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Orthogonal Partial Least Squares Model for Rapid Prediction of Antioxidant Activity of Pereskia bleo by Fourier Transform Infrared Spectroscopy (Article)

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Abstract

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Pereskia bleo is a species of primitive cactus. In the present study, infrared spectroscopy was used to characterize the antioxidant activity of P. bleo leaves by multivariate analysis. A total of twenty-four extracts were prepared in different solvents. Antioxidant activities were measured by 1,1-diphenyl-2-picrylhydrazyl assay and fingerprinted by infrared spectroscopy between 4000 and 400 cm^{-1} at a resolution of 2 cm^{-1}. A three component multivariate orthogonal partial least squares model with R^2Y of 0.88 and Q^2 of 0.86 was developed to correlate infrared spectra with antioxidant activity and evaluated by internal cross-validation and a true external test. For external validation, bioactivity of new extracts of P. bleo was predicted using the model, and -OH, -NH, and -CH were identified as functional groups responsible for the activity. In summary, a successful orthogonal partial least squares model was developed using infrared spectroscopy as a rapid method to predict antioxidant activity. © 2014 Copyright Taylor & Francis Group, LLC.

Author keywords

Antioxidant activity Fourier transform infrared spectroscopy Orthogonal partial least squares Pereskia bleo

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