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ORIGINAL PAPER

PARAFAC modeling of dandelion phenolic compound fluorescence relation to antioxidant properties

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Abstract

The phenolic compounds in dandelion were extracted using different ethanol percentage solutions, identified with HPLC-MS, and their scavenging capabilities of DPPH, ABTS and OH radicals were determined. Then the excitation-emission matrix fluorescence spectroscopy coupled with parallel factor analysis (PARAFAC) was conveyed to analyze the relationship between phenolics, components scores of PARAFAC model and antioxidant capacities, based on linear regression method. The results showed that the relative content of chicoric acid, esculetin, caffeic acid, gallic acid monohydrate, eupatilin, caffeic acid-3-glucoside, corchorifatty acid F, and luteolin was higher than 0.5%, and the extraction solutions with 100% and 75% water had a better scavenging capacity of DPPH, ABTS and OH radicals. Two components PARAFAC model was identified with the comparatively higher sum of squares, core consistency values, and lower interactions numbers, and the established equations indicated the component scores had a linear regression relationship with antioxidant capacities of DPPH, and ABTS. The paper was proposed for the first time that the component scores of PARAFAC model might be treated as a useful indication for antioxidant capacity evaluation.

Keywords Dandelion · Phenolic compound · Excitation-emission matrix · Parallel factor analysis · Antioxidant

Introduction

Oxidative stress is regarded as one of the key reasons causing human pathological processes, it originated from the generation of reactive oxygen species (ROS) and reactive nitrogen species (RNS), the harmful byproducts generated during the normal cellular functions, and lead to cardiovascular diseases, inflammation and cancer [1]. Natural products, such as phenolic compounds, play an important role in disease prevention, free radical scavenging, oxidative damage prevention and antioxidant effects, by modulating important processes in blood platelets, interfering various stages of coronavirus entry and replication cycle [2–4].

Dandelion (*Taraxacum mongolicum*) is a perennial herbaceous plant belonging to the Asteraceae family, it consists of more than 2500 species and is cultivated almost anywhere worldwide [5]. Numerous studies have linked dandelion to antioxidant properties in vitro and vivo, including the functions of oxidative stress and superoxide radical inhibiting activity, for the high levels of (poly)phenols [6–8]. Since the (poly)phenols could directly react in one-electron reactions with free radicals to prevent oxidative damage [9], or regulate various signals pathways induced by oxidative stress, the dandelion has also been investigated as a potential ingredient with anti-inflammatory, anti-obesity, antineoplastic effects. So it is widely used in the health care industry as dandelion tea, milk juice, tonic, diuretic, laxative, and wine [10].

In the last decades, the chemical components in the whole dandelion plant have been studied extensively, and an increasing number of dandelion (poly)phenol was discovered, such as luteolin, luteolin-7–O–glucoside, luteolin-7-diglucosides, apigenin, chicoric acid, chlorogenic and caffeic acid [11–14]. Caffeic acid, and chlorogenic acid, rich in leaves, flowers, roots, and stems, demonstrates good performance on tyrosinase inhibitory, DPPH radical, and superoxide anion radical scavenging ability [15]. Quercetin could protect DNA from

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oxidative damage from the attack of ·OH, H_2O_2, and O^{2-} [16]. While luteolin, apigenin, quercetin, and catechin showed inhibitory effects on the MAPK pathway to reduce oxidative stress [15, 17]. Based on these health beneficial effects, different extracts with various phenolic compounds were prepared and their antioxidant capacities were determined as well. The phenolic of chicoric acid was proved as the predominant compound in the 50 and 85% ethanol extract of leaf, and 50% ethanol extraction of petal, but the 85% ethanol extractions did not contain any phenolic acids. In addition, the 50% ethanol extraction of leaf could reduce the oxidation of platelet lipid peroxidation with a hydroxyl radical donor (H_2O_2/Fe^{2+}) and thiol groups in plasma proteins, and the inhibition effect was only about 70% for individual chicoric acid at the same content in extractions [7]. The results indicated that the antioxidant activities of the extracts from different parts of dandelion were different, and the phenolic compounds structure and content lead to the difference [18, 19]. Therefore, determining the species and content of phenolic compounds is the basis for evaluating their antioxidant activities.

Due to the rapid detection of various chemical components and biological activity in a non-destructive and non-polluting manner, Excitation-Emission Matrix is commonly used to investigate fluorescence spectroscopy [20, 21]. It plays important roles in the application of the detection of chemical components and quality characteristics investigating through multivariate data analysis [20]. The extreme complexity of food components, along with the phenomena such as quenching and the reaction of several components, cause the interpretation of EEM challenge. But the conjunction with powerful chemometric tools, such as (parallel factor analysis) PARAFAC analysis, can simplify data analysis of the EEM as the sum of several fluorescence compounds exist in the analyzed sample, which could be used for phenolic compounds evaluation.

In order to explore the relationship between the dandelion phenolic compounds species, contents, and their antioxidant activity, the dandelion phenolic compounds in different extractions were determined with HPLC-MS, the excitation-emission matrix spectra (EEMs) coupled with PARAFAC analysis, antioxidant capacities of DPPH, ABTS, and OH radicals were conveyed. And the series of regression equations were established to determine the regression models of phenolics content, antioxidant capacities, and component characteristics from EEMs coupled with the parallel factor analysis algorithm.

Materials and methods

Materials and chemicals

Dandelion powder (3000 mesh) of the whole grass plant (Hebei, China), purchased from a local pharmacy (Taian, Shandong), stored in sealed light-resistant packaging at − 20 °C before use. The ethanol and formic acid used for HPLC-MS analysis were of chromatographic grade and obtained from Tianjin KaiTong Chemical Reagent Co., LTD (Tianjin, China). Diphenyl-1-picrylhydrazyl (DPPH), Diammonium 2,2′-azino-bis (3-ethylbenzothiazoline-6-sulfonate) (ABTS), salicylic acid, and ferrous sulfate were of analytical grade and purchased from Shanghai Macklin Biochemical Co., LTD (Shanghai, China). Amberlite XAD-7HP macroporous resin was obtained from Shanghai Aladdin Bio-Chem Technology Co., Ltd. (Shanghai, China).

Preparation of phenolic extractions from dandelion

Thirty grams of dandelion powder was mixed with 300 ml ethanol solutions (acidified with 1 ‰ formic acid, containing different ethanol percentages of 0, 25, 50, 75, and 100%). Phenolic compounds in powder were extracted for 20 min using an ultrasonic extractor operated at a frequency of 40 kHz. The solution was centrifuged at 8000 rpm for 30 min, then filtered with qualitative filter paper (15–20 μm, 15 cm). The obtained extract was loaded to the Amberlite XAD-7HP macroporous resin column (50 × 1.6 cm), then the column was washed with 20-fold resin volumes of 0.1% formic acid–water solution at a flow rate of 2.0 ml/min to remove the hydrophilic compounds, followed with tenfold volume of 0.1% formic acid–ethanol solution to collect a phenolic fraction [22]. The eluents were collected and filtered through a 0.22 μm nylon filter for HPLC-MS analysis.

Determination of phenolic compounds

Phenolic compounds in the eluents were separated and identified with HPLC-MS/MS (LTQ Orbitrap Elite, Thermo Scientific™ Technologies) [23]. The mobile phase was composed of 1 ‰ formic acid–water (eluent A) and 1 ‰ formic acid–ethanol (eluent B) at a flow of 0.3 ml/min in gradient elution mode. Gradient elution started at 30.0% B, increased the concentration linearly to 60.0% within 30 min, held for 10 min; and rise to 70% within 10 min, maintain for 20 min; increased to 80% in following 20 min and stayed for another 10 min; then increased to 100% with 20 min. An aliquot (10 μl) of the sample was injected into a Venusil MP C18 column (4.6 × 250 mm, 5 μm) (Agela Technologies, USA) for separation, the wavelength was set at 280 nm. Electrospray ionization (ESI) source was set in negative ion mode and full scan mode, and other conditions as follows: mass spectral range, 100–1000 m/z; capillary temperature, 325 °C; heat block temperature, 300 °C; source voltage, 3.50 kV.

The obtained mass spectrometry data were then uploaded to the XCMS online platform (http://xcmsonline.scripps.edu) for retention time correction, peak alignment, feature detection, annotation, and statistical analysis [24]. Default

parameters were accepted for mass tolerance of 5 parts per million, minimum peak width of 10 s, and maximum peak width of 60 s. Phenolic compounds with contents for comparison larger than 0.5% were chosen and subjected for qualitative analysis using the daughter scan with the default tuning parameters and optimized collision energy of 15 eV. All the daughter peaks were identified by matching the fragmentation patterns to experimentally documented in former literature.

Antioxidant capacity determination

(1). DPPH· radical scavenging activity

DPPH· radical scavenging activity of dandelion phenolic compounds extracted from different ethanol percentage solvents was determined using the modified methods [25, 26]. DPPH· has an intense violet color with the maximum absorbance at 517 nm, but turns colorless when scavenged by antioxidants. Reaction solutions containing 2 ml of alcoholic solution of DPPH· (0.2 mM) and 2 ml dandelion phenolic extracts were incubated in a water bath at 25 °C for 30 min, an aliquot of sample from the reaction solution was placed into a cuvette, and the absorbance was measured at 517 nm. The radical scavenging activity was calculated as follows:

$$\text{DPPH}\cdot \text{ radical scavenging percentage}\,(\%) = \left(1 - \left(A_1 - A_S\right)/A_0\right) \times 100 \quad (1)$$

where A_0 is the absorbance of DPPH· solution, A_1 is the absorbance of DPPH· and phenolic solution, and A_S is the absorbance of phenolic solution.

(2). $ABTS^{\cdot+}$ radical cation scavenging activity

The antioxidant capacity of dandelion phenolic solutions was analyzed by investigating the ability to scavenge the $ABTS^{\cdot+}$ radical using the modified method [27]. The $ABTS^{\cdot+}$ cation radical solution was prepared by mixing $ABTS^{\cdot}$ solution (7 mM) and potassium persulfate solution (2.45 mM), incubated in the dark for 12 h and diluted to the absorbance of 0.70 ± 0.02 at 734 nm. Then 2 ml of $ABTS^{\cdot+}$ cation radical solution was mixed with the same volume of dandelion phenolic extract, the mixture absorbance was measured at 734 nm [28, 29]. The $ABTS^{\cdot+}$ radical scavenging percentage was calculated according to the following equation:

$$ABTS^{\cdot+} \text{ radical scavenging percentage}\,(\%) = \left(\left(A_c - A_s\right)/A_c\right) \times 100 \quad (2)$$

where A_c is the absorbance of $ABTS^{\cdot+}$ solution, A_s is the absorbance of ABTS and phenolic extract solution.

(3). $^{\cdot}OH$ radical scavenging activity

The ·OH radical scavenging activity of dandelion phenolic solutions was carried out using the modified method [30]. The reaction solution, containing 100 µl of ferric sulfate (9 mM), salicylic acid (9 mM) and hydrogen peroxide (8.8 mM), was mixed with 100 µl of phenolic extracts and incubated at 37 °C for 30 min. Then 200 µl of the mixture was transferred to the 96-well plate, and absorbance at 510 nm was measured. The $^{\cdot}OH$ radical scavenging activity of the extracts was calculated:

$$^{\cdot}OH \text{ radical scavenging percentage}\,(\%) = \left(1 - \left(A_1 - A_S\right)/A_0\right) \times 100 \quad (3)$$

where A_0 is the absorbance of the reaction solution, A_1 is the absorbance of reaction, and A_S is the absorbance of the phenolic extract solution.

Acquisition of EEMs

The dandelion phenolic extractions were diluted fivefold with particle-free water, and filtered with a 0.22 µm tube filter to avoid inner filter effects [31]. The samples were transferred into a 1 cm path length cuvette at 20 °C, and the excitation-emission matrix fluorescence spectra were recorded at an integration time of 0.1 s using the FL6500 fluorescence spectrometer (PerkinElmer, U.S.A.). EEM spectra were collected with subsequent scanning emission spectra from 250 to 500 nm at 5 nm increments by varying the excitation wavelength from 200 to 390 nm at 1 nm increments. Both excitation and emission slits were set as 5 nm.

PARAFAC model and analysis

After removing outliers with the preliminary examination of data, PARAFAC statistically decomposes the three-way excitation-emission matrix spectra into individual fluorescence components and a residual matrix. The individual fluorescence components are directly proportional to the component concentration in the sample, and could be converted into actual concentration when excitation and emission of each component is known.

$$x_{ijk} = \sum_{n=1}^{F} a_{in} b_{jn} c_{kn} + \varepsilon_{ijk}$$

where, X_{ijk} is the fluorescence intensity of the ith dandelion phenolic extraction at the kth excitation and jth emission wavelength, a_{in} is directly proportional to the concentration of the nth fluorophore in the ith sample, b_{jn} and c_{kn} are estimates of emission and excitation spectra of nth fluorophore at wavelength j and k. F is the number of the components, and ε_{ijk} is the residual matrix [32].

The PARAFAC analysis with the EEMizer algorithm [32, 33] was performed using the PLS toolbox software (Eigenvector Research, Inc. trial license) developed for MATLAB. This software first eliminated Rayleigh and Raman scattering peaks of each scan centered on the respective scatter peak by excising portions (10 and 20 nm at each excitation wavelength), and the default PARAFAC constraints (no negative values in concentration, emission and excitation wavelength) were applied to process the data. The PARAFAC models were tested with a range from one component to five components by the fit-values, core consistency, and split-half quality calculation. Samples with high leverage (the elements on the diagonal of the hat matrix of the score matrix) or high sum-squared residual were removed until no samples were assessed as the outliers, and the PARAFAC model of proper component number was identified.

Statistical analysis

All the samples for the EEM scan were repeated six times, and data were expressed as mean ± standard deviation. The linear regression and one-way analysis of variance (ANOVA) analysis were carried out using the Origin 7.5 software (Origin Lab, Northampton, USA). The Duncan's multiple range test was used to determine the significance of the differences among the means (differences were considered statistically significant at $p < 0.05$).

Results and discussion

EEM fluorescence spectra

The raw EEM was obtained in the excitation range of 200–390 nm and the emission range of 250–550 nm. As shown in Fig. 1, the different polarity extractions showed fluorescence fingerprints with three relatively intense bands, and their maximum excitation/emission wavelength was about 220 nm/330 nm, 280 nm/330 nm, and 330 nm/450 nm, which is related to phenolic compounds in this experiment. In addition, the intensity fluorescence band of 330 nm/450 nm was around 6.6×10^6, while the intensity

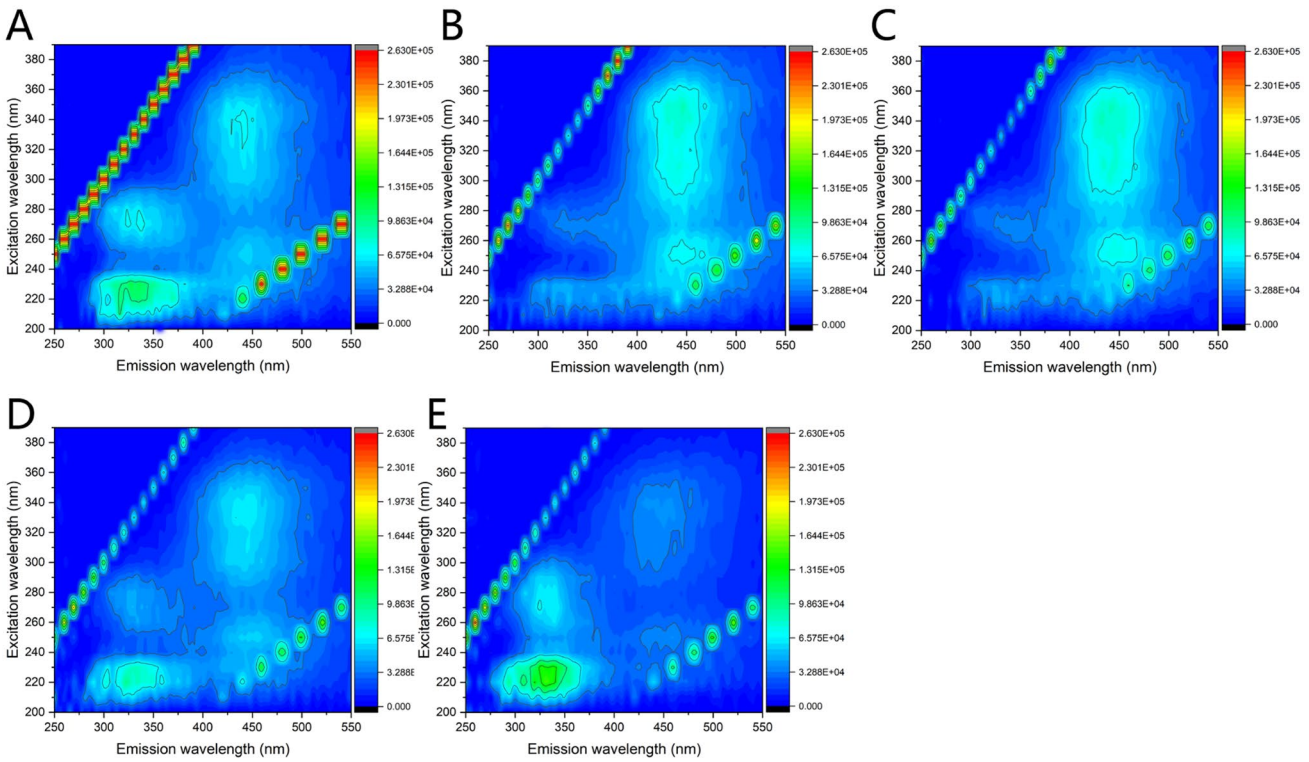

Fig. 1 Contour maps of EEM fluorescence of dandelion phenolic compounds solutions (letter **A**–**E** referred the solutions containing 0%, 25%, 50%, 75% and 100% ethanol)

of fluorescence bands of 220 nm/330 nm, 280 nm/330 nm varied significantly among extractions. As ethanol percentage increases, the water-soluble phenolic compounds content increased first and decreased with lower polarity and hydrophilicity [19]. To compare and evaluate the phenolic compounds species and concentration effects on the fluorescence spectra, the PARAFAC method was used to determine the fluorescent components and corresponding spectral characteristics.

PARAFAC analysis

After removing the Rayleigh and Raman scattering from the fluorescence spectra, the PARAFAC models were tested from a component number of 1–5. In order to identify proper component number, the residual sum of the square, core consistence, and interaction number were compared and evaluated. As shown in Fig. 2A–C, the residual sum of the squares, decreased as more components were selected. The core consistency analysis of the first two components models remained at 100 and decreased of the three, four and five components models, while the interaction number decreased slightly at the two components model. Based on the higher core consistency and lower interaction number, the two components model was identified for the fluorescence dataset with some variability remaining in the residuals, while the three, four and five components models were rejected for their lower core consistency and higher interaction numbers. Although the two components model was determined, it does not suggest that only two types of fluorophores were

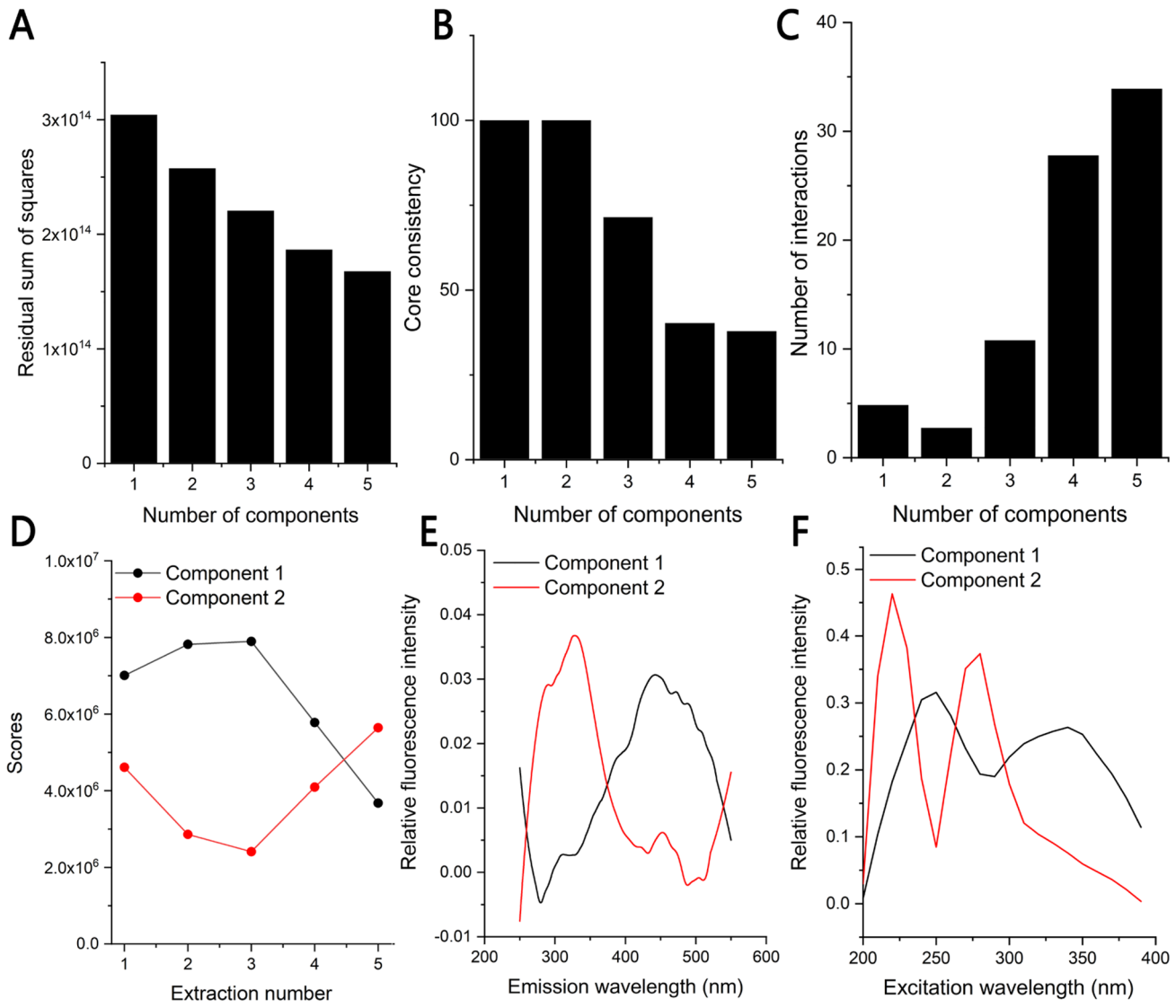

Fig. 2 Identification and characteristics of PARAFAC model (letter **A**–**C** referred the residual sum of squares, core consistency, and interaction number analysis of PARAFAC model, letter **D**–**F** were corresponding component scores, emission and excitation spectra)

present in these extractions, the model only suggested that two components were present in the majority of the samples. Figure 2D–F showed the excitation and emission loadings and relative concentrations identified from the two component PARAFAC model. The first component with black color had two excitation wavelengths of 230 and 330 nm, and one emission wavelength of 450 nm, while the second component with red color had two excitation maximum wavelengths at about 220 and 280 nm, and one emission maximum at about 330 nm. The excitation and emission fluorescence spectra of the second component were the same as the classic phenolic compounds fluorescence, and the first component fluorescence characteristics might be related to the energy transfer or interactions of phenolic molecules [34]. The scores of component one increased at ethanol percentage of 25 and 50%, then decreased at higher ethanol proportion, while the scores of component two showed the opposite tendency.

Determination of phenolic compounds in extract solutions

The HPLC-MS was used to separate and identify the phenolic compounds in different ethanol percentage extractions. As shown in supplement Fig. S1, all the phenolic compounds in different extractions were isolated using the optimized liquid system. The isolated compounds were then analyzed using the full scan model, and the mass data were submitted to the XCMS website for data analysis. The relative content of phenolic compounds higher than 0.5% were selected and their fragment ions information was obtained using the daughter scan model. Supplement Fig. S2 showed the m/z information of nine selected phenolic compounds, which were identified as chicoric acid, esculetin, caffeic acid, gallic acid monohydrate, eupatilin, caffeic acid-3-glucoside, corchorifatty acid F, luteolin [14, 35, 36]. As shown in Table 1 and Fig. 3, relative intensities and changes of phenolic compound in the majority were analyzed. All the phenolics content changed significantly in different ethanol percentage extractions, and a downtrend phenomenon occurred with a higher ethanol ratio. Chichoric acid, esculetin, caffeic acid, and gallic acid monohydrate were the top four phenolic compounds in dandelion, and their content decreased with the increases of the ethanol percentage, while the luteolin and unknown one showed reversed trend. The content of eupatilin and caffeic acid-3-glucoside decreased and reached to the lowest at 50% ethanol, and increased with higher ethanol percentage.

Antioxidant capacities analysis

Three determination methods of DPPH, ABTS and OH radicals were conveyed to compare the antioxidant potential

Table 1 Content analysis of phenolic compounds in different extractions

Compounds	m/z	0% ethanol		25% ethanol		50% ethanol		75% ethanol		100% ethanol	
		Peak area	Percentage	Peak area	Percentage	Peak area	Percentage	Peak area	Percentage	Peak area	Percentage
Chicoric acid	473	7.60E+07	7.8607	3.20E+08	2.9178	3.58E+07	2.4008	3.70E+07	2.4420	–	–
Eupatilin	343	3.63E+07	3.7550	3.41E+08	3.0315	2.25E+07	1.5108	3.01E+07	1.9924	8.72E+06	2.2027
Caffeic acid-3-glucoside	341	9.05E+06	0.9354	9.34E+07	0.8305	6.57E+06	0.4404	1.04E+07	0.6899	3.15E+06	0.6321
Corchorifatty acid F	327	3.84E+07	3.9688	4.88E+08	4.3517	3.58E+07	2.4000	6.77E+07	4.4737	1.43E+07	2.2027
Unknown	309	3.74E+06	0.3868	7.33E+07	0.6557	1.24E+07	0.8345	2.69E+07	1.7776	1.73E+07	2.2027
Luteolin	285	6.71E+05	0.0694	5.86E+07	0.6761	7.58E+07	5.0830	6.08E+07	4.0154	3.77E+07	2.0055
Gallic acid monohydrate	187	5.45E+07	5.6361	3.79E+08	3.2853	3.62E+07	2.4311	4.39E+07	2.9039	1.59E+07	1.9856
Caffeic acid	179	6.39E+07	6.6025	4.39E+08	3.8669	3.48E+07	2.3333	2.25E+07	1.4861	7.68E+06	1.0627
Esculetin	178	8.94E+07	9.2415	1.15E+09	10.2721	9.71E+07	6.5099	8.09E+07	5.3474	4.38E+07	1.2067

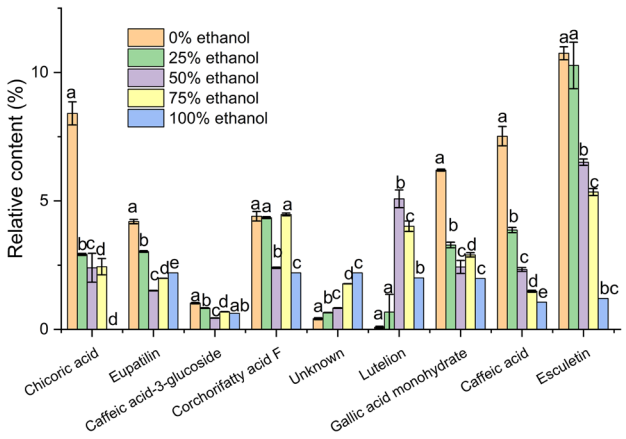

Fig. 3 Relative content of phenolic compounds in extractions

of different phenolic compounds extractions. The DPPH-colorimetric method mainly uses the free radical scavenger to provide an electron to pair with the lone pair of DPPH free radicals, making itself purple into yellow, absorbance wavelength decreasing, and the color change value is linear with the free radical scavenging capacities [37]. ABTS can be oxidized by $K_2S_2O_8$ to generate blue-green free radical cation $ABTS^{\cdot+}$, it is stable and could react with antioxidants, losing color and absorbance at 734 nm [29]. For OH radical scavenging reaction, salicylic acid quickly produces a purple compound of 2,3-dihydroxybenzoic acid with ·OH, which has the maximum absorption at 510 nm and can be reduced by antioxidants [38]. And the extraction absorbance change was in a linear relationship with their free radical scavenging ability.

The DPPH, ABTS, and OH radical scavenging activity of phenolic compounds extractions were determined and shown in Fig. 4. For DPPH and ABTS assay, the scavenging activities were 94.44% and 98.91%, and no significant difference existed in the extractions with ethanol percentage ranging from 0 to 75%, while the antioxidant activities of pure ethanol extraction decreased significantly to 44.39 and 87.30% respectively. Although the content of chicoric acid, gallic acid monohydrate, and esculetin decreased with higher ethanol percentage, the stable antioxidant potential might be related to the undetected phenol and other compounds (eupatilin, corchorifatty acid, luteolin, and the unknown) content change, whose content increased at higher ethanol percentage or remained. The OH radical scavenging activity of extraction with 0, 25 and 50% ethanol increased from 10.02% to the maximum of 25.68% at 75% ethanol percentage, and decreased to 26.44% at 100% ethanol extraction. The relatively higher errors might cover the OH scavenge capacities difference between the extractions of lower ethanol percentage, but its tendency was the same as DPPH, ABTS antioxidant potential.

Analysis of PARAFAC modeling of phenolic compounds and antioxidant potential

According to the mass spectra analysis, the content of individual phenolic compounds in extractions varied with different ethanol percentages, and this difference leaded to the EEMs change, as well as the scores of the corresponding component obtained from the PARAFAC model. And the antioxidant capacities of DPPH, ABTS, and OH radicals were also related to the phenolic content. So a series of regression models were established to explore the relationship between these characteristics.

(1). Analysis of phenolic compounds content and antioxidant potential

In order to find the most effective phenolic compounds, the stepwise linear regression models between identified phenolic compounds concentration (chicoric acid, corchorifatty acid F, luteolin, esculetin, eupatilin, caffeic acid-3-glucoside, gallic acid monohydrate, caffeic acid, and total phenolics content) and antioxidant parameters of DPPH, ABTS, and OH radicals scavenging activity were set respectively. Chicoric acid, corchorifatty acid F, luteolin, and

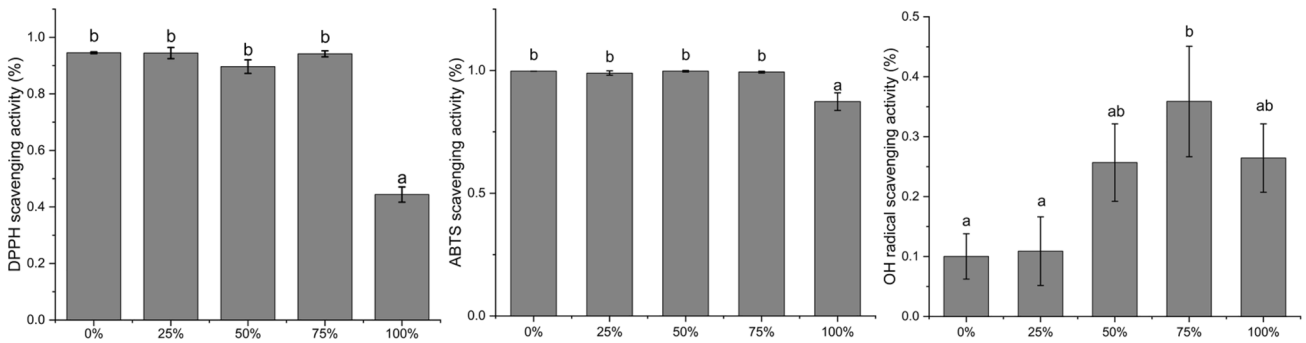

Fig. 4 Antioxidant capacities of DPPH, ABTS and OH radical scavenging activity of dandelion phenolic compounds extractions

esculetin were included in the model, while others phenolic, as well as the total phenolics content were excluded from all these linear models. The normalized regression coefficients were 0.13, 0.29, 0.71 and 0.83 in linear model related with DPPH, 0.33, 0.42, 0.61 and 0.80 in model of ABTS, and 0.11, 0.55, 0.68 and 0.91 in OH radical scavenging model. In addition, the regression coefficients of esculetin and luteolin were larger than other phenolics, and this might be related with their comparatively higher content.

(2). Analysis of phenolic compounds content and PARAFAC models

Two components PARAFAC model was selected and the corresponding scores were calculated when the excitation and emission spectra identified. The linear regression models of phenolic compounds content and components scores were established to explore the inner relationship. Similar to the antioxidant analysis results, chicoric acid, corchorifatty acid F, luteolin, esculetin were included in the linear model, their normalized coefficients were − 0.28, − 0.30, 0.45, and 1.48 in the regression model of component I, 0.76, 0.26, − 0.63, and − 1.61 in the regression model of component II. The excitation and emission spectra of component II was consistent with the classic phenolic compounds, and the higher normalized coefficients of scores could also indicated the close relationship when compared to component I. The PARAFAC model indicated two fluorophores were in majority of these extractions, but the obtained components have not been identified yet. Esculetin or chicoric acid might be the component II, for their higher coefficient, but more research is needed to discover the relationship.

(3). Analysis of PARAFAC components scores and antioxidant potential

The relationship between the components scores from PARAFAC model and antioxidant potential was also explored based on linear models. The normalized coefficients of components I and II were 1.06 and 0.21 with the dependent variable of ABTS scavenging value, 1.10 and 0.29 with the dependent variable of DPPH, and − 1.64 and − 1.31 with OH radical scavenging. The determination coefficients of the three linear models were 0.77, 0.74, and 0.64, indicating the PARAFAC model cores were not well fit linear regression with antioxidant potential, but the inner relationship between the computed component scores and their antioxidant potential was proved. Phenolic compounds content difference leads to the change of antioxidant potential, excitation-emission matrix, as well as the component scores in PARAFAC model. The errors of default PARAFAC limitation, component number selection and antioxidant potential evaluation might account for the lower determination coefficients, and more work focusing on the used defined limitation in PARAFAC model establishment are needed to improve the fitness between computed scores and antioxidant potentials.

Conclusion

The species and content of phenolic compounds in dandelion were determined, and their DPPH, ABTS, and OH radical scavenging activity, emission-excitation fluorescence spectra, and PARAFAC analysis were conveyed. Then regression models of the predominant phenolic compounds content, components score, and antioxidant capacities were established to explore the inner relationship. The result indicated that the two components model was successfully identified with EEMs and PARAFAC method, and the corresponding component scores were in linear regression with DPPH, ABTS radical scavenging activity. The chicoric acid, corchorifatty acid F, luteolin, esculetin were the majority compounds in extraction and were proved to have a linear relationship with antioxidant capacities, as well as the components score. The paper proved that component scores from two components PARAFAC model of phenolic compounds extractions could be used as a useful indicator for phenolic content and antioxidant capacity evaluation.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/s11694-022-01389-z.

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Author contributions PW: Data curation, Conceptualization, Methodology, Software, Formal analysis, Writing—original draft. TB: Visualization, Validation. HZ: Writing—review & editing, Supervision, Visualization, Project administration. YC: Writing—review & editing, Supervision, Visualization, Resources, Project administration, Funding acquisition.

Declarations

Conflict of interest The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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