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PREDICTING IN VITRO SECONDARY METABOLISM OF VITIS VINIFERA UNDER THE EFFECT OF NACL USING ARTIFICIAL NEURAL NETWORK COMBINED WITH PRINCIPAL COMPONENT ANALYSIS

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This work proposes a procedure for the forecasting the targeted phenolic profile of vitis vinifera under in vitro NaCl stress. Hence, a combination of principal component analysis (PCA) to decrease the dimensionality of the dataset and artificial neural networks (ANN) for predicting purposes was used. The results obtained were compared with those obtained by linear regression (LR) modeling. NaCl concentration (0, 25, 50, 75 and 100 mM) and grape genotype (Sorkhak, rishbaba, Sahebi, Keshmeshi, Angosht Arous, Perlet, Yaghouti, Laal, Sahebi, Sefid Fakhri, Shahroudi) as inputs and 12 polyphenol compounds including flavonoids catechin, kaempferol, quercetin, rutin, naringenin and isoquercitrin, phenolic acids gallic acid, *p*-coumaric acid, *o*-coumaric acid and *m*-coumaric acid, stilbene resveratrol and coumarin as outputs were used to make the models. Different grape varieties showed various responses of increasing and decreasing phenolics content by enhancing NaCl concentration in culture medium. The effect of genotype varied depending on the type of measured phenolic. In this study, PCA-ANN revealed a considerably higher accuracy of prediction than for regression models. PCA-ANN modeling method is suggested to get inside information on the effect of NaCl on secondary metabolism of grape.

Keywords: artificial neural network, phenolic compounds, principal component analysis, *Vitis vinifera*