XXI Encontro Sociedade Portuguesa de Eletroquímica

XVIII Encontro Ibérico de Eletroquímica

XXI Meeting of the Portuguese Electrochemistry Society
&
XVIII Iberian Electrochemistry Meeting
Abstract Book

XXI Encontro da Sociedade Portuguesa de Eletroquímica
&
XVIII Encontro Ibérico de Eletroquímica
Livro de Resumos

Bragança, Portugal ◆ 14-17 setembro 2016

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XVIII Encontro Ibérico de Eletroquímica

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PC

POSTER COMMUNICATIONS

COMUNICAÇÕES EM POSTER

PC16

Sugars quantification using an Electronic Tongue: multivariate calibration with a genetic algorithm for sensor selection.

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Sugar analysis contributes to the assessment of their impact on the human health and their physiological effects, allowing to better understand their relation with sensory attributes and acting on quality control and authenticity of food products [1,2]. Although, several analytical methods are routinely used in the identification and quantification of sugars in foods, in general, these methods have several disadvantages such as, slowness of the analysis, high consumption of chemicals and the need for destructive pretreatments of samples. The development of new reliable methods have been proposed [3] to avoid theses disadvantages and, in this follow-up, it was decided to apply a potentiometric electronic tongue, built with cross-selectivity polymeric sensors that were selected considering the sensitivities towards sugars, previously reported [4]. The analysis of sugars (glucose, fructose and sucrose) in this study aimed to establish an analytical methodology and mathematical framework to quantify these compounds. For this purpose, analyzes were performed using standard solutions of ternary mixtures of these sugars, by applying an orthogonal experimental design to establish different concentration levels [5]. It was then made an exploratory data analysis using principal component analysis to verify data variability. To establish a multiple linear relationship between the concentration of sugars and the potentiometric signals obtained by the electronic tongue, a genetic algorithm was used to select the best subset of sensors and cross-validation with K-folds, to optimize the model in prediction. Satisfactory results were obtained in each sugar analysis. For instance, the multiple linear regression model for fructose analysis allowed to have, by cross-validation using K-folds (dividing analytical data randomly into 7 groups), a $R^2_{ajusted}$ above 0.99 and RMSE less than 0.5. Moreover, the linear relationship between the predicted values by the obtained model and the respective fructose experimental values allowed to obtain a slope of 0.98±0.02 (close to unity) and an intercept value statistically equal to zero.
The multisensor system used proved to be a suitable tool for the analysis of sugars, when present in majority concentrations and alternative to the instrumental reference methods, such as HPLC. It allowed to decrease the time and price of each analysis, and also, to reduce sample preparation work and eliminate pollutants in the analysis procedure.

References:

[1] LG Dias, C Sequeira, AC Veloso, MC Sousa, AM Peres, Analytica Chimica Acta, 2014, 848, 32-42
[2] L Escuder-Gilabert, M Peris, Analytica Chimica Acta, 2010, 665, 15-25
[3] T Sakata, K Faceli, T Almeida, A Júnior, W Steluti, 11th International Conference on Machine Learning and Applications, 2012, 538-541
[4] LG Dias, AM Peres, TP Barcelos, JS Morais, A Machado, Sensors Actuators B: Chemical, 2011, 154, 111-118
[5] RG Brereton, Applied Chemometrics for Scientists, 2007, Wiley, Chichester, United Kingdom

Sugars quantification using an Electronic Tongue:
multivariate calibration with a genetic algorithm for sensor selection

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OBJECTIVES

ELECTRONIC TONGUE ANALYSIS

QUANTIFY 3 SUGARS IN MIXED SOLUTIONS: glucose, fructose and sucrose

INTEREST:

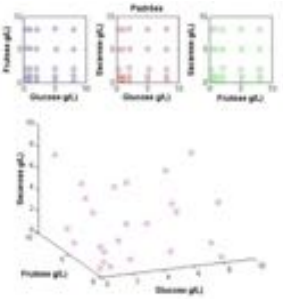
- impact on the human health and their physiological effects, allowing to better understand their relation with sensory attributes and acting on quality control and authenticity of food products

TERNARY MIXED SOLUTIONS

ORTHOGONAL EXPERIMENTAL DESIGN

≠ CONCENTRATION LEVELS

0,2 – 8 g/L
Glucose
Fructose
Sucrose



ELECTRONIC TONGUE DATA

EXPLORATORY ANALYSIS → PRINCIPAL COMPONENT ANALYSIS

MULTIPLE LINEAR REGRESSION → **GENETIC ALGORITHM** select the best subset of sensors → CROSS-VALIDATION with K-folds

ELECTRONIC TONGUE (taste sensor array)

Chemical sensors with high stability and cross sensitivity to different species in solution

OBTAIN signal pattern which corresponds to the overall information on the sample

APPLY chemometric methods for multivariate calibration

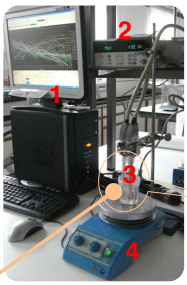
ALLOW multicomponent analysis

25 MIXED SOLUTIONS

Sugars standards dissolved in water according to an experimental design

POTENTIOMETRIC DEVICE (all-solid-state electrodes)

20 lipid polymeric membranes
Ag/AgCl reference electrode



MULTI-SENSOR ANALYTICAL SYSTEM:
1 - PC for data acquisition;
2 - DataLogger Agilent;
3 - Etongue device;
4 - Magnetic stirrer.

Analysis with two sensor arrays: 40 sensors

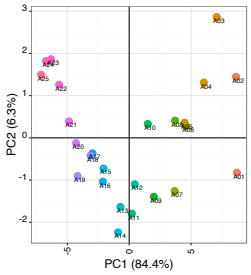
COMPOSITION OF **LIPID POLYMERIC MEMBRANE**:
31.9-32.3% of PVC
64.7-65.2% of one of the plasticizers
2.8-3.2% of one membrane additive

MEMBRANE ADDITIVE SUBSTANCE
[1] Octadecylamine
[2] Oleyl alcohol
[3] Methyltrioctylammonium chloride
[4] Oleic acid

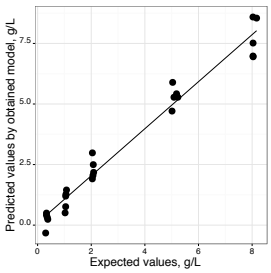
PLASTICISER SUBSTANCE
[A] Bis(1-butylpentyl) adipate
[B] Dibutyl sebacate
[C] 2-Nitrophenyl-octylether
[D] Tris (2-ethylhexyl) phosphate
[E] Bis (2-ethylhexyl) ftalate

ELECTRONIC TONGUE RESULTS: MULTIVARIATE ANALYSIS

PRINCIPAL COMPONENT ANALYSIS
using all sensors selected for the calibrations



MULTIPLE LINEAR REGRESSION MODEL → GENETIC ALGORITHM FOR SENSOR SELECTION → K-FOLD (7 FOLDS) CROSS-VALIDATION



		Results for the K-FOLDS cross-validation		Relation between expected and predicted by model [*1]		
Compound	N sensors	RMSE (g/L)	R^2	Slope (± sd)	R	$R^2_{adjusted}$
Glucose [*2]	17	0.85 (± 0.57)	0.88 (± 0.30)	0.998 (± 0.009)	0.997	0.981
Fructose [*3]	16	1.57 (± 0.57)	0.84 (± 0.23)	0.99 (± 0.02)	0.994	0.987
Sucrose [*4]	15	1.06 (± 0.18)	0.92 (± 0.06)	0.99 (± 0.02)	0.997	0.994

*1) intercept without statistical significance;
*2) sensors selected: S2, S6, S8, S16, S18, S22, S24, S25, S28, S30, S31, S32, S34, S35, 3S6, S37, S38;
*3) sensors selected: S1, S4, S8, S9, S15, S18, S19, S21, S22, S23, S24, S27, S32, S33, S36, S39;
*4) sensors selected: S1, S2, S4, S5, S9, S15, S18, S19, S22, S23, S28, S30, S31, S32, S36.

CONCLUSION

The proposed approach can be used as a practical tool for the analysis of sugars, when present in majority concentrations and an alternative to the instrumental reference methods, such as HPLC.
It allowed to decrease the time and price of each analysis, and also, to reduce sample preparation work and eliminate pollutants in the analysis procedure.

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SOCIEDADE PORTUGUESA DE ELECTROQUÍMICA
PORTUGUESE ELECTROCHEMICAL SOCIETY

grupo especializado electroquímica

CERTIFICADO

A Comissão Organizadora do
XXI Encontro da Sociedade Portuguesa de Eletroquímica
&
XVIII Encontro Ibérico de Eletroquímica
que decorreu nos dias 14 a 17 de Setembro de 2016,
no Instituto Politécnico de Bragança, Portugal,
informa que a
Comunicação em poster
intitulada
Sugars quantification using an Electronic Tongue: multivariate calibration with a genetic algorithm for sensor selection
e com o(s) autor(es)
Vinicius da Costa Arca, António M. Peres, Evandro Bona, Luís G. Dias
foi apresentada.

Conceição Angélico

Presidente da
Comissão Organizadora

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