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Development and Validation of First Derivative Method and Artificial Neural Network for Simultaneous Spectrophotometric Determination of Two Closely Related Antioxidant Nutraceuticals in Their Binary Mixture”

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Abstract : Background: Two new, simple and specific methods; First, a Zero-crossing first-derivative technique and second, a chemometric-assisted spectrophotometric artificial neural network (ANN) were developed and validated in accordance with ICH guidelines. Both methods were used for the simultaneous estimation of the two closely related antioxidant nutraceuticals ; Coenzyme Q10 (Q) ; also known as Ubidecarenone or Ubiquinone-10, and Vitamin E (E); alpha-tocopherol acetate, in their pharmaceutical binary mixture. Results: For first method: By applying the first derivative, both Q and E were alternatively determined; each at the zero-crossing of the other. The D1 amplitudes of Q and E, at 285 nm and 235 nm respectively, were recorded and correlated to their concentrations. The calibration curve is linear over the concentration range of 10-60 and 5.6-70 µg mL-1 for Q and E, respectively. For second method: ANN (as a multivariate calibration method) was developed and applied for the simultaneous determination of both analytes. A training set (or a concentration set) of 90 different synthetic mixtures containing Q and E, in wide concentration ranges between 0-100 µg/mL and 0-556 µg/mL respectively, were prepared in ethanol. The absorption spectra of the training sets were recorded in the spectral region of 230–300 nm. A Gradient Descend Back Propagation ANN chemometric calibration was computed by relating the concentration sets (x-block) to their corresponding absorption data (y-block). Another set of 45 synthetic mixtures of the two drugs, in defined range, was used to validate the proposed network. Neither chemical separation, preparation stage nor mathematical graphical treatment were required. Conclusions: The proposed methods were successfully applied for the assay of Q and E in laboratory prepared mixtures and combined pharmaceutical tablet with excellent recoveries. The ANN method was superior over the derivative technique as the former determined both drugs in the non-linear experimental conditions. It also offers rapidity, high accuracy, effort and money saving. Moreover, no need for an analyst for its application. Although the ANN technique needed a large training set, it is the method of choice in the routine analysis of Q and E tablet. No interference was observed from common pharmaceutical additives. The results of the two methods were compared together

Keywords : coenzyme Q10, vitamin E, chemometry, quantitative analysis, first derivative spectrophotometry, artificial neural network

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