ABSTRACT

Andrographis paniculata with a local name of Sambiloto is known for its pharmacological activities for treating common-cold, anti-inflammatory, immunomodulatory, antihyperglycemic, hepatoprotective, antimicrobial and antiparasitic, anticancer, cardiovascular effect, antihyperlipidemic, antipyretic, and antioxidant effect. One of the main active constituents in *A. paniculata* is andrographolide (ANDR). This research aimed to determine the levels of ANDR by correlating the absorbances of FTIR spectra with ANDR contents as determined by HPLC chromatogram, assisted by multivariate calibrations. *A. paniculata* herbs from several regions were powdered. The powdered samples were measured in terms of FTIR spectra. Besides, a weighted sample was subjected to the extraction procedure. The extracts were measured in terms of the HPLC chromatogram. Data obtained are then used as variables during chemometrics analysis using principal component regression (PCR) and partial least square regression (PLSR). These multivariate calibrations were compared and used to build the prediction models at optimized FTIR spectra regions. The selection of multivariate calibrations, wavenumbers region, and FTIR spectra modes based on the highest R^2 for the correlation between actual values of ANDR as determined by HPLC and FTIR predicted values and lowest values of root mean square error of calibration (RMSEC) and root mean square error of prediction (RMSEP). The result indicated that HPLC method was useful to evaluate ANDR content in *A. paniculata* herb. PLSR using second derivative FTIR spectra at the wavenumbers region of 3700-665 cm^{-1} was selected for quantification of ANDR with *R* values of 0.9997 and 0.9765 in calibration and validation models, respectively and R^2 values of 0.9994 and 0.9536 in calibration and validation models, respectively. The values RMSEC and RMSEP obtained were 0.005% and 0.055%, respectively. Fourier transform infrared (FTIR) spectroscopy in combination with PLSR was successfully used for quantitative analysis of ANDR.

Keywords: *Andrographis paniculata*, FTIR spectra, HPLC, Partial Least Square Regression, Principal Component Regression

ABSTRAK

Andrographis paniculata atau biasa disebut dengan Sambiloto diketahui memiliki berbagai aktivitas farmakologi yaitu dalam pengobatan *common-cold*, antiinflamasi, imunomodulator, antihiperglikemi, hepatoprotektor, antimikroba, antiparasit, antikanker, efek kardiovaskular, antihiperlipid, antipiretik, serta efek antioksidan. Salah satu kandungan aktif utama dalam *A. paniculata* adalah andrographolide (ANDR). Penelitian ini bertujuan menentukan kandungan ANDR dengan korelasi antara nilai absorbansi pada spekra FTIR dengan kandungan ANDR berdasarkan pengukuran kromatogram HPLC menggunakan kalibrasi multivariat. Herba *A. paniculata* dari berbagai daerah diserbukkan. Spekta FTIR dari serbuk sampel dibaca. Selain itu, sejumlah serbuk sampel diekstraksi. Kromatogram HPLC dari ekstrak dianalisis. Data yang diperoleh digunakan sebagai variabel dalam analisis kemometri menggunakan principal component regression (PCR) dan partial least square regression (PLSR). Kedua kalibrasi multivariat dibandingkan dan digunakan untuk membentuk model prediksi pada daerah spektra FTIR optimal. Pemilihan jenis kalibrasi multivariat, daerah bilangan gelombang, dan spektra FTIR ditentukan berdasarkan nilai R^2 tertinggi pada korelasi antara nilai ANDR sebenarnya yang ditentukan berdasarkan HPLC dan nilai prediksi berdasarkan FTIR dan nilai terendah dari root mean square error of calibration (RMSEC) dan root mean square error of prediction (RMSEP). Hasil penelitian menunjukkan metode HPLC berguna dalam evaluasi kandungan ANDR pada herba *A. paniculata*. PLSR menggunakan derivat-2 spektra FTIR pada daerah bilangan gelombang 3700-665 cm^{-1} digunakan dalam kuantifikasi ANDR dengan nilai *R* 0.9997 dan 0.9765 berturut-turut pada model kalibrasi dan validasi serta nilai R^2 0.9994 dan 0.9536 pada model kalibrasi dan validasi secara berurutan. Nilai RMSEC and RMSEP yang diperoleh adalah 0.005% dan 0.055% secara berurutan. Fourier transform infrared (FTIR) spektroskopi dikombinasikan dengan PLSR dapat digunakan dalam analisis kualitatif ANDR.

Keywords: *Andrographis paniculata*, spektra FTIR, HPLC, Partial Least Square Regression, Principal Component Regression