



XV

MADEIRA

ENCONTRO DE QUÍMICA DOS ALIMENTOS

5-8 DE SETEMBRO DE 2021



ESTRATÉGIAS PARA A EXCELÊNCIA,
AUTENTICIDADE, SEGURANÇA
E SUSTENTABILIDADE ALIMENTAR



<http://xvega.events.chemistry.pt/>

Livro de Resumos

XV Encontro de Química dos Alimentos



XV ENCONTRO DE
QUÍMICA DOS
ALIMENTOS
MADEIRA 5-8 DE SETEMBRO DE 2021



ESTRATÉGIAS PARA A EXCELÊNCIA,
AUTENTICIDADE, SEGURANÇA
E SUSTENTABILIDADE ALIMENTAR

CQM
CENTRO DE QUÍMICA
DA MADEIRA

UNIVERSIDADE da MADEIRA

SOCIEDADE PORTUGUESA DE QUÍMICA

ROYAL SOCIETY
OF CHEMISTRY

EuChemS
European Chemical Society

<http://xveqa.events.chemistry.pt/>

Hotel Meliã Madeira Mare,
Funchal, Madeira
5 a 8 de setembro de 2021

Ficha Técnica

Titulo

Livro de Resumos do XV Encontro de Química dos Alimentos: Estratégias para a Excelência, Autenticidade, Segurança e Sustentabilidade Alimentar

Autores

José S. Câmara

Jorge A. M. Pereira

Rosa Perestrelo Gouveia

Edição

José S. Câmara

Jorge A. M. Pereira

Rosa Perestrelo Gouveia

Editor

Universidade da Madeira, Centro de Química da Madeira

ISBN

978-989-8805-68-3

Data

Setembro de 2021

OC29: Phenolic compounds and antioxidant activity modeling in strawberry by using artificial neural networks (ANNs) technique

Iman Golpour, ¹ Fernando Gonçalves, ² Paula M. R. Correia, ² Raquel P. F. Guiné ²

¹ Grupo de Investigaciones Termoenergéticas (GIT), Universidad Politécnica de Madrid, Madrid, Spain

² Centro de Investigação CERNAS-IPV, Instituto Politécnico de Viseu, Campus Politécnico, Repeses, 3504-510 Viseu, Portugal

Email: raquelguine@esav.ipv.pt

Extraction constitutes a vital procedure when attaining bioactive compounds from plant matrices. Conventional extraction using solvents is highly dependent on variables such as time, temperature, solid to liquid ratio or type of solvent, among others, leading to the need for optimising process variables in order to increase the yield. ^{1,2}

This research study focuses on the evaluation of total phenolic compounds (TPC) and antioxidant activity (AOA) of strawberry fruits according to different experimental extraction conditions by application of Artificial Neural Networks (ANNs) technique. The experimental data was applied to train ANNs using feed and cascade forward back propagating models by Levenberg-Marquardt and Bayesian regulation algorithms. Three independent variables (solvent concentration, volume/mass ratio and extraction time) were used as ANNs inputs whereas the three variables of total phenolic compounds, DPPH and ABTS Antioxidant Activities were considered as ANNs outputs. The results demonstrated that the best neural network cascade and feed forward back-propagation topologies for the prediction of total phenolic compounds and DPPH and ABTS antioxidant activity factors were the 3-9-1, 3-4-4-1 and 3-13-10-1 structures with the training algorithm of trainlm, trainbr, trainlm and threshold functions of tansig-purelin, logsig-tansig-tansig and tansig-tansig-purelin, respectively. The best R² value for the predication of total phenolic compounds and DPPH and ABTS antioxidant activity factors were 0.9806 (MSE=0.0047), 0.9651(MSE=0.0035) and 0.9756 (MSE=0.00286), respectively. According to the comparison of ANNs, the results showed that cascade forward back propagation network had better performance than feed forward back propagation network for the prediction of TPC as feed forward back propagation network in predicting the DPPH and ABTS antioxidant activity factors had more precision than cascade forward back propagation network. According to the obtained results, it was possible to predict TPC and AOA as a function of extraction time, volume/mass ratio, solvent concentration and volume.

Acknowledgements: We would like to thank the CERNAS-IPV Research Centre and the Polytechnic Institute of Viseu for their support.

Funding: This work is funded by National Funds through the FCT - Foundation for Science and Technology, I.P., within the scope of the project Ref^o UIDB/00681/2020.

References:

1. A.A. Kamarudin, N.M. Esa, N. Saad, et al., *Ind. Crops Prod.* (2020) 112064.
2. Ö. Aybastier, E. Işık, S. Şahin, et al., *Ind. Crops Prod.* 44 (2013) 558.