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Bioactive phytochemicals in wheat: Extraction, analysis, processing, and functional properties

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ABSTRACT

Whole wheat provides a rich source of bioactive phytochemicals namely, phenolic acids, carotenoids, tocopherols, alkylresorcinols, benzoxazinoids, phytosterols, and lignans. This review provides information on the distribution, extractability, analysis, and functional properties of bioactive phytochemicals present in wheat. Understanding the impact of processing on wheat phytochemicals allows us to develop improved processes with higher retention of bioactive compounds in processed wheat foods. Details of extraction, analytical methodologies and processing effects on bioactive phytochemicals in wheat are presented in tabulated form.

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1. Introduction

In 2013, Food and Agriculture Organization (FAO) of the United Nations forecasted world cereal production will reach around 2500 million tonne and wheat production to be around 700 million tonne (FAO, 2014). Grains and its processed products are consumed globally as important energy sources. Grain-based foods provide the majority of the carbohydrates, some proteins, oils, dietary fiber, and other micronutrients in many diets. During the past few decades research publications from universities, governmental, non-profit health, industrial, and trade organizations have encouraged increased consumption of whole grain food products due to their positive health benefits (Chanson-Rolle et al., 2014; Shahidi & Chandrasekara, 2013). According to United States Food and Drug Administration (FDA), cereal grains that consist of the intact, ground, cracked or flaked caryopsis, whose principal anatomical components (the starchy endosperm, germ, and bran) are present in the same relative proportions as they exist in the intact caryopsis, should be considered a whole grain food (FDA, 2006). The germ contains the plant embryo and the endosperm contains starch and storage proteins. Bran is the outermost layer which protects the inner portion of the grain from external weather, insect molds, and other microorganisms attack.

Previous studies have indicated that consumption of whole grain foods can significantly reduce the risk of some chronic health conditions such as type 2 diabetes, cardiovascular disease, and cancer (Landberg, Marklund, Kamal-Eldin, & Åman, 2014; Seo et al., 2015; Tucker et al., 2014). Initially, the health beneficial effect of whole grains was primarily attributed to its high fiber content. However, recent research indicates that the beneficial effect of whole grain may arise from the combined action of several components such as fiber, vitamins, phenolics,

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carotenoids, alkylresorcinols, and other phytochemicals (Piironen, Lampi, Ekholm, Salmenkallio-Marttila, & Liukkonen, 2009). The major grains include wheat, rice, corn, oats, rye, barley, sorghum, triticale, millet, amaranth, and teff. In Asia, nearly half of the annually consumed grain is rice, while the major grain consumed in Europe and US is wheat. The bioactive phytochemicals in wheat can be broadly subdivided into the following categories: phenolic acids, carotenoids, tocopherols, alkylresorcinols, and other miscellaneous compounds (sterols, steryl ferulates, benzoxazinoids and lignans).

Phenolic acids recognized as simple phenols can be divided into two subgroups. One is hydroxybenzoic acid derivatives, which include vanillic, syringic, *p*-hydroxybenzoic, and gallic acids. The other is hydroxycinnamic acid derivatives, which include ferulic, *p*-coumaric, caffeic, and sinapic acids (Luthria & Liu, 2013; Verma, Hucl, & Chibbar, 2009). The concentration of phenolic acids in whole wheat ranges from approximately 200 to 1200 mg/g dry matter basis (DMB) (Andersson, Dimberg, Aman, & Landberg, 2014). Ferulic acid is the primary and most abundant phenolic acid in wheat grain. Smaller concentrations of *p*-hydroxybenzoic, vanillic, syringic, *o*-coumaric, *p*-coumaric, salicylic, sinapic acids are also present in wheat (Liyana-Pathirana & Shahidi, 2006; Moore et al., 2005).

Whole wheat grain also provides moderate sources of vitamin E. The vitamin E includes four tocopherols and tocotrienols. Tocopherols have saturated phytyl side chains, while tocotrienols have isoprenyl side chain with three double bonds. Previous studies have confirmed the presence of α-, β-, δ-, and γ-tocopherols in soft and hard wheat grain (Moore et al., 2005; Panfili, Alessandra, & Irano, 2003). The spelt, durum, and soft wheat grains from Italy contained vitamin E in a range from 56.5 to 74.3 μg/g dry weight, respectively, with 66–77% tocotrienols (Panfili et al., 2003). In addition, the concentration of total tocopherols and tocotrienols in whole wheat samples varied between 27.6 and 79.7 μg/g (Lampi, Nurmi, Ollilainen, & Piironen, 2008).

In whole wheat grains, color has been most commonly used as a quality indicator. The color is primarily attributed to the presence of carotenoids and their esters. The concentration of total carotenoids in whole wheat ranged from 0.8 to 2.17 μg/g (Moore et al., 2005). Lutein and zeaxanthin were the most predominant carotenoids present in whole wheat, with concentrations of 0.5–1.44 and 0.2–0.39 μg/g grain, respectively (Moore et al., 2005). In addition, lower concentrations of carotenoids including β-cryptoxanthin at 0.01–0.13 μg/g, and β-carotene at 0.09–0.21 μg/g have also been detected in wheat.

Phenolic lipids, also known as alkylresorcinols (ARs), are commonly present in wheat (Gunenc, Hadinezhad, Tamburic-Ilincic, Mayer, & Hosseninian, 2013). Structurally the ARs are similar to tocopherols except for the presence of a straight aliphatic hydrocarbon side chain and a single phenolic ring. The alkyl side chain may contain between 13 and 27 carbon atoms. 5-N-alkylresorcinols, 5-alkenylresorcinols, 5-oxoalkylresorcinols, 5-oxoalkenylresorcinols, and 5-hydroxyalkenylresorcinols are the five major classes of ARs reported in the whole wheat. ARs in whole wheat range from 489 to 1429 μg/g (Ross et al., 2003).

Other bioactive phytochemicals have also been extracted and identified in whole wheat. In this review, they are grouped together as a "miscellaneous" group. The miscellaneous group consists of benzoxazinoids, lignans, phytosterols and steryl ferulates. Benzoxazinoids are a group of potent natural compounds which have recently been identified in whole grain wheat and rye grains and in bakery products of these cereals (Hanhineva et al., 2011; Pedersen, Laursen, Mortensen, & Fomsgaard, 2011). The total benzoxazinoids content in wheat is very low (5 μg/g DMB). Phytosterols are isoprenoid compounds, which are biosynthetically derived from squalene. Phytosterols are mostly found in free or esterified forms, including esters of fatty acids and phenolic acids, as well as glycosides or acylated glycosides. According to the study of Nurmi, Nyström, Edelmann, Lampi, and Piironen (2008), the content of phytosterols range is 670–959 μg/g DMB in whole grain winter wheat and 797–949 μg/g DMB in spring wheat. A portion of the phytosterols occurs in ferulic acid ester form, i.e. as steryl ferulates.

This contribution provides an overview of bioactive phytochemicals such as phenolic acids, carotenoids, tocopherols, alkylresorcinols, and other miscellaneous bioactive compounds that are commonly found in wheat grain (Table 1). The distribution of bioactive phytochemicals, their extraction, analysis, changes during processing, varietal differences, and functional properties will be presented and discussed.

2. Distribution of bioactive phytochemicals in wheat

All whole wheat grain products contain bran, germ, and endosperm fractions. It is well documented in the published literature that the bioactive phytochemicals are not uniformly distributed. Germ and bran fractions generally contain higher concentration of bioactive phytochemicals. This is evident from number of pearling studies described in the literature (Blandino et al., 2013; Liyana-Pathirana, Dexter, & Shahidi, 2006). Liyana-Pathirana et al. (2006) studied the effect of sequential removal of the outermost layers (pearling) on the phenolic composition of wheat grains. Higher levels of phenolic compounds have been reported in the bran fraction as compared to the refined grain fraction that primarily comprises endosperm. In a recent study, it was reported that most of the phenolic acids existed in bound insoluble form (80%) as compared to free soluble form, and high concentrations of phenolic acids were detected in whole grain which contains the bran fraction (627.8–745.6 μg/g dry weight) as compared to the refined grain (66.0–97.0 μg/g dry weight) (Lu, Fuerst et al., 2014).

The concentration of total carotenoids in wheat ranges from 0.7 μg/g in durum wheat from Spain to as high as 13.6 μg/g in Einkorn accessions from Italy. The highest concentrations of carotenoids are observed in the germ fraction followed by the bran and endosperm fractions. Similarly, tocopherols and tocotrienols are not uniformly distributed in grain. Higher concentrations of tocopherols are found in the germ or the outer layers and the concentration of tocopherols in the endosperm fraction is comparatively lower. Similarly, tocotrienols are found at higher concentrations in outer layer of the grain (85%, pericarp, testa, and aleurone) and only 15% in the endosperm fraction (Piironen et al., 2009).

In a recent study, Tanwir, Fredholm, Gregersen, and Fomsgaard (2013) investigated the levels of benzoxazinoids in