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Metabolite Profiling of Wheat Grains (*Triticum aestivum* L.) from Organic and Conventional Agriculture

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In some European community countries up to 8% of the agricultural area is managed organically. The aim was to obtain a metabolite profile for wheat (*Triticum aestivum* L.) grains grown under comparable organic and conventional conditions. These conditions cannot be found in plant material originating from different farms or from products purchased in supermarkets. Wheat grains from a long-term biodynamic, bioorganic, and conventional farming system from the harvest 2003 from Switzerland were analyzed. The presented data show that using a high throughput GC−MS technique, it was possible to determine relative levels of a set of 52 different metabolites including amino acids, organic acids, sugars, sugar alcohols, sugar phosphates, and nucleotides from wheat grains. Within the metabolites from all field trials, there was at the most a 50% reduction comparing highest and lowest mean values. The statistical analysis of the data shows that the metabolite status of the wheat grain from organic and mineralic farming did not differ in concentrations of 44 metabolites. This result indicates no impact or a small impact of the different farming systems. In consequence, we did not detect extreme differences in metabolite composition and quality of wheat grains.

KEYWORDS: Wheat grain; *Triticum aestivum*; organic; conventional; metabolite profiling; GC−MS

INTRODUCTION

Wheat (*Triticum aestivum*) is the most important cereal crop worldwide, with a production of 585×10^6 metric tons of grain per year (*1*). In the past decade the discussion about safer food with respect to the environment and residues of pesticides has changed consumer behavior to favor organically produced foods (*2*). In 2005, in some European community countries up to 8% of the agricultural area is managed organically according to European Union Regulation (EEC) No. 2092/91 (www.organic.aber.ac.uk/statistics/index.shtml). Consumers purchase organic products in special stores. Supermarkets also offer more and more food from organic agricultural production. But how healthy are these products in comparison to the conventional counterparts, and are there differences in metabolite composition? There are a number of studies comparing a limited number of key nutrients of wheat from organic and conventional origin. However, most of these studies have serious shortcomings. Food from the supermarket shelf and material with a lack of rigorously controlled conditions were used. Decisions on appropriate sites, cultivars, and harvest criteria can differ between organic and nonorganic products. Therefore, organic food claims cannot be substantiated through testing of samples derived form the marketplace (*3*). Some studies comparing organic and nonorganic foods continue to source products from retailers (*2*). Moreover, some analytical methods used are subject to criticism from the current point of view (*4*−*6*). Our aim was to obtain a metabolite profile for wheat rather than to determine the levels of some key nutritional substances. Such a profile is valuable, for example to assess the nutritional status of the grain and to compare wheat that originates from different growing regimes. The metabolite profile comparing conventional and organic wheat is meaningful only if the material is grown under comparable conditions. For example, the nitrogen, sulfur, phosphorus, and potassium fertilization of the plants of organic and conventional wheat has to be in the same range, considering that the plant nutrition orginates from organic matter, farmyard manure, or mineral fertilizer. Additionally the plants must originate from the same cultivar and must be grown in the same microclimate and in similar soil conditions. These conditions cannot be found in plant material originating from different farms or from products purchased in supermarkets.

In the past decade, metabolite profiles of some plants have been published especially from the perspective of stress physiology research, e.g., involving leaf tissue metabolite profiles (*7*, *8*). However, comparable scientific evaluations using biochemical data and metabolite profiles are lacking. For this purpose it

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is necessary to directly compare different farming systems. We used wheat grain from the controlled DOK field trial that has been conducted continuously since 1978 by the research Institute of Organic Agriculture (FiBL, Frick, CH) including a biodynamic (dyn) and a bio-organic system (org) and a system with farmyard manure (conv) and a mineral system (min). Field plots have been managed for 21 years with the "DOK" system comparison trial which is based on a lay rotation with grass-clover. For further information see Mäder et al. (*9*). Data comprising several growing periods were collected from the "DOK" material, including macro- and microelements, protein content, milling and baking properties, and also quality impairing substances such as mycotoxins (Mäder et al., unpublished data). Despite exclusion of fungicides from the organic production systems, the concentrations of mycotoxins detected in wheat grains were low in all systems and did not differ (*10*, Mäder et al., unpublished data). A previously published study based on the DOK field experiment has shown better soil fertility, higher biodiversity in organic field plots, a higher energy and nutrient efficiency in organic systems, and crop yields that were 21% lower in the organic systems (*9*).

The aim of the work presented here was to determine relative levels of a large set of metabolite components such as sugars, sugar alcohols, amino acids, or organic acids from wheat grain. Based on these data it was a further aim to compare organic and nonorganic field trials from the harvest of 2003.

MATERIALS AND METHODS

Plant Material. Wheat grains were harvested in 2003 from the "DOK" field trial near Basel, Switzerland. Material from two organic farming systems, namely, biodynamic (dyn, D) and bioorganic (org, O), and from two conventional systems (conv, K; mineralic), one using mineral fertilizer and the other using mineral fertilizer plus farmyard manure, were used. Crop rotation, varieties, and tillage were identical in all systems (*9*). Plants in the crop rotation were (1) potatoes; (2a) winter wheat; (2b) green manure; (3a) soy; (3b) green manure; (4) maize; (5) winter wheat (cv. Titlis, for the year 2003). Additionally, there were plots which received no fertilizer at all, (none) except green manure and N-entries by air (ca. 40 kg/ha). Four samples of each wheat cultivation form, originating from independent field plots from the DOK trial, were taken.

Metabolite Extraction. Wheat grains (100 g) were crushed in a Teflon laminated mill using a 0.5 mm sieve (Retsch, Germany). The material was then ground using a mortar to a fine homogeneous powder denoted meal. The metabolites were extracted from 10 to 20 mg of meal with 1 mL of 80% methanol, containing 10 μM ribitol as internal standard in a FastPrep Instrument (Qbiogene, Heidelberg, Germany), using 1 mm zirconia beads (Roth, Karlsruhe, Germany). Extracts were treated three times at 6.5 m/s for 45 s. Metabolite extraction was enhanced by incubation at 70 °C for 15 min with 1400 rpm in a Thermomixer (Eppendorf, Hamburg, Germany). After 10 min of centrifugation at 15000*g* at room temperature, the clear supernatant was transferred to 1 mL glass vials (Supelco, Bellfonte, California) and evaporated in a nitrogen stream. Metabolites were derivatized with 75 μL of methoxylamine hydrochloride in pyridine (20 mg/mL; w/v) for 90 min at 37 °C and 75 μL of MSTFA for 30 min at 37 °C (*11*). All chemicals and standard compounds were purchased from Sigma-Aldrich-Fluka (Taufkirchen, Germany), Merck (Darmstadt, Germany), or Macherey-Nagel (Düren, Germany).

GC−MS Analysis. Sample volumes of 1 μL were analyzed with a TraceGC gas chromatograph coupled to a PolarisQ ion trap mass spectrometer equipped with an AS2000 auto sampler (Thermo Electron, Dreieich, Germany). Derivatized metabolites were evaporated at 250 °C in splitless mode and separated on a 30 m × 0.25 mm VF-5MS capillary column with 0.25 μm coating equipped with an integrated 10 m guard column (Varian, Darmstadt, Germany). Helium carrier gas flow was adjusted to 1 mL/min. The interface and ion source temperatures were set to 250 °C. Oven temperature was kept constant for 3 min at 80 °C and subsequently raised to 325 °C at 5 °C/min. The system was equilibrated for 5 min at 80 °C after each analysis. Mass spectra were recorded at 2 scans/s with a scanning range of 50−550 *m/z*. Metabolites were identified by comparison to purified standards and the NIST 2005 database (NIST, Gaithersburg, MD). In addition, the freely available Golm Metabolome Database (*12*) was of particular help to identify several metabolites. Relative levels of selected metabolites were determined automatically by integrating the peak areas of selective ions (*7*) using the processing setup implemented in the Xcalibur 1.4 software (Thermo Electron, Dreieich, Germany). Relative response ratios were calculated by normalizing the respective peak areas to the peak area of the internal standard and dividing the value by the weight of the extracted sample.

Data, Replication, and Statistics. Four biological replicates from each condition originating from a field plot each (D, O, K, M, K, N) were analyzed. Statistical treatment was checked on the basis of the 5% level using the Tukey-test algorithm of the Student's range using SAS software (Institute Inc., Cary, NC). Concerning reproducibility six aliquots of one sample were extracted in parallel and taken separately through the sample preparation and GC−MS analysis procedure for all individual metabolites. Of these six analyses standard deviations were calculated. Relative standard deviations for levels of 52 metabolites were below 10%. In the subsequent analyses of all wheat samples only levels of the 52 metabolites were determined. In order to analyze the accuracy of the system seven internal technical replications were made; values were accepted only when the standard error was below 5%. In addition, we generated calibration curves for 30 commercially available metabolites (data not shown). These measurements revealed linearity of detection for most metabolites in the range of 100 fmol to 1 nmol. Samples were randomized prior to GC−MS injection in order to prevent bias due to instrument performance.

RESULTS AND DISCUSSION

Comparison of the Metabolite Profiles of Wheat from Organic and Conventional Farming. At present, there is a good deal of information available about certain ingredients of metabolites in wheat grains originating from various cultivars grown at different nutrient regimes, for example a report of components measured in glyphosate tolerant and conventional wheat (*13*). However, there are not many comprehensive data collections, i.e., a metabolite profile of grains which is discussed with respect to nutrition. We have recorded broad metabolic profiles, and we investigated whether grains from organic and conventional origin are different.

We were able to detect 250 and to identify 52 metabolites by gas chromatography−mass spectrometry in hydrophilic extracts from wheat. In the following the metabolites were arranged in five groups containing 14 amino acids, 11 sugars and sugar derivates, 5 sugar alcohols, 12 organic acids, and 10 other metabolites (**Table 1**). A comparison of the chromatograms revealed little variation of metabolites between all farming systems (**Figure 1**). GC−MS chromatograms contained about 250 compound peaks. In total 52 substances were identified from the methanolic extracts of wheat. Of these 52 metabolites only eight showed significant differences (**Figure 2**).

Although a principal component analysis was calculated, no separation into groups could be detected (data not shown).

Amino Acids. A total of 14 amino acids were detected in methanolic extracts of wheat (**Table 1, Figure 2**). The levels of tryptophan, phenylalanine, lysine, and threonine were too low for reliable quantification. Lysine and threonine have been reported to occur at a low concentration in whole wheat meal (*14*). In our work, we detected only for alanine and valine significant differences in levels between the field cultivations. The amounts of alanine decreased in the order mineralic > none > conv, dyn, org. Valine levels where highest also in mineralic, decreased in none, org, and conv, and were lowest in dyn. In

Table 1. Compilation of the Metabolites Identified and Quantified by Gas Chromatography–Mass Spectrometry in Hydrophilic Extracts of *Triticum aestivum* L. from Organic and Nonorganic Grains[a]

amino acids	sugars	sugar alcohols	organic acids	others
α-alanine (116)	erythrose 4-P (357)	glycerate (189, 192)	2-phosphoglycerate (277, 299, 459)	α-glycerophosphate (357)
β-alanine (248)	fructose (307)	pinitol (260)	isocitrate (245, 319)	homocysteine (234)
aspartate (232)	fructose-6-P (315)	*myo*-inositol (305)	2-methylcitrate (287)	adenosine (236)
proline (142)	gluconate 6-P (387)*	*myo*-inositol-P (318)	citrate (257)	thymine (255)
glutamate (154)	gluconate (333)	ribitol (IS)	fumarate (245)	uracil (255, 241)
asparagine (188)	glucose (319)		malate (245, 307)	urea (189)
glycine (174)	glucose-6-P (387)		succinate (247, 409)	shikimate (204)
isoleucine (158)	saccharose (361)		pyruvate (174)	pantothenic acid (201)
lysine (204)	raffinose (361)*		lactate (191)	cystathionine (218)*
threonine (101)	ribose-5-P (217)		α-ketocaproate (110)	spermidine (144)
tyrosine (218)	maltose (361)		α-ketoglutarate (198)	
tryptophan (202)			2-hydroxyglutarate (203, 247)	
valine (144)				
methionine (176)				

[a] Abbreviations: P, phosphate; IS, internal standard. *m*/*z* values in parentheses are the selective ions used for quantification. (*) Metabolites identified using the NIST 2005 database, others through purified standards.

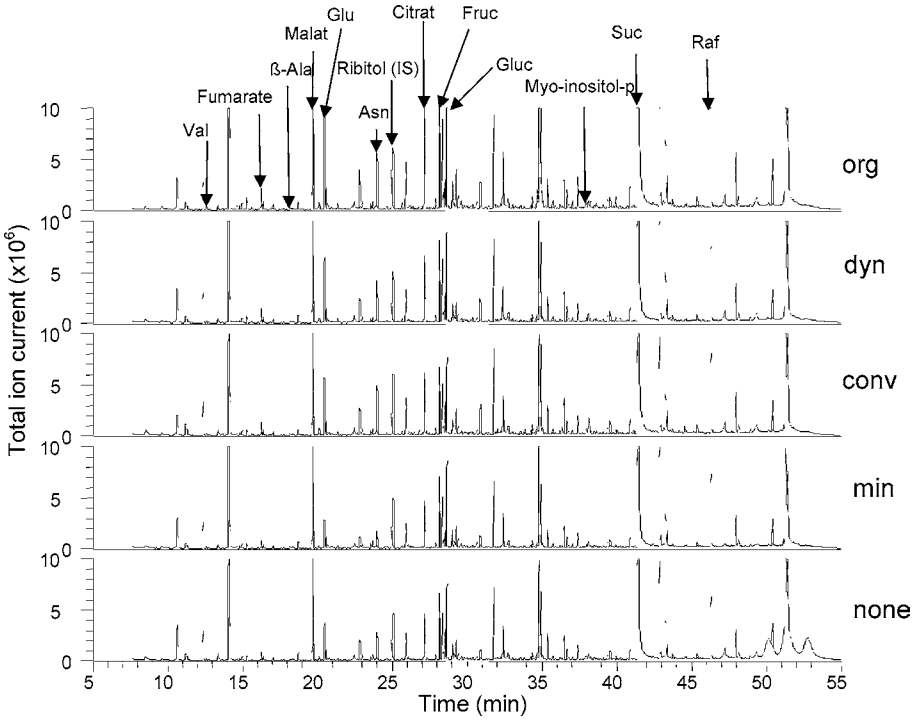

Figure 1. Gas chromatography–mass spectrometry total ion chromatograms of methanolic metabolite extracts from grains of wheat from biodynamic (dyn), bioorganic (org), and two nonorganic (conv, min) systems and no fertilization (see Materials and Methods). Val, valine; β-Ala, β-alanine; Glu, glutamate; Asn, aspartate; Fruc, fructose; Gluc, glucose; Suc, sucrose; Raf, rafinose; Ribitol (IS), internal standard.

contrast, Mäder et al. (unpublished data) found no significant differences in levels of any amino acids, including alanine and valine in wheat of the DOK trial from the different growing conditions in the 1998 harvest. Since ratios of N supply (i.e., fertilization) in the various field cultivations were unaltered in the growing seasons of 1998 and 2003, these contrasting findings for alanine and valine were most likely not due to variations in nutrient supply of the plants. The altered levels of alanine and valine might be explained by variations in the growing season. For example, the wheat used in our study was grown in the exceptionally dry and warm European summer of 2003. The magnitudes of changes in levels of alanine and the essential amino acid valine were relatively small, indicating that these differences would have a negligible effect on the nutritional value of wheat from the different growing conditions.

β-Alanine is a non-protein amino acid that serves as a precursor for pantothenic acid. β-Alanine will therefore be dealt with in the section Nucleotides, Urea, and Vitamin B5.

Stress Markers. The hypothesis has been put forward that organic crops would generally grow under stress conditions because of insufficient nutrient supply. In stress physiology, the accumulation of compatible solutes is a widespread response that may protect plants against environmental stresses and additionally will have an impact on the taste of foodstuffs. Compatible solutes include proline, betaines, polyols, and trehalose (*15*). Osmotic stress is often found as a consequence of various other stresses such as chilling, water logging, heat, or biotic stress (*16*). No significant differences could be detected by comparing the levels of osmotic stress markers proline and trehalose from mineralic and organic farming. The similar levels

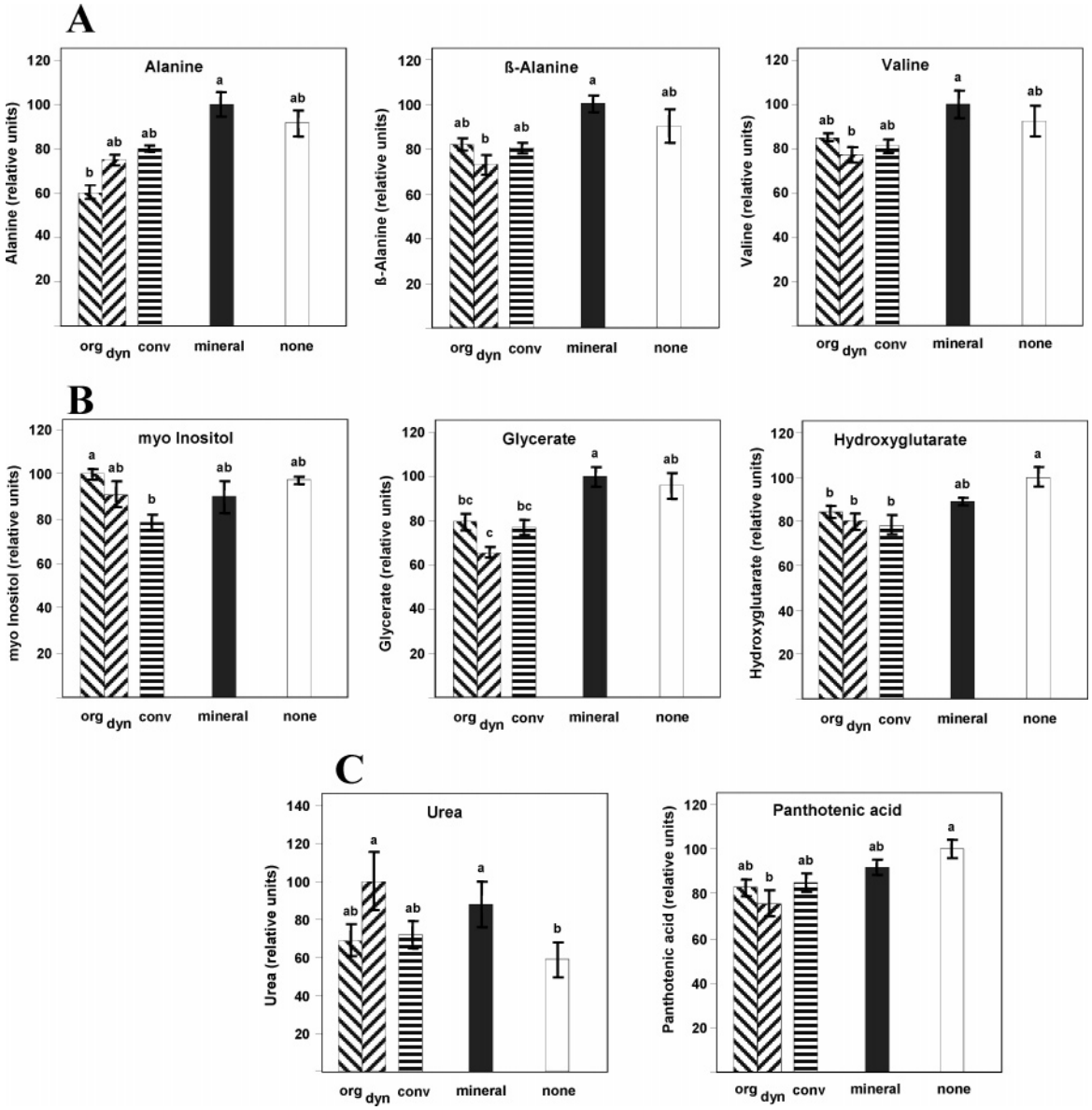

Figure 2. Metabolite content of wheat grains influenced by the conditions of cultivation. Values are means of replicates from 4 independent field trials and from 8 technical replications each ± standard error. Statistical significance tests ($p = 0.05$) were performed after the Tukey-test algorithm of the Student range. Different letters indicate significant differences of the means. (**A**) Amino acids. (**B**) Sugar and sugar alcohols. (**C**) Others.

did not support the hypothesis that the organic growth conditions reflect a stress to wheat.

Sugars and Sugar Alcohols. For many organisms there is a correlation between the levels of sugars and sugar alcohol accumulation and osmotic stress resistance, but the mechanisms underlying this protection remain elusive (*17*, *18*). Sugars and sugar alcohols are also important for taste and quality of the grain (*19*). No significant differences in glucose, fructose, saccharose, maltose, and erythrose-4-P of organic and conventional wheat were detected (**Table 1**). By contrast, significant, though small, differences were detected in amounts of *myo*-inositol which was reduced in the conventional farming system (org > dyn, min, none > conv; **Figure 2B**). The accumulation of *myo*-inositol in organic wheat suggests that the grain was well supplied with sufficient assimilate source.

Organic Acids. Significant differences between the glycerate levels in organic and nonorganic wheat were detected. Glycerate decreased from mineralic> none > org, conv > dyn. Glycerate is involved in various metabolic processes, e.g., photorespiration in green tissue. The photorespiration is an important pathway for amino acid metabolism. Glyoxylate (glycolate) acts as acceptor for NH_3, forming the amino acid glycine. Two molecules of glycine are converted into serine with simultaneous liberation of CO_2 in the photorespiration. In this reaction ammonia is also released. In order to prevent both ammonia toxicity and losses by volatilization, reassimilation of ammonia is required via the formation of glutamine from glutamate (*20*). The nitrogen supply plays a role for the grain filling phase of wheat in which the standing grain is photosynthetically active. The differences in glycerate levels could be described as a function of lower nitrogen availability or slower mobilization of nitrogen in the dynamic and organic wheat cultivation.

The content of hydroxyglutarate was significantly different between nonfertilized and organic wheat. Little information is available for hydroxyglutarate in plants and especially in wheat grains. However, it is known that hydroxyglutarate is involved in the biosynthesis of the amino acids tryptophan and lysine (*14*). Thus, it is possible that the high level of hydroxyglutarate

is a result of an imbalance in the C and N metabolism of the nonfertilized wheat plants. Taken together significant though small differences in levels of two organic acids occurred in wheat grain. The levels of 10 organic acids were not influenced by the cultivation method (**Table 1**). We conclude from these data that the small differences in levels of the two organic acids are negligible with respect to human or animal nutrition.

Nucleotides, Urea, and Vitamin B5. Adenosine, thymine, and uracil were not changed in organic and nonorganic wheat (**Table 1**). Analyses of urea showed that concentrations decreased in the order dyn, mineralic > org, conv, none (**Figure 2C**). Urea is often used as a rapidly available nitrogen fertilizer and is an important nitrogen metabolite in plants (*21*).

Pantothenic acid (vitamin B5) is a water-soluble vitamin essential for the synthesis of CoA and acyl-carrier proteins, cofactors in energy yielding reactions including carbohydrate metabolism and fatty acid synthesis (*22*). **Figure 2C** shows that the content differed between none and dynamic fertilization in the order none > min, org, conv > dyn.

Also, β-alanine is a precursor in the synthesis of pantothenic acid. It is interesting that β-alanine decreased in a similar order, mineralic > none, org, conv > dyn (**Figure 2A**). It appears that the pantothenic acid pathway is sensitive to the β-alanine level in wheat grain.

Agronomic Parameters. Concerning the characterization of metabolite levels of organic and nonorganic wheat, results from this study and the literature have to be combined. Mäder et al., 2002 (*9*, *23*), and others reported a decreased harvest in organic wheat production of about 30%. A reason for the reduction of grain harvest was the reduction of the grain number but not the reduction of the grain weight (*24*). This indicates a physiological main feature of plant metabolism, i.e., reduction of the number of grains in order to achieve the production of healthy and vigorous seeds. The nutrient availability has to be recognized and the wheat plant has to manage the number of tillers and the number of grains which can be sufficiently supplied with assimilates and ripened till seed maturity. In consequence, we did not detect extreme differences in metabolite composition and quality of the grains.

The presented data show that by using GC−MS it was possible to detect a set of 52 different metabolites including amino acids, organic acids, sugars, sugar phosphates, and sugar alcohols and nucleotides from wheat grains. Within the metabolites from all field trials including mineralic and no fertilizer, there was at the most a 50% reduction by comparing highest and lowest mean values. Differences, validated by statistical analysis, between dynamic, bio-organic, and conventional wheat grain were found in 8 of 52 detected metabolites. Values differed in the range of 10% to 40% (**Figure 2**). According to the statistics the data show that the metabolite status of the wheat grain from organic and mineralic farming did not differ in concentrations of 44 metabolites. Probably, this result indicates no or only a small impact of the different farming systems on the nutritional value of their products.

A decreased nutrient supply of the grains could not be confirmed by our data, because assimilate production, mirrored in sugar and sugar alcohol amounts in grains, was not significantly affected. According to our data, we could also not conclude that photosynthesis was limited in plants from organic fertilized field trials. The production of seeds was regulated by the nutrient availability of the wheat plant. In consequence we did not detect extreme differences in metabolite composition and quality of wheat grains.

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