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RESEARCH ARTICLE

Evaluation of Essential and Toxic Element Concentrations in Buckwheat by Experimental and Chemometric Approaches

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Abstract

The essential and toxic element concentrations in buckwheat were analyzed by inductively coupled plasma optical emission spectrometer (ICP-OES). The concentration data were subjected to common chemometrics analyses, including correlation analysis (CA), principal component analysis (PCA) and hierarchical cluster analysis (HCA), to gain better understanding of the differences among the tested samples. Our results indicated that the essential and toxic element concentrations were not different between *Fagopyrum tataricum* (L.) Gaertn and *F. esculentum* Moench. The element concentrations varied among buckwheat samples from different sources. Commercial tartary buckwheat tea contained several essential elements, thus, could be used as the source of essential elements. The detection of toxic heavy metals in commercial tartary buckwheat tea suggested that safety issue of such buckwheat products should be seriously concerned. Our results also revealed that the place of origin and the processing protocol of tartary buckwheat affected the element concentrations of the commercial form. The implications to the quality control and safety evaluation of buckwheat were extensively discussed.

Key words: buckwheat, ICP-OES, trace element, toxic element, chemometrics

INTRODUCTION

Originated from China, buckwheat belongs to *Fagopyrum* (Polygonaceae) and is widely planted worldwide (Wijngaard and Arendt 2006). Currently, there are 15 species and many mutations of buckwheat reported. The most planted buckwheat species are *Fagopyrum tataricum* (L.) Gaertn and *F. esculentum* Moench. Buckwheat becomes more and more popular these years, because it holds great values from the nutriological and pharmacological perspectives (Christa and Soral-Smietana 2008). The proteins, vitamins and trace elements in buckwheat are generally higher than those in rice, wheat and also corn. More importantly, the amino acids in buckwheat are more balanced, making buckwheat more valuable (Pomeranz and Robbinas 1972). Previously, we found that trace emodin, a bioactive compound, existed in tartary buckwheat and its products (Peng *et al*. 2013). Buckwheat also helps controlling the blood glucose, blood cholesterol, blood pressure, and oxidative stress

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(Yao *et al*. 2008; Lin *et al*. 2008; Kim *et al*. 2009; Inglett *et al*. 2011). Buckwheat might even be useful in cancer treatment (Kim *et al*. 2007). Thus, commercial buckwheat products are produced and distributed rapidly. While great efforts are paid to the market development, the quality control and safety evaluation of buckwheat are scarce currently. Many studies have focused on the amino acids and other nutrition of buckwheat (Christa and Soral-Smietana 2008).

Trace elements are important and essential for human health. The lack and/or excess of certain element would lead to unwanted toxicity. Moreover, there might be toxic elements in buckwheat, considering that heavy metal pollutions occur frequently in China. Unfortunately, the information on the element concentrations of buckwheat is still lacking. Only several pilot studies concerned the trace element concentrations of buckwheat. Bonafaccia *et al*. (2003) reported the Se, Cr, Rb, Zn, Fe, Co, Sb, Ba, Ni, Ag, Hg, and Sn contents in the flour and bran of buckwheat, where most trace elements are concentrated mainly in the bran. Mestek *et al*. (2007) analyzed the Co, Cu, Fe, Mn, Mo, Ni, P, and Zn in extract of buckwheat flour. Other studies reported the metal concentrations in different parts of buckwheat (Liu *et al*. 2007). However, previous studies only analyzed several metals. The elemental pattern in buckwheat has not been determined yet. Only very recently, we published a paper concerning the element concentrations in different parts of buckwheat (Huang *et al*. 2013).

However, available information is far away from the thorough understanding of the elements in buckwheat. The influences of source, place of origin and species on the element concentrations of buckwheat have not been well documented yet. These factors are crucial in the production and quality control of buckwheat tea and other buckwheat products. Herein, we studied the essential and toxic element concentrations in buckwheat. The aim of our study is to compare the element concentrations in buckwheat by inductively coupled plasma optical emission spectrometer (ICP-OES). Different original and commercial forms of *F. tataricum* (L.) Gaertn and *F. esculentum* Moench were investigated, and the data were analyzed by correlation analysis (CA), principal component analysis (PCA) and hierarchical cluster analysis (HCA) to reveal the distribution rules of these elements. The implications to the quality control and safety evaluation of buckwheat were extensively discussed.

RESULTS

Element concentrations in buckwheat

The essential and toxic elemental concentrations were listed in Table 1 and Appendixes A and B. There were 23 elements detected in buckwheat samples. Generally, there were essential elements and also toxic elements in buckwheat samples. For example, K14 had the highest Zn concentration (48.7 $\mu g\ g^{-1}$) and the lowest value was detected in K1 (20.24 $\mu g\ g^{-1}$). The highest Pb concentration was found in K10 (21.155 $\mu g\ g^{-1}$) and the value was 0.79 $\mu g\ g^{-1}$ for K13. To reach a better understanding, the data were subjected to chemometrics analyses.

Correlation analysis

The correlation matrix analysis of 23 essential and toxic elements was presented in Table 2. Positive/negative correlation coefficients (r) indicate positive/negative correlations between the two elements. When the absolute value of r is close to 1, there is strong correlation between the two elements. When the r value is close to 0, the two elements are weakly or not related at all. For example, the toxic element Pb was highly correlated with Cr (r=0.90) and Sn (r=0.90). The element V was highly correlated with Al (r=0.99), Fe (r=0.89), Cu (r=0.71), and Ti (r=0.84).

Principal component analysis

To highlight the relationships between the 23 essential and toxic elements, the data were subjected to PCA. The first five principal components explained 82% of the total variance in the data. The loading values were listed in Table 3. The loadings expressed how well the principal components correlated with the old variables. The first principal component explained 28.1% of variance. It was positively correlated with Ca, Al, Fe, Si, Mn, Sr, and V very well. The second principal component explained 24.3% of variance and correlated closely with K, Mg, P, and Zn. The third principal component correlated well with Cr, Sn and Pb positively. It accounted for 14.6% of variance. The fourth principal component nega-