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Analysis of closely related antioxidant nutraceuticals using the green analytical methodology of ANN and smart spectrophotometric methods

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Abstract:

Two new, simple, and specific green analytical methods are proposed: zero-crossing first-derivative and chemometric-based spectrophotometric artificial neural network (ANN). The proposed methods were used for the simultaneous estimation of two closely related antioxidant nutraceuticals, coenzyme Q10 (Q10) and vitamin E, in their mixtures and pharmaceutical preparations. The first method is based on the handling of spectrophotometric data with the first-derivative technique, in which both nutraceuticals were determined in ethanol, each at the zero crossing of the other. The amplitudes of the first-derivative spectra for Q10 and vitamin E were recorded at 285 and 235 nm respectively, and correlated with their concentrations. The linearity ranges of Q10 and vitamin E were 10-60 and 5.6-70 μg·mL^{-1}, respectively. The second method, ANN, is a multivariate calibration method and it was developed and applied for the simultaneous determination of both analytes. A training set of 90 different synthetic mixtures containing Q10 and vitamin E in the ranges of 0-100 and 0-556 μg·mL^{-1}, respectively, was prepared in ethanol. The absorption spectra of the training set were recorded in the spectral region of 230-300 nm. By relating the concentration sets (x-block) with their corresponding absorption data (y-block), gradient-descent back-propagation ANN calibration could be computed. To validate the proposed network, a set of 45 synthetic mixtures of the two drugs was used. Both proposed methods were successfully applied for the assay of Q10 and vitamin E in their laboratory-prepared mixtures and in their pharmaceutical tablets with excellent recovery. These methods offer advantages over other methods because of low-cost equipment, time-saving measures, and environmentally friendly materials. In addition, no chemical separation prior to analysis was needed. The ANN method was superior to the derivative technique because ANN can determine both drugs under nonlinear experimental conditions. Consequently, ANN would be the method of choice in the routine analysis of Q10 and vitamin E tablets. No interference from common pharmaceutical additives was observed. Student's t-test and the F-test were used to compare

the two methods. No significant difference was recorded.

Reference:

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