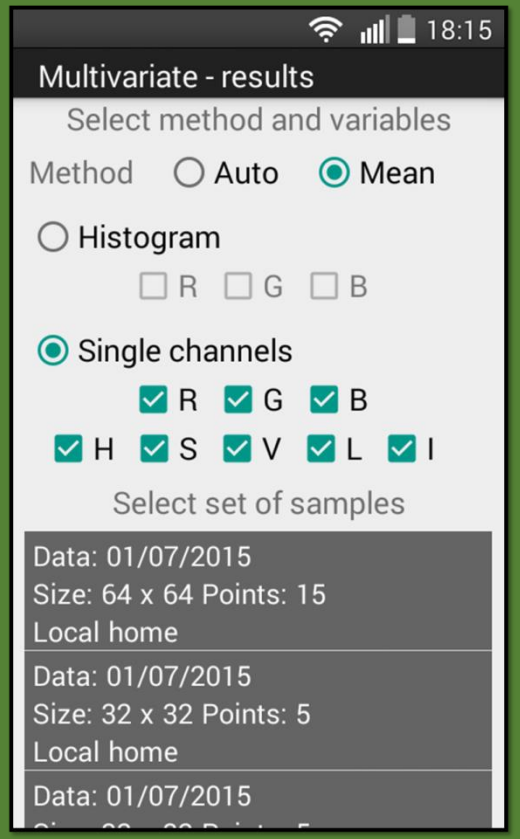
PHOTOMETRIX: Aplicativo Android em constante desenvolvimento

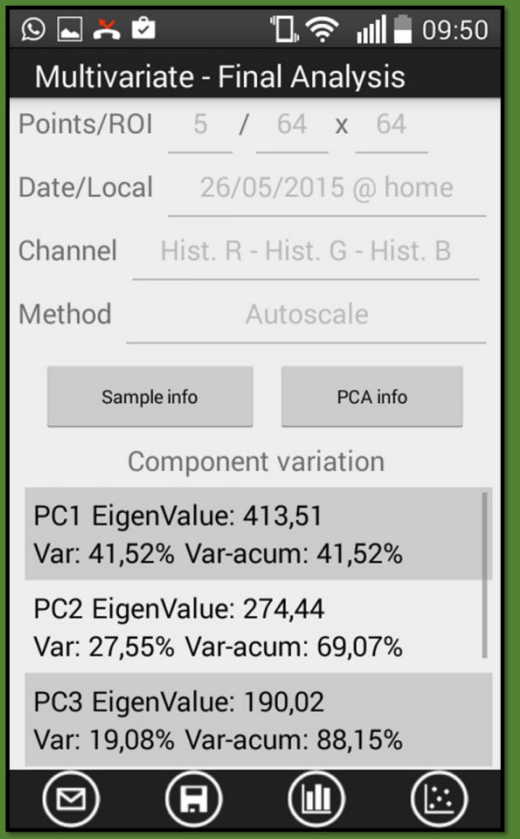
PhotoMetrix

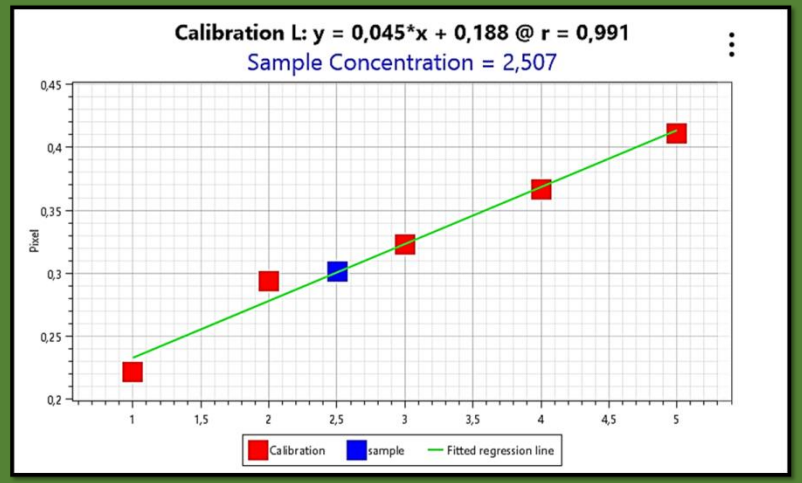


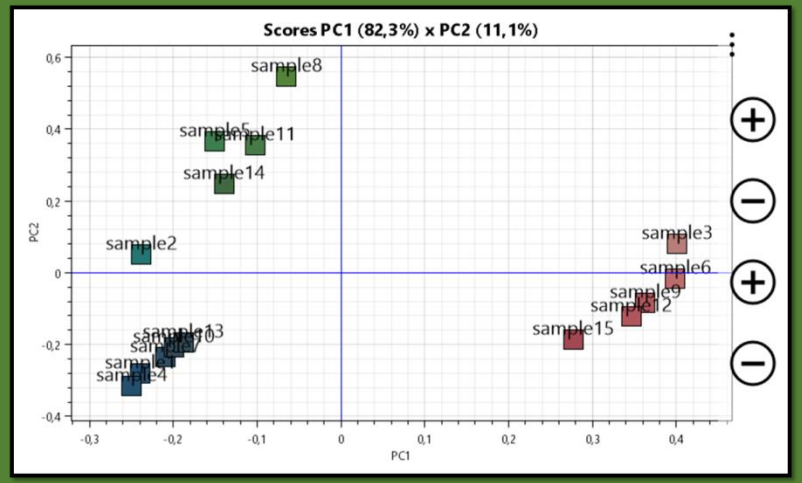

f(x)


12:47
Calibration - Univariate - Final
Points/ROI 5 / 48 X 48
Date/Local 25/05/2015 @ home
Send
Calibration data
Linear equation
Linear equations - tap to plot
Channel V
y = 0,043*x + 0,503 @ r = 0,979
Channel G
y = 12,522*x + 122,481 @ r = 0,960
Channel L
y = 0,036*x + 0,325 @ r = 0,945
Channel I
y = 0,037*x + 0,381 @ r = 0,936
Channel B
y = 8,498*x + 131,715 @ r = 0,931
Channel H


18:15
Multivariate - results
Select method and variables
Method Auto Mean
Histogram
R G B
Single channels
R G B
H S V L I
Select set of samples
Data: 01/07/2015
Size: 64 x 64 Points: 15
Local home
Data: 01/07/2015
Size: 32 x 32 Points: 5
Local home
Data: 01/07/2015


09:50
Multivariate - Final Analysis
Points/ROI 5 / 64 x 64
Date/Local 26/05/2015 @ home
Channel Hist. R - Hist. G - Hist. B
Method Autoscale
Sample info
PCA info
Component variation
PC1 EigenValue: 413,51
Var: 41,52% Var-acum: 41,52%
PC2 EigenValue: 274,44
Var: 27,55% Var-acum: 69,07%
PC3 EigenValue: 190,02
Var: 19,08% Var-acum: 88,15%


Calibration L: y = 0,045*x + 0,188 @ r = 0,991
Sample Concentration = 2,507
Pixel
Calibration
sample
Fitted regression line


Scores PC1 (82,3%) x PC2 (11,1%)
PC1
PC2
sample8
sample5
sample11
sample14
sample2
sample3
sample6
sample15

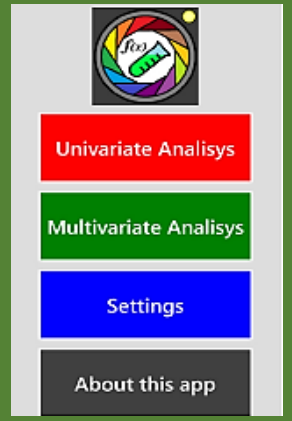
ESTRATÉGIAS DIDÁTICAS PARA A ANÁLISE POR COMPONENTES PRINCIPAIS EMPREGANDO DISPOSITIVOS MÓVEIS VIA PHOTOMETRIX

Layane Lenardon, Camila Correa, Carla Ruschel, Gilson A. Helfer, Adilson B. Costa, Marco Flôres Ferrão, Ana Maria Bergold

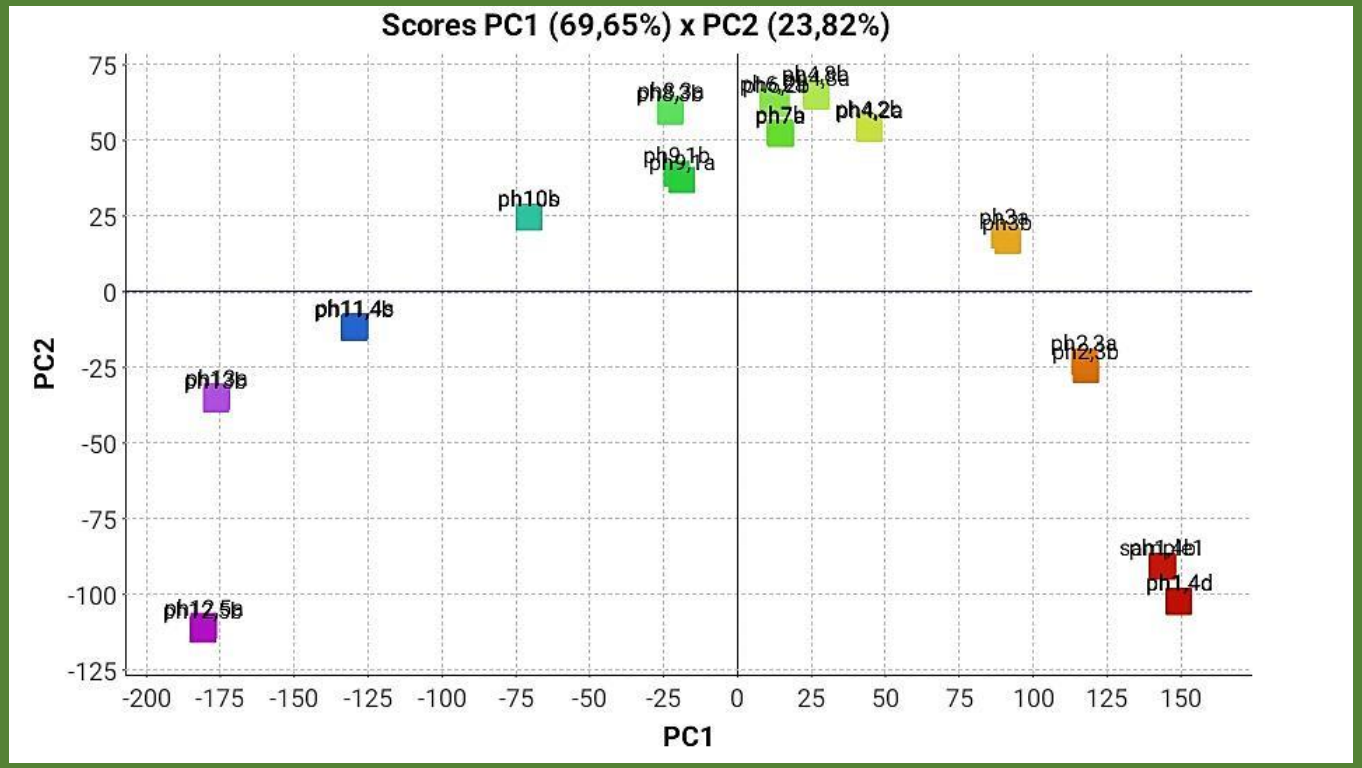
App Photometrix

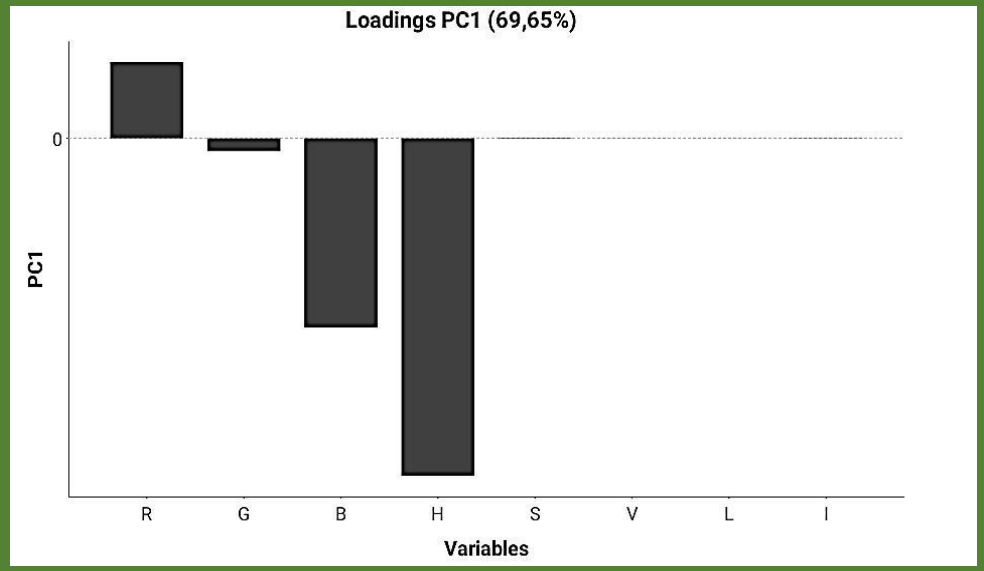
Dispositivo

Móvel (celular)



cuqa 4
4to Congreso Uruguayo de Química Analítica
Montevideo-Uruguay 25 al 28 de setiembre 2016





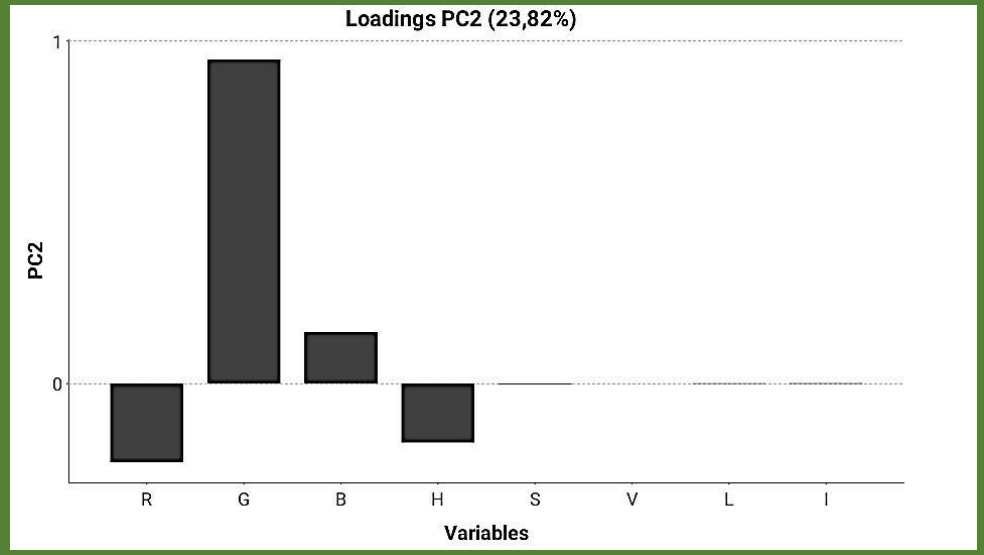


Figura 1: Gráfico da PC1xPC2 das amostras com diferentes escalas de pH.

MONITORING ACID-BASE TITRATIONS ON WAX PRINTED PAPER MICROZONES USING A SMARTPHONE

Sandro A. Nogueira , Lucas R. Sousa , Nathália K. L. Silva ,
Pedro H. F. Rodrigues and Wendell K. T. Coltro

Micromachines **2017**, *8*(5), 139

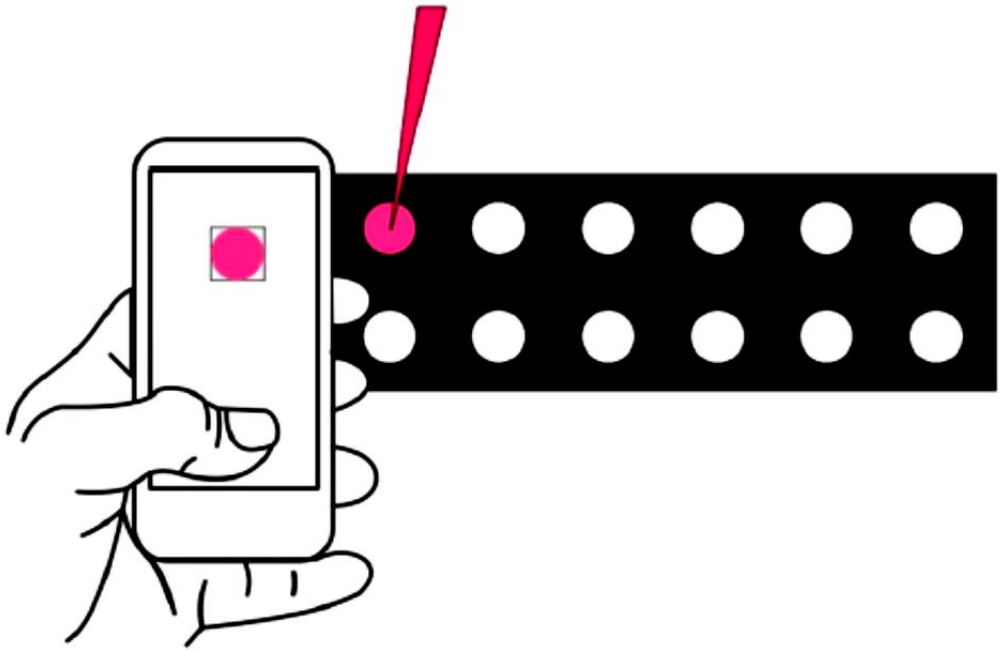
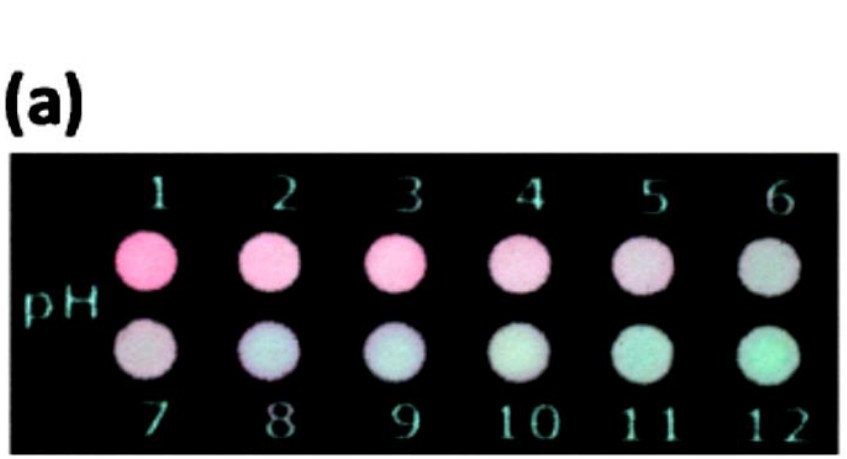


Figure 1. Scheme of paper devices for acid–base reactions and procedure for colorimetric reading by smartphone.



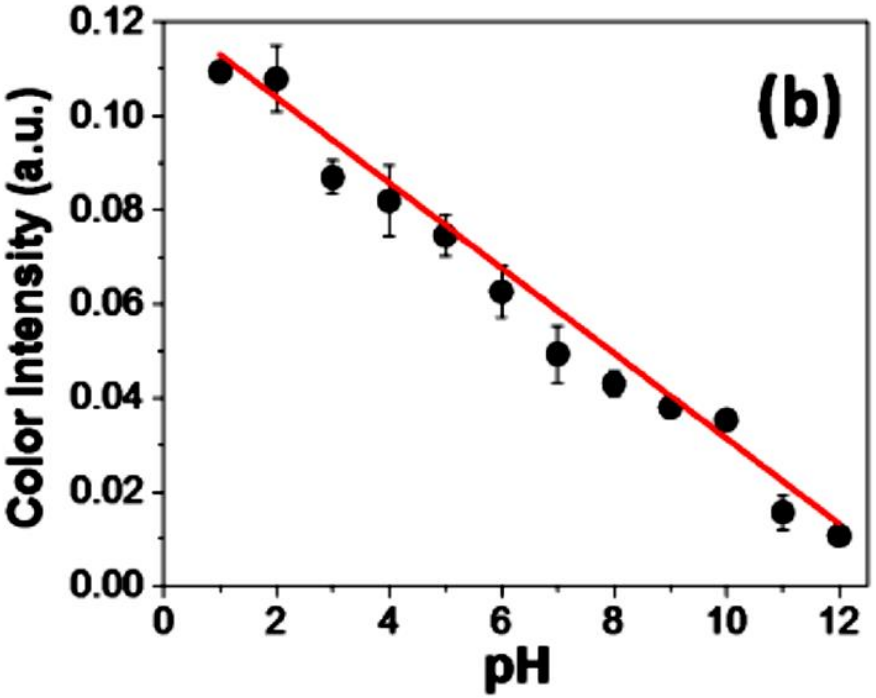


Figure 2. Presentation of (**a**) an optical micrograph showing the color changes on printed zones and (**b**) color intensity analysis over different pH values. In (a), microzones were first spotted with 5 µL of the natural indicator. Then, 5 µL of different solutions prepared at pH range from 1 to 12 were added on microzones prior to image capture. The labels depicted in (a) indicate the used microzones for each pH value.

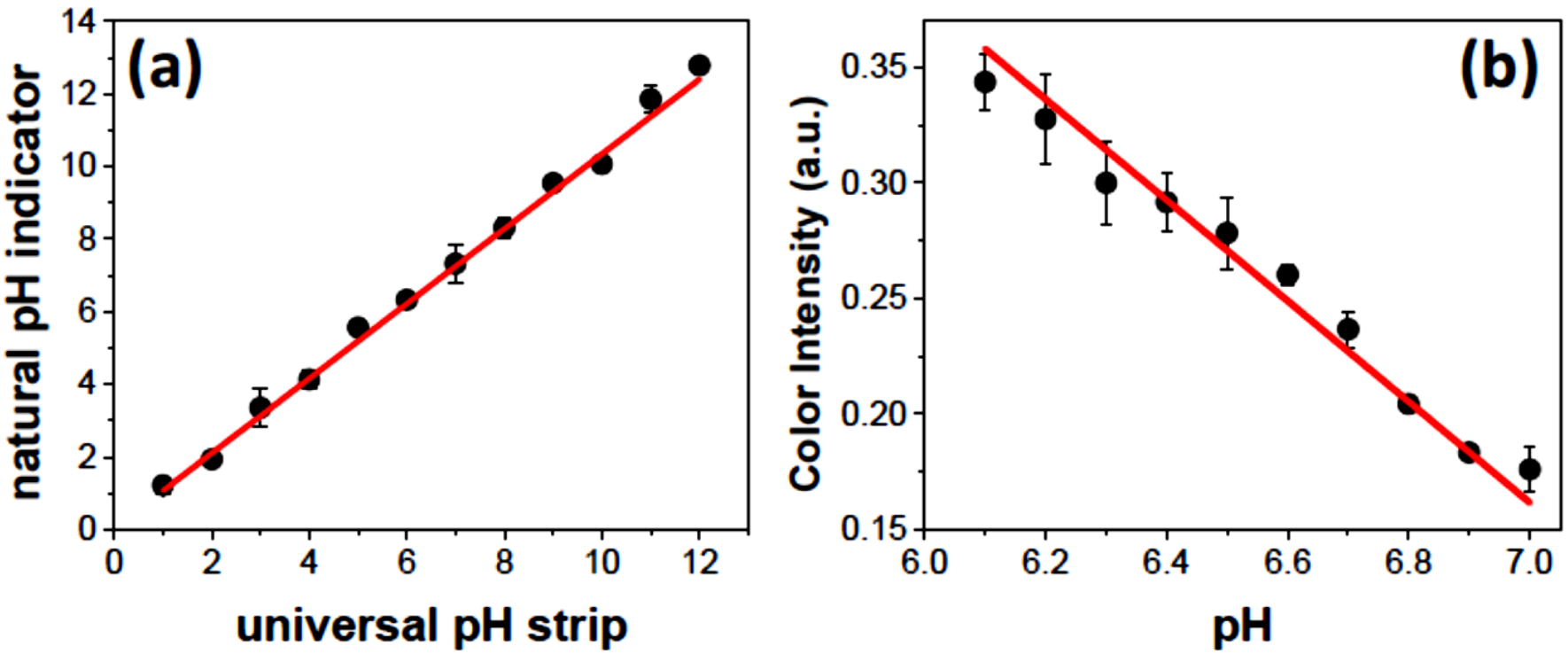


Figure 3. Presentation of (a) pH values measured with universal pH strip and wax printed paper zones previously spotted with natural pH indicator and (b) pH resolution measured on paper zones. In (a), all measurements were recorded for standard solutions prepared in a pH range between 1 and 12. For the readings using universal pH strips, each device was introduced inside sample solution requiring a volume of ca. 1 mL to obtain coloration and allow the comparison with a pH scale defined in a color gradient as reference. In (b), the color intensity was determined in phosphate buffer solutions prepared in a pH range between 6.1 and 7.0. For pH determination on paper zones spotted with natural indicator, see Figure 2.

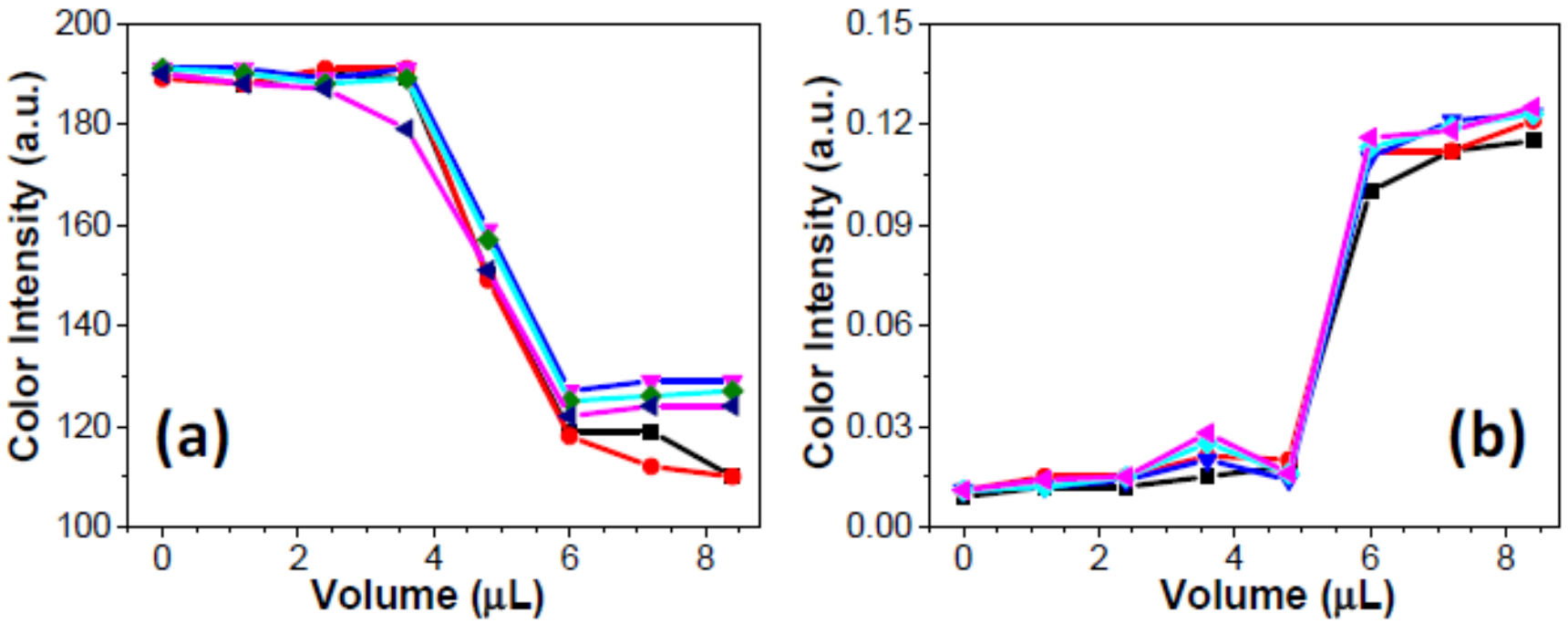
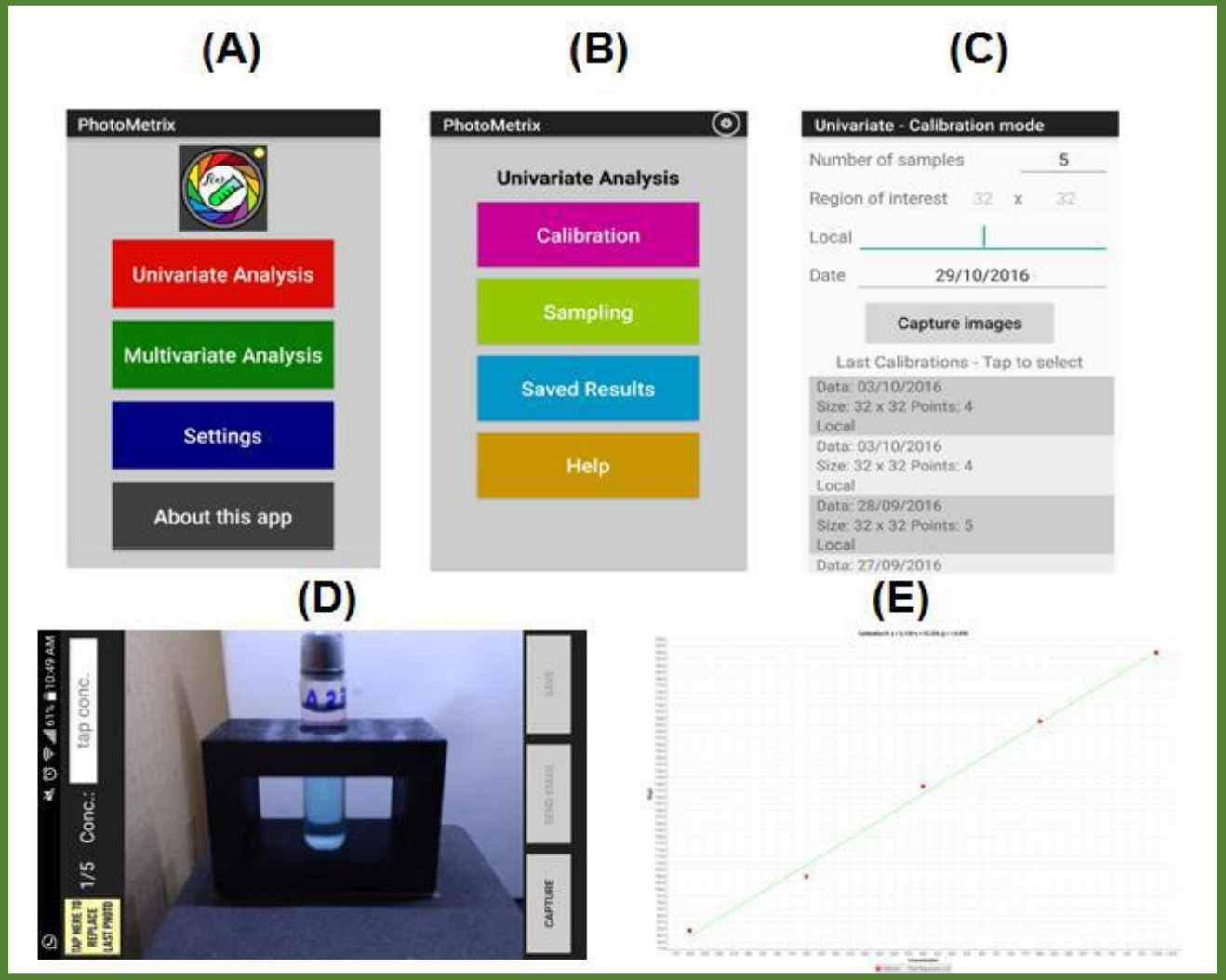


Figure 4. Titration curves performed on wax printed paper microzones showing examples of (a) NaOH versus HCl and (b) HCl versus NaOH titrations. In both examples, titrations were carried out using equimolar solutions (0.1 mol/L). For each titration, microzones were first spotted with 5 µL of the natural indicator. In (a,b), the color intensities were recorded after adding 1.2 µL aliquots of HCl and NaOH, respectively. Color intensity was captured by smartphone and analyzed through the Photometrix® App.

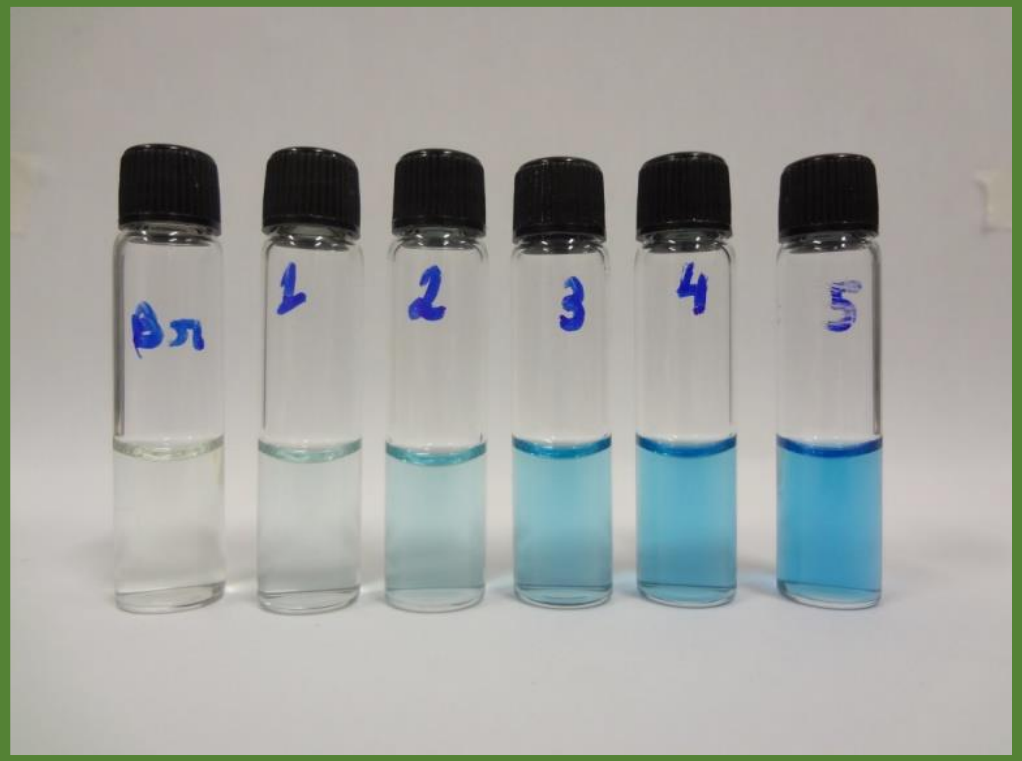
Medidas colorimétricas com smartphones para identificação de amostras de cocaína e quantificação de alguns adulterantes

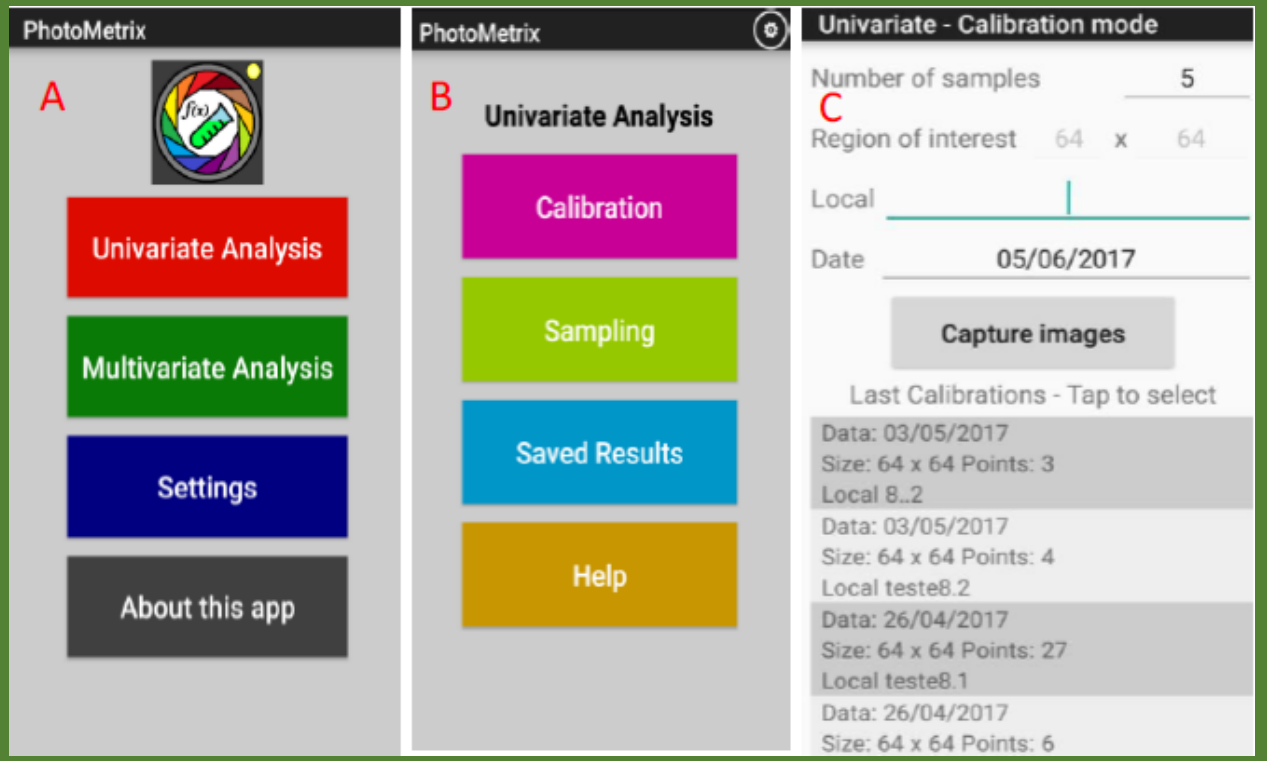
Msc. Pâmela Anália Costa de Oliveira – UNB 2017



Avaliação do uso de imagens digitais obtidas por smartphones para determinação de amônia total em águas

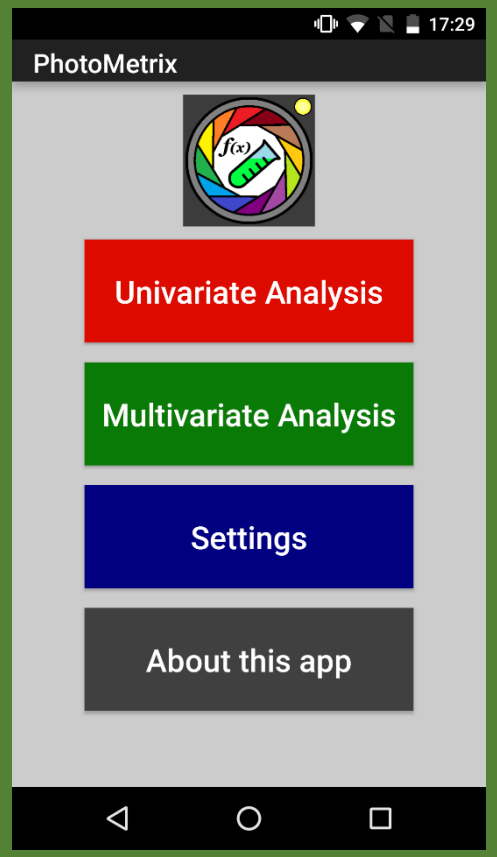
TCC de Katharina Monteiro Plácido – UNB 2017

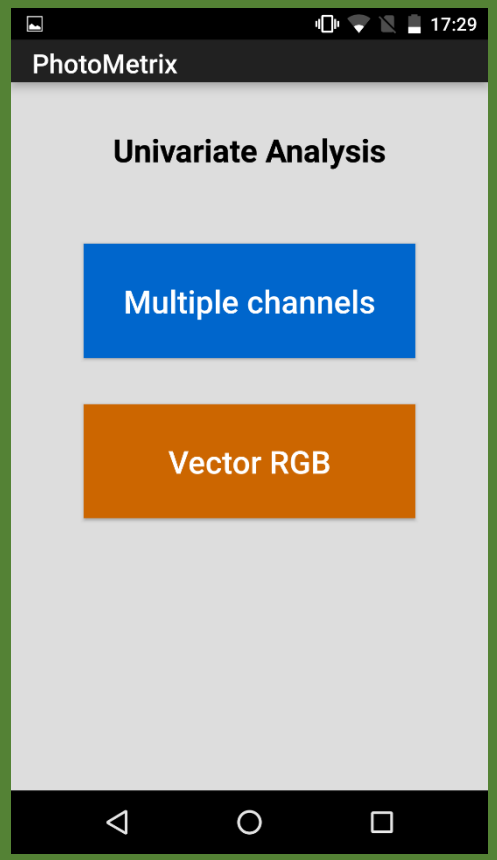


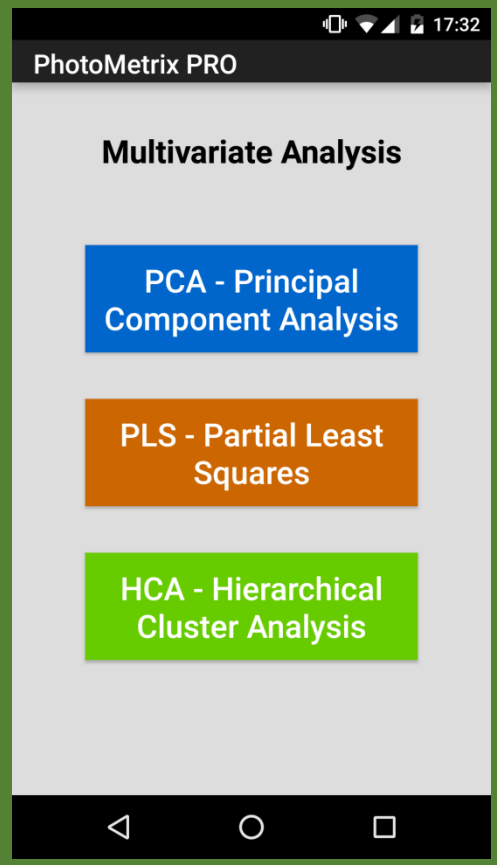


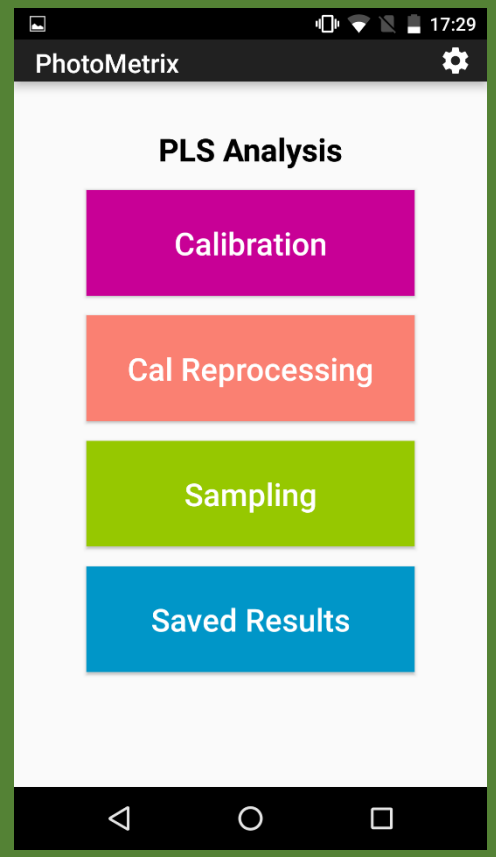
PhotoMetrix PRO

Google Play









RAPID DETERMINATION OF ETHANOL IN SUGARCANE SPIRIT USING PARTIAL LEAST SQUARES REGRESSION EMBEDDED IN SMARTPHONE

Fernanda C. Böck, Gilson A. Helfer, Adilson B. da Costa,
Morgana B. Dessuy, Marco F. Ferrão

$(NH_4)_2Ce(NO_3)_6$ + ROH $\rightleftarrows$ $(NH_4)_2Ce(NO_3)_6$ + HNO_3

Ceric ammonium nitrate (yellow) — alcohol — (red)

Table 1 Experiment planning ethanol determination, where X_1 corresponds to CAN and X_2 to NA concentrations

Experiment	X_1 (mol L^{-1})	X_2 (mol L^{-1})
1	0.15 (0)	0.10 (0)
2	0.15 (0)	0.20 (+1)
3	0.20 (+0.866)	0.15 (+0.5)
4	0.15 (0)	0 (−1)
5	0.10 (−0.866)	0.05 (−0.5)
6	0.10 (−0.866)	0.15 (+0.5)
7	0.20 (+0.866)	0.05 (−0.5)

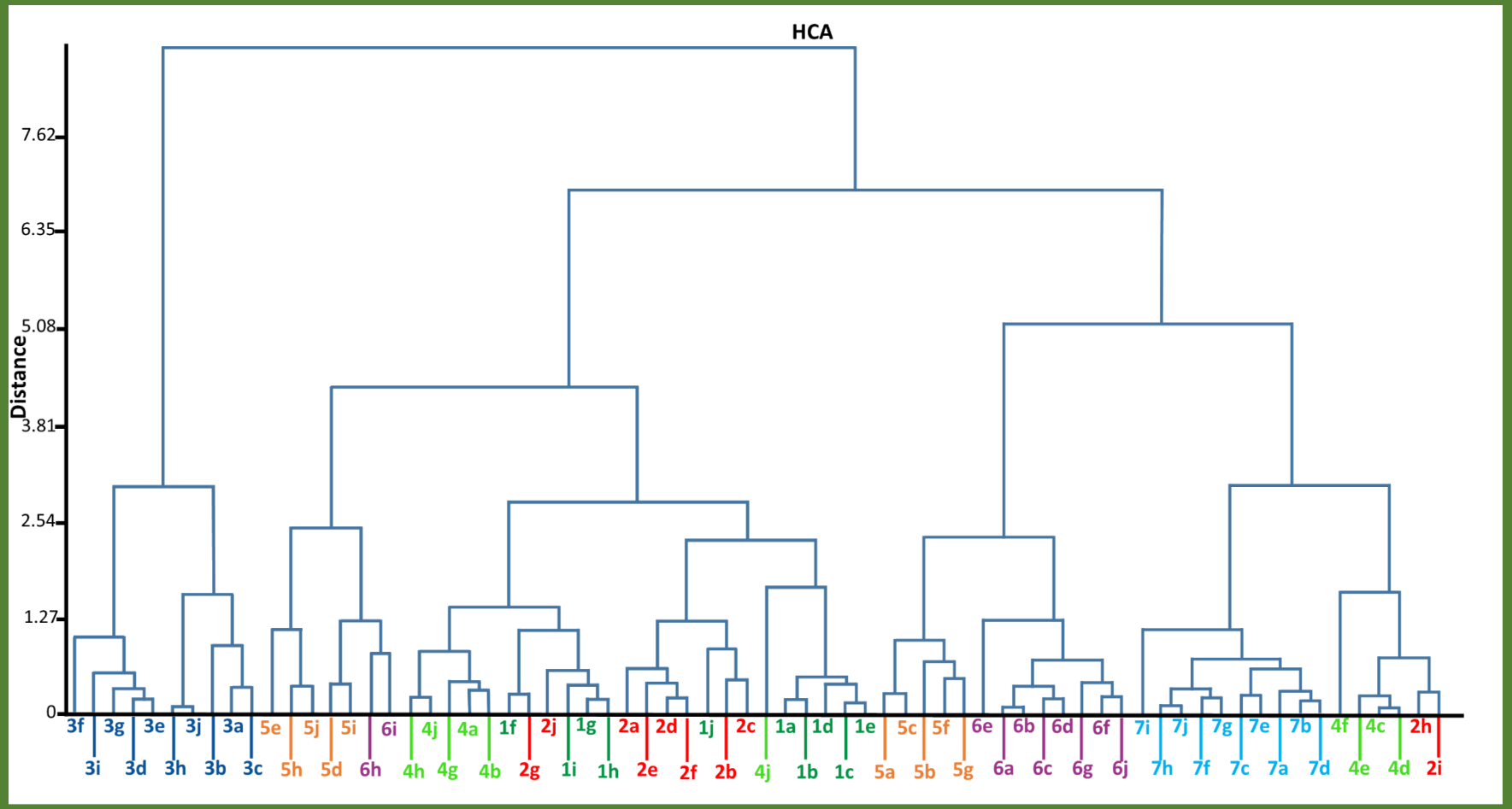
Table 2 Example of image acquired by the scanner in the reaction time of 5 min that was used in the HCA analysis

Condition / Time	1	2	3	4	5	6	7
5 min							

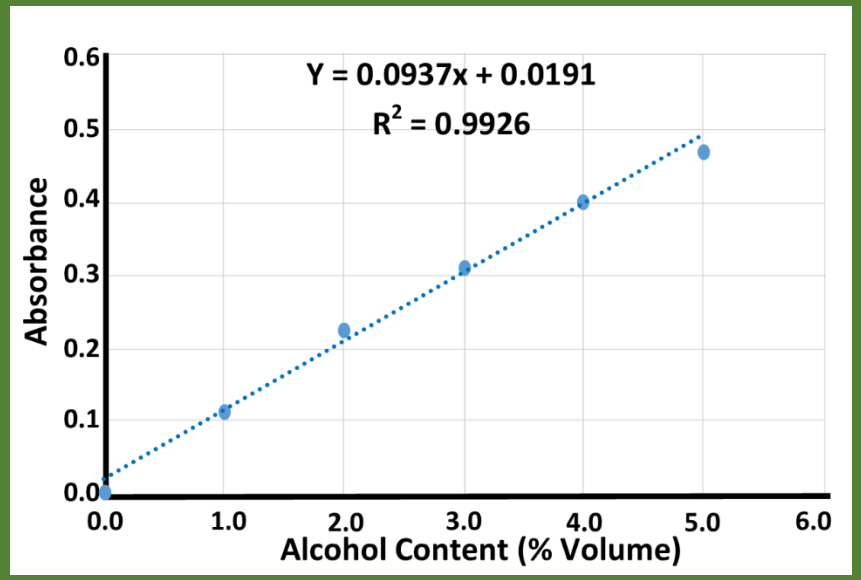
The numbers from 1 to 7 correspond to the experiments in Table 1

RAPID DETERMINATION OF ETHANOL IN SUGARCANE SPIRIT USING PARTIAL LEAST SQUARES REGRESSION EMBEDDED IN SMARTPHONE

Fernanda C. Böck, Gilson A. Helfer, Adilson B. da Costa,
Morgana B. Dessuy, Marco F. Ferrão



UV-VIS



PhotoMetrix

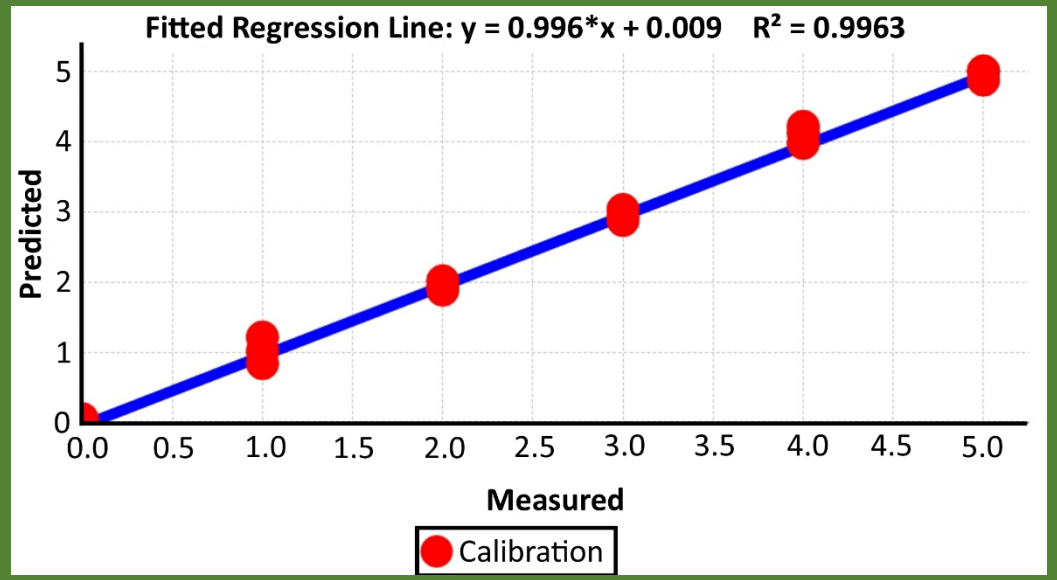


Table 3: Results obtained by the reference method and by PLS image analysis.

Sample	UV-VIS (% v/v)	Relative Deviation (% v/v)	PLS (% v/v)	Relative Deviation (% v/v)	Relative Error (% v/v)
A	37.6	<0.1	37.6	0.2	0.0
B	39.2	<0.1	40.5	0.1	3.4
C	38.9	<0.1	38.4	0.1	-1.4
D	39.3	<0.1	39.7	0.1	-3.6
E	37.9	<0.1	38.5	0.2	1.5
F	36.3	<0.1	35.2	0.1	-3.0

A New Tool for Interpretation of Thermal Stability of Raw Milk by Means of the Alizarol Test Using a PLS Model on a Mobile Device

G. A. Helfer, B. Tischer, P. F. Filoda, A. B. Parckert, R. B. dos Santos, L. L. Vinciguerra, M. F. Ferrão, J. S. Barin, A. B. da Costa

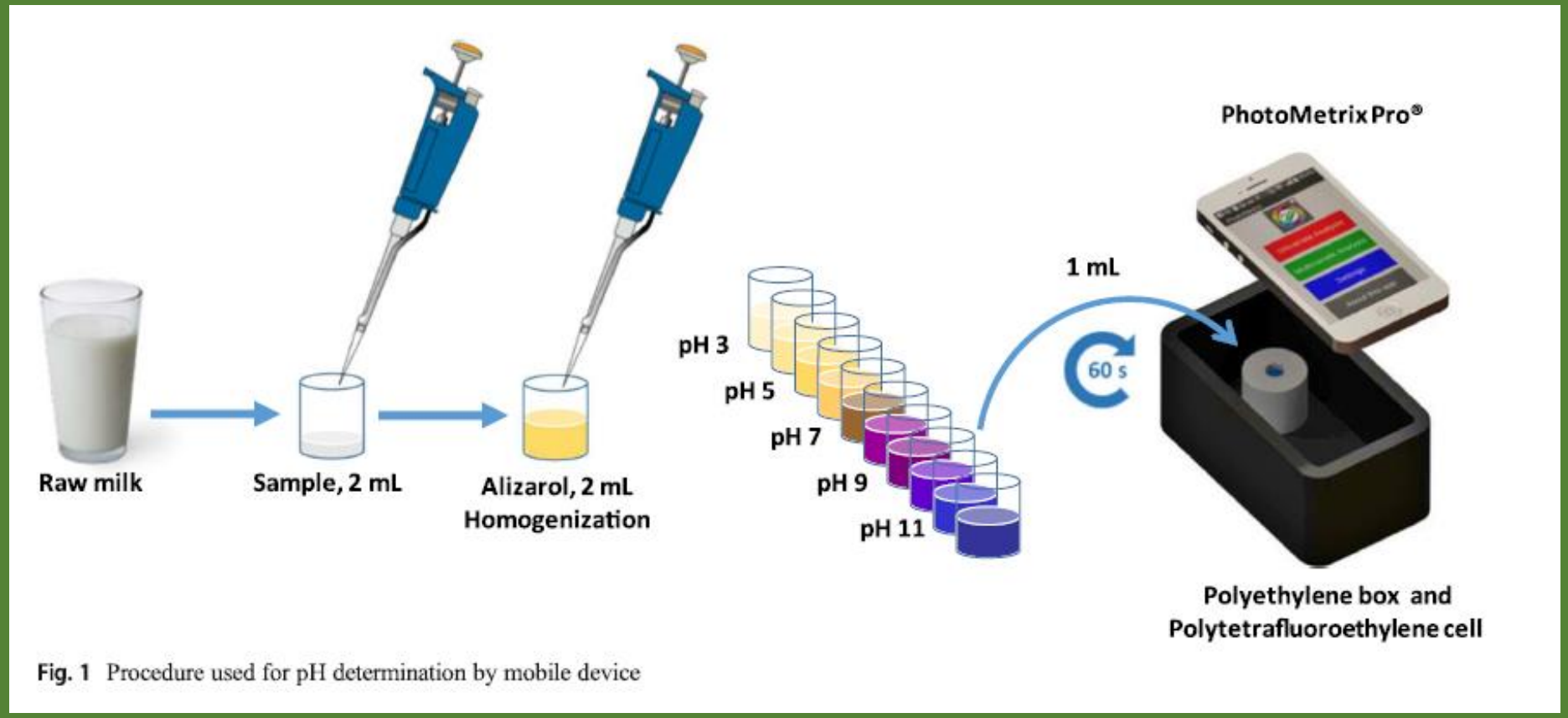
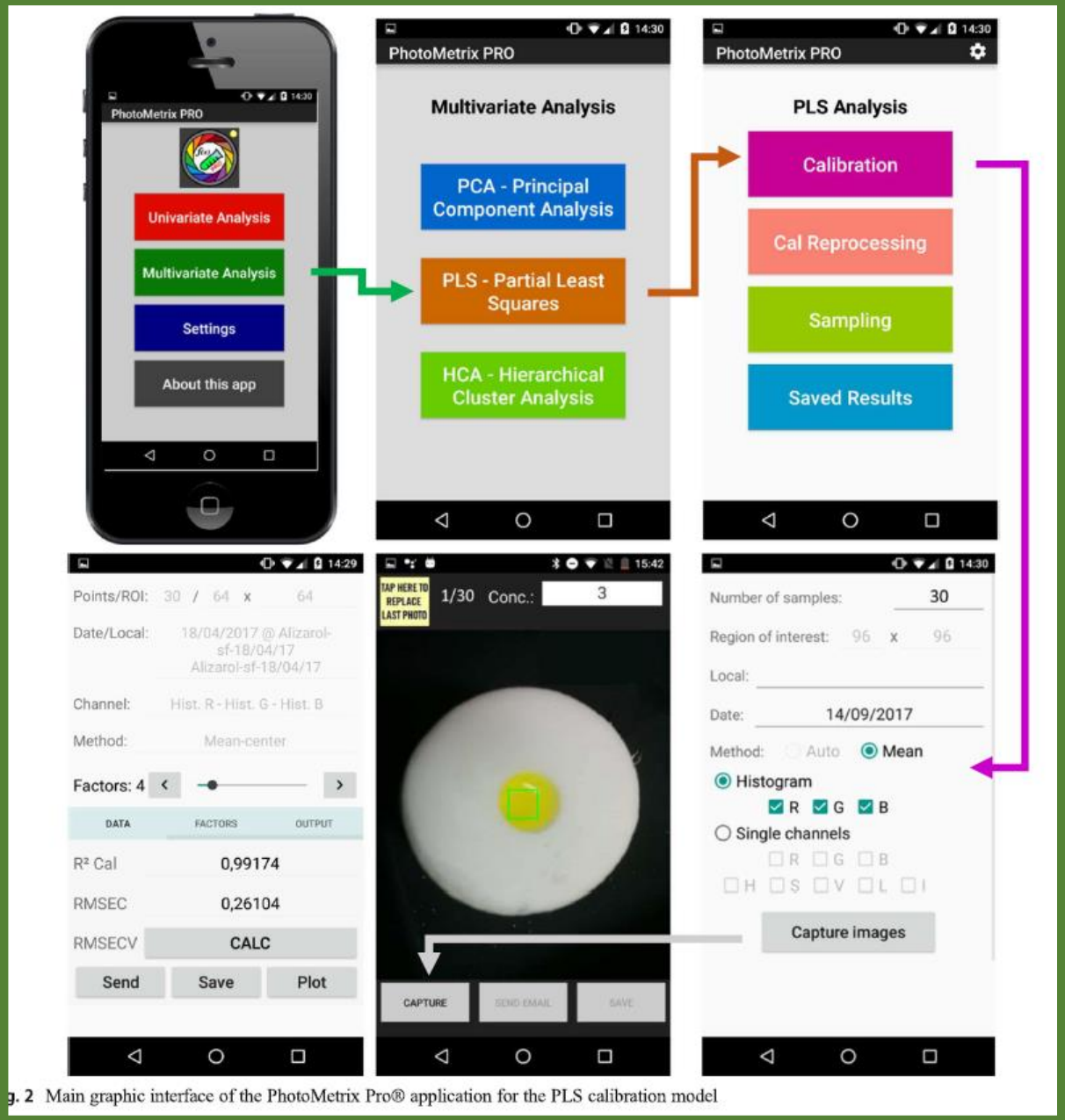


Fig. 1 Procedure used for pH determination by mobile device



g. 2 Main graphic interface of the PhotoMetrix Pro® application for the PLS calibration model

Table 1 PLS regression results using PhotoMetrix Pro® for milk analysis

Parameter	Calibration	Prediction
Samples	30	7
Number of factors	4	4
Slope	0.992	0.999
Offset	0.06	−0.11
R^2	0.992	0.994
RMSEC	0.25	–
Bias	0.0007	0.0980
RMSEP	–	0.30

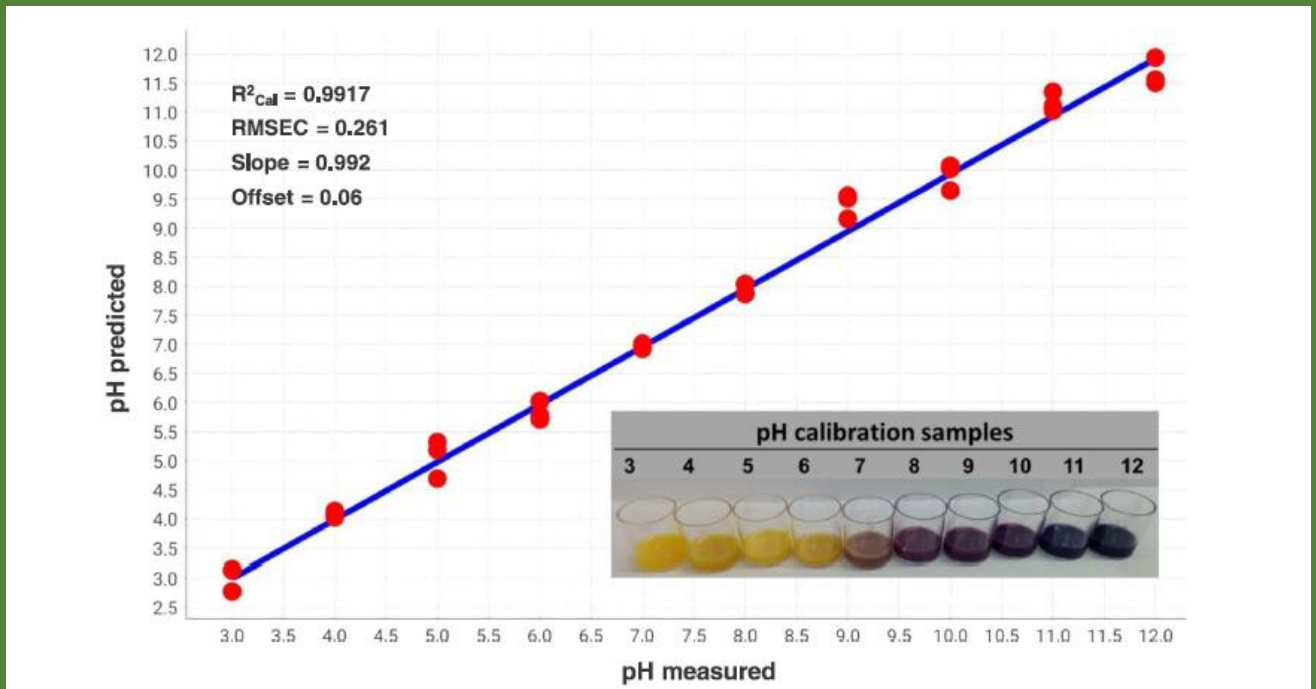
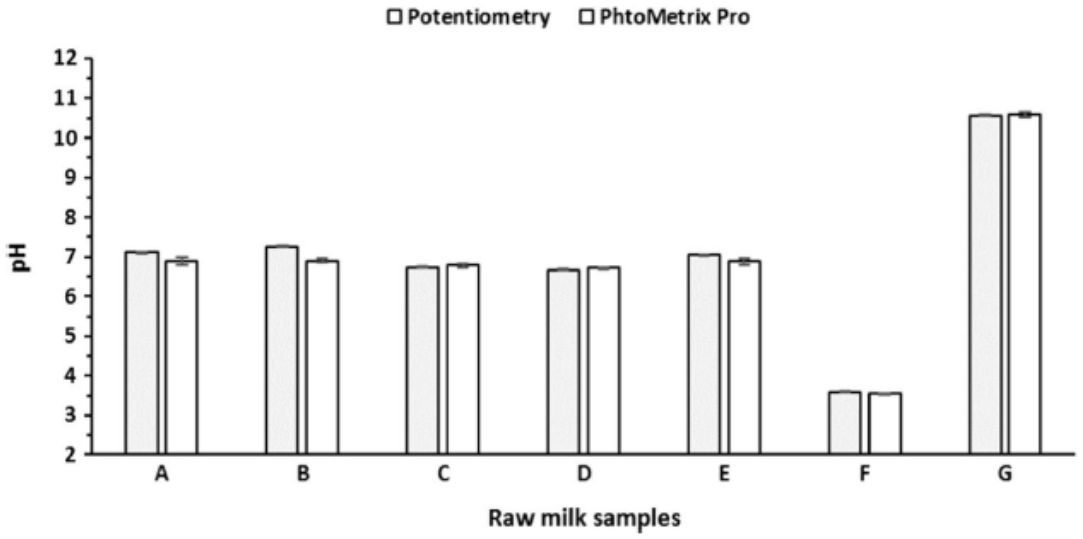


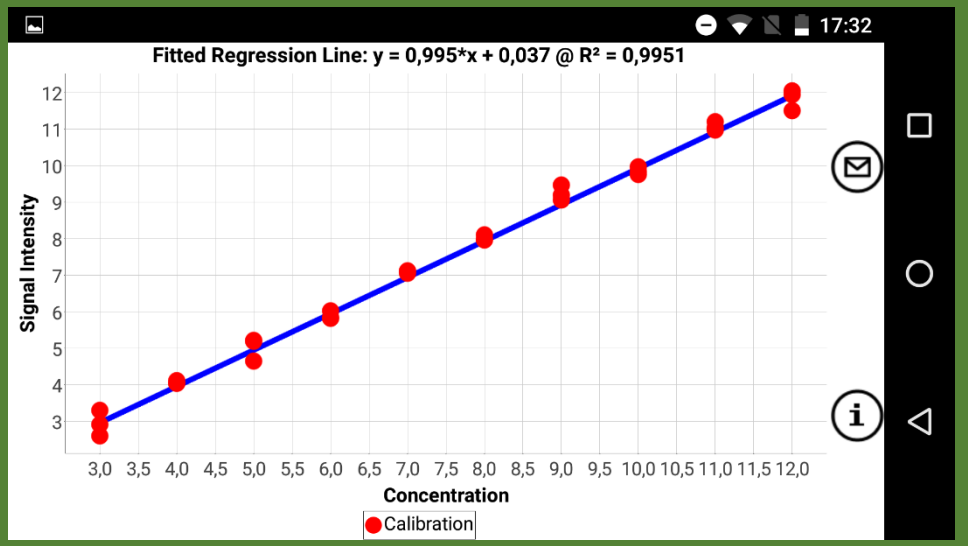
Fig. 3 Correlation between raw milk pH values measured by the reference methodology (pH measured) and results predicted by PhotoMetrix Pro®, using a PLS regression model with four factors and mean center data preprocessing

Fig. 4 Comparison of counting results for raw milk pH by the reference methodology (potentiometry) and by PhotoMetrix Pro®. Mean and standard deviation are shown ($n = 3$)



PhotoMetrix PRO

Enqa nas Escolas



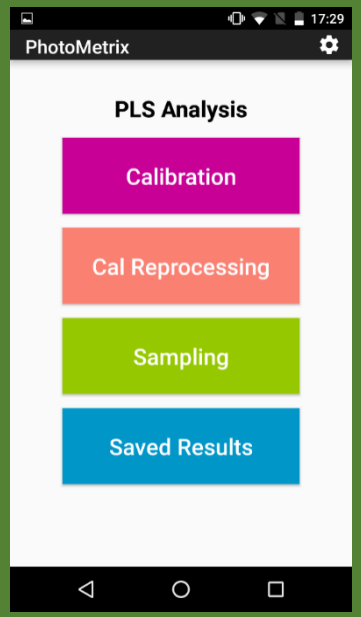
1	2	3	4	5	6	7	8	9	10	11	12	13

PhotoMetrix UVC

PhotoMetrix UVC

Determinação de Cobre em Cachaça Através de Quimiometria de Imagens em Celulares Empregando Regressão por PLS

Böck, F. C. (PG), Leandro, I. S. (IC), Dessuy, M. B. (PQ), Helfer, G. A. (PQ), Costa, A. B. (PQ), Ferrão, M. F. (PQ)



Espectroscopia Molecular: UV-VIS/Celular

Espectrometria Atômica: GFAAS

Obrigado pela Atenção!