20°ENQA | 8°CIAQA

Encontro Nacional de Química Analítica
20th Brazilian Meeting on Analytical Chemistry

Congresso Ibero-Americano
de Química Analítica

September 25th to 28th • 2022 • Dall'Onder Grande Hotel
Bento Gonçalves • RS • Brazil

BOOK OF ABSTRACTS

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Realization

Sociedade Brasileira de Química

Universidade Federal de Santa Maria 1960 UFSM

Universidade Federal de Pelotas RS-Brasil UFPEL

UFN Universidade Franciscana

PRESENTATION

The **Brazilian Meeting on Analytical Chemistry (20th ENQA)** returns to Rio Grandedo Sul state, where a previous edition (10th ENQA) was organized in the Federal University of Santa Maria (UFSM), in 1999. This is the first edition of ENQA after the beginning of Covid-19 pandemic. In addition to the inherent difficulties of organizingany presential meeting, we still face challenges related to this pandemic. Nobodyimagined in 1999 that in this century we would be facing anti-vaccine and anti-science movements. However, despite all the losses and adversities, we have much to celebrate because good science proved again that it is the only safe way to managesuch problems. In this sense, analytical chemistry has provided many contributions to help in the management of this pandemic as well as to the science development.

The **20th edition of ENQA** will be hosted together with the 8th Ibero-American Congress of Analytical Chemistry (CIAQA). It is worth noting that the historical and cultural affinity among members of the analytical chemistry communities of Ibero-America is important to promote the integration among researchers from these regions.

Therefore, the **20th ENQA/8th CIAQA** aims to provide a discussion forum on the advances in analytical chemistry through conferences, workshops, oral sessions, technical lectures, short courses, presentations of posters and company exhibitions. From **September 25 to 28th, 2022**, the scientific advances in analytical chemistry will be presented by national and international conference attendees and speakers, contributing to the update of knowledge in this area. **20th ENQA/8th CIAQA** will also be fostering direct contact among participants and the leading companies active in the field of analytical chemistry.

In addition to the scientific program, the city of Bento Gonçalves offers many tourist attractions and excellent hospitality and gastronomical infrastructure.

Welcome to 20th ENQA/8th CIAQA.

Érico Marlon de Moraes Flores

Chair of the 20th ENQA/8th CIAQA

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PROGRAM

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GENERATION OF SECOND-ORDER ELECTROCHEMICAL DATA FOR INTERFERENCE-FREE CALIBRATION OF GALLIC ACID IN RED WINES

Montemerlo A[b,c] , Azcarate S [a,b] Camiña J [a,b], Messina G

[a] Facultad Ciencias Exactas y Naturales, Universidad Nacional de La Pampa, Av.Uruguay 151, (6300) Santa Rosa, La Pampa, Argentina. Tel: 02954-245220 int 7433

[b] Instituto de Ciencias de la Tierra y Ambientales de la Pampa (INCITAP-CONICET-UNLPam), Santa Rosa, La Pampa, Argentina.

[c] Instituto de Química de San Luis, "Dr. Roberto Antonio Olsina" (INQUISAL-CONICET-UNSL), San Luis, Argentina.

*e-mail:amontemerlo@gmail.com

Wine consists of a solution of ethanol in water, which also contains a variety of organic compounds, such as organic acids, amino acids, sugars, volatile compounds and polyphenols in different concentrations. In particular, the interest in the latter is continuously growing due to its bioactive nature and its close relationship with the final qualities of the resulting product. Specifically, gallic acid is one of the most widely used phenolic compounds as a marker for the characterization of wine products. The use of sulfur dioxide is a common practice in oenology that is currently considered essential for the correct finish of wines. However, there is a growing concern about the reduction of its levels in the final product, which makes it necessary to search for complementary agents. Among the possible alternatives is ascorbic acid or vitamin C. In recent years, its use as an additive for winemaking has been reported due to its antioxidant properties, its reducing nature and because it is a healthy compound. It is important to note that ascorbic acid will never replace the use of sulfites, but it can be an excellent complement to it. The rise of multidirectional calibration enabled the quantification of numerous analytes in complex samples without interference, even in the presence of components not modeled in the calibration, commonly referred to as a second-order advantage. However, classical chemometric methodologies assume that the data comply with the property of bilinearity, which is sometimes not possible to achieve with all instrumental methods. Among them, electrochemistry is capable of providing information with high potential to be used in the development of novel second-order calibration methodologies, although they may not meet the aforementioned conditions. This work raises the possibility of developing a simple and versatile methodology for the interference-free quantification of gallic acid in the presence of ascorbic acid, based on chemometric modeling of electrochemical data. Second-order data were generated by cyclic voltammetry (CV) at different scanning speeds and various modeling strategies were implemented to treat the data obtained. The quantification of gallic acid in the presence of ascorbic acid was possible using a model based on the resolution of multivariate curves-alternating least squares (MCR-ALS). It was found that the optimal number of estimated components for calibration is equal to one. While the analytical figures of merit found, REP% 9.4, LOD 6.094×10^{-5} mol L^{-1}, show the possibility of using this methodology for the quantification of gallic acid in complex samples. The studies carried out open the doors for wine quality analysis through new and innovative methodologies based on the potential of electrochemical data, combined with chemometric techniques, which make it possible to obtain results in a simple, fast and reliable way for quality control in the wine industry.

1 F. Tekos *et al.*, "Assessment of antioxidant and antimutagenic properties of red and white wine extracts in vitro," *Metabolites*, vol. 11, no. 7, 2021, doi: 10.3390/metabo11070436.

2 F. A. Chiappini, F. Gutierrez, H. C. Goicoechea, and A. C. Olivieri, "Achieving the analytical second-order advantage with non-bilinear second-order data," *Anal. Chim. Acta*, vol. 1181, p. 338911, 2021, doi: 10.1016/j.aca.2021.338911.