Prediction of Antioxidant Capacity of Thai Indigenous Plant Extracts by Proton Nuclear Magnetic Resonance Spectroscopy

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ABSTRACT

Antioxidant capacities of the ethanol extracts from 28 Thai indigenous plants were determined by FCRC, DPPH, ABTS and FRAP assays. Proton nuclear magnetic resonance spectra of the extracts dissolved in D_2O were measured at 300 MHz. The antioxidant capacity and integrated peaks of nuclear magnetic resonance (NMR) spectra were analyzed by partial least square (PLS) regression. Linear correlation was found between the actual and predicted antioxidant capacities of all assays with R^2 more than 0.84 for calibration models and more than 0.54 for cross-validation models. However, these values were lower than those using infrared (IR) spectroscopy in our previous study. The lower efficiency of NMR-PLS regression might be due to the integrated NMR spectra having lower resolution than the whole IR spectra. Therefore, full NMR spectra should be further investigated for predicting the antioxidant capacity or other biochemical properties of plant extracts.

Keywords: Thai plants, Antioxidant capacity, Nuclear magnetic resonance spectroscopy, Partial least square regression

INTRODUCTION

Plants are important sources of phytochemicals with various biological activities, including antioxidant activity, which has been studied extensively. Antioxidants inhibit free radicals by hydrogen atom transfer or electron transfer. Various assays should be conducted to evaluate the total antioxidant capacity of a sample (Karadag et al., 2009). Commonly used antioxidant assays include 1,1-diphenyl-2-picrylhydrazyl (DPPH), 2,2′-azinobis (3-ethylbenzothiazoline-6-sulfonic acid) diammonium salt (ABTS), ferric reducing antioxidant power (FRAP),