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Artificial Neural Network in predicting the extraction yields for anti-cancer compounds

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ABSTRACT Artificial Neural Networks (ANNs) were used to predict the extraction yields for the anti-cancer compounds, Saponins from the particles of Saponaria vaccaria L seeds (particle size = 0.297 mm to 0.840 mm; moisture content = 15.35% to 61.40% d. b.). A total of 120 extractions were prepared from the factorial design with four levels of methanol concentrations (MeOH), 30%, 50%, 70%, and 90% (vol., aq.) and three levels of temperatures (T), 30˚C, 45˚C, and 60˚C at ten extraction interval times (t) between 1 and 180 min. A calibration equation developed as a part of this work using the known mass of the "standard" Saponins, and their corresponding liquid-chromatogram-mass spectroscopy (LC-MS) peaks was used to quantify the extract yields. An ANN based upon error back propagation algorithm and Bayesian regularization with three inputs, MeOH, T, and t predicted the extraction kinetics and the saponins yields, in general, with less than 12% error. It also slightly outperformed the complex diffusional model (DM) in predicting both the yields and the extraction kinetics based upon the MSE and R values making the prediction simple, and faster at the same time eliminating the estimation of the partition coefficient and the effective diffusivity required for DM. Therefore an ANN can be a simple tool to predict the saponins yields, and may have same potential for the predictions of other pharmaceutical and neutraceutical products with satisfactory accuracy and speed, which otherwise would be very time consuming and tedious

Keywords: Saponaria vaccaria, diffusion model, ANN