Leibniz Institut
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1. STRUCTURE AND FUNCTION OF LOW MOLECULAR WEIGHT FOOD COMPONENTS

1.1. Aroma and taste (hedonic value) as quality parameters

1.1.1. Characterization of important odorants in freshly squeezed juices of Valencia late and Navel oranges

Twenty-five odor-active compounds were quantified in hand-squeezed juices of Valencia late and Navel oranges using stable isotope dilution assays. Odor activity values (OAVs, ratio of the concentration to odor thresholds) based on odor thresholds in water were calculated for the entire set of aroma compounds in both varieties. Due to their high OAVs, the fruity smelling esters 2-methyl-propanoic acid ethyl ester, butanoic acid ethyl ester, (S)-2-methyl-butanoic acid ethyl ester and 3a,4,5,7a-tetrahydro-3,6-dimethyl-2(3H)-benzofuranone (winelactone), the grassy smelling (Z)-hex-3-enal and the citrus-like decanal were characterized as the most potent odorants in both juices. The weaker fruity note in the Navel oranges was clearly correlated with significantly lower OAVs of all fruity smelling esters but a higher OAV of (Z)-3-hexenal compared to Valencia late. Aqueous model solutions simulating the odor of both orange varieties based on a mixture of reference odorants in the "natural" concentrations confirmed the findings of the quantitation studies.

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1.1.2. Characterization of key aroma compounds in hand-squeezed grapefruit juice by quantitation and aroma recombination

Twenty-five odor-active compounds were quantified in the fresh, hand-squeezed juice of White Marsh seedless grapefruits using stable isotope dilution assays. By calculation of odor activity values (ratio of their concentrations in the juice to their odor thresholds in water) it was shown that the fruity smelling esters 2-methyl-propanoic acid ethyl ester, butanoic acid ethyl ester and (S)-2-methyl-butanoic acid ethyl ester and the fruity, sweet winelactone, as well as the grassy smelling (Z)-hex-3-enal and trans-4,5-epoxy-(E)-dec-2-enal with a metallic odor were among the most potent odorants of the fresh grapefruit juice. The typical sulfurous, grapefruit-like odor quality was mainly evoked by the catty, blackcurrant-like 4-mercapto-4-methyl-pentan-2-one and the grapefruit-like smelling 1-p-menthene-8-thiol. These findings were confirmed by reconstitution experiments which successfully simulated the aroma of the fresh grapefruit juice.

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1.1.3. 3,4-Dihydroxy-3-hexen-2,5-dione - an intense caramel-like smelling aroma compound

3,4-Dihydroxy-3-hexen-2,5-dione (DHHD) was identified in a thermally treated mixture of cysteamine and fructose. GC/MS and 13C-NMR measurements revealed that its flavor activity is present only in the open chain form, while the cyclic species (acetylformoin) was shown to be odorless. The flavor quality of DHHD was similar to that of 4-hydroxy-2,5-dimethyl-3(2H)-furanone (Furaneol), its odor threshold was determined to be 10 µg/l in sunflower oil. NMR measurements, however, showed that the odor-active open chain tautomer is present only in aprotic solvents, such as oils while the cyclic, odorless tautomer (acetylformoin) is immediately formed in aqueous solution.

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1.1.4. Model studies on the Strecker-reaction: On the role of Amadori compounds

Alpha-dicarbonyls, generated by sugar degradation, catalyze the formation of the so-called Strecker aldehydes from alpha-amino acids. To check the effectiveness of Amadori compounds, suggested as important intermediates in alpha-dicarbonyl formation from carbohydrates, in Strecker aldehyde formation, the amounts of phenylacetaldehyde (PA) formed from either an aqueous solution of L-phenylalanine/glucose or the corresponding Amadori compound N-(1-deoxy-D-fructosyl-1-yl)-L-phenylalanine (ARP-Phe) were compared. The results revealed the ARP-Phe as a much more effective precursor in PA generation. On the contrary, a binary mixture of glucose/phenylalanine yielded preferentially phenylacetic acid, in particular, when reacted in the presence of oxygen and copper ions. Further model experiments gave evidence that a transition metal catalyzed oxidation of the ARP-Phe by air oxygen into the 2-hexosulose-(phenylalanine) imine is the key step responsible for the favored formation of phenylacetaldehyde from the Amadori compound. This mechanism might explain differences in the ratios of Strecker aldehydes and the corresponding acids depending on the structures of carbohydrate degradation products involved and indicates a new pathway in the formation of Strecker aldehydes without catalysis by alpha-dicarbonyls.

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1.1.5. Characterization of Maillard reaction products imparting "cooling" effect in beer malt

Gel permeation chromatography (GPC) of the solvent-extractables isolated from a thermally treated glucose/L-proline mixture and sensory analysis of the fractions collected led to the discovery of the presence of "cooling" compounds in Maillard reactions. To characterize the compounds imparting this oral cooling sensation, the Taste Dilution Analysis was applied to the cooling-active GPC fraction by determining the taste threshold of reaction products in serial dilutions of HPLC fractions. MS, NMR, [13C] labeling experiments, followed by synthesis led to the unequivocal identification of 3-methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one (3-MPC), 5-methyl-2(1-pyrrolidinyl)-2-cyclopenten-1-one (5-MPC) and 2,5-dimethyl-4-(1-pyrrolidinyl)-3(2H)-furanone (3(2H)-DMPF) as the most intense "cooling" compounds formed from hexoses. Comparative studies on pentose/L-proline mixtures led to the identification of the odorless 5-methyl-4-(1-pyrrolidinyl)-3(2H)-furanone (3(2H)-MPF),

exhibiting a "cooling" sensation at the low concentration of 1.5-3.0 mg/kg (water), as one of the most active "cooling" agents reported so far. To the best of our knowledge, these are the first Maillard reaction products reported to cause intense cooling sensations by degustation. Finally, the detection of 5-MPC, 3-MPC, 3(2H)-DMPF, and 3(2H)-MPF in dark roasted beer malts verified their natural occurence in thermally processed foods and demonstrated 3(2H)-MPF as the most active, odorless cooling agent reported so far in nature.

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1.2. Physiology and techno-functional properties

1.2.1. Influence of the carbohydrate skeleton on structure, formation and anti-oxidative potential of non-enzymatic browning products

The influence of the carbohydrate moity on the formation of 2-(3-oxo-4-pyrrolidino-4-cyclopentene-1-ylidene)-2H-furan-3-one chromophores during food-related Maillard reactions from pentoses, hexoses and disaccharides is reported. The orange compounds (E)/(Z)-4-hydroxy-5-methyl-2-(3-oxo-4-pyrrolidino-4-cyclopentene-1-ylidene)-2H-furan-3-one and (E)/(Z)-5-methyl-2-(3-oxo-4-pyrrolidino-4-cyclo-pentene-1-ylidene)-4-pyrrolidino-2H-furan-3-one were isolated and identified in a roasted xylose/L-proline by 1D- and 2D-NMR, LC/MS, UV/VIS spectroscopy as well as synthetic experiments. Studies on their formation revealed that these chromophores are formed upon condensation of pentose-derived 4-hydroxy-5-methyl- and 5-methyl-4-pyrrolidino-2H-furan-3-one, respectively, with 2-hydroxy-2,4-cyclopentadien-1-one and L-proline. Substitution of the pentose with glucose led to the identification of the structurally related colored (Z)/(E)-2-(2-hydroxy-2-methyl-3-oxo-4-pyrrolidino-4-cyclopenten-1-ylidene)-4-hydroxy-5-methyl-2H-furan-3-one and to the characterization of 2,4,5-trihydroxy-5-methyl-2-cyclopenten-1-one and 5-hydroxy-5-methyl-3-cyclopentene-1,2-dione as key intermediates in chromophore formation from hexoses. Comparative studies on disaccharides revealed that not 2-(3-oxo-4-pyrrolidino-4-cyclopentene-1-ylidene)-2H-furan-3-one chromophores, but the colorless 4-(alpha-D-glucopyranosyloxy)-2-hydroxy-2-methyl-2H,6H-pyran-3-one and 4,5-dihydroxy-2-(alpha-D-glucopyranosyloxy)-5-methyl-2-cyclopenten-1-one are formed amongst the major degradation products of maltose. It could be shown that their aglycons cannot be liberated upon food-related heating conditions, thus, inhibiting the formation of the chromophores. These data gave strong evidence that the 1,4-glycosidic linkage of disaccharides is responsible for their lower effectivity in browning development compared to pentoses or hexoses. In addition, the antioxidative capacity of these chromophores was measured in vitro showing that not the phenol-type hydroxy group in the furanone ring, but the free methylene group in (E)/(Z)-4-hydroxy-5-methyl-2-(3-oxo-4-pyrrolidino-4-cyclopentene-1-ylidene)-2H-furan-3-one is the most active structural feature determining the antioxidative activity of the chromophore.

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1.2.2. Metabolism of S-(+)- und R-(-)-carvone in humans

To identify the in vivo metabolites of carvone in humans under the most realistic conditions the MICA (Metabolism of Ingestion-Correlated Amounts) approach was developed, meaning the amount metabolized in the experiment was not as-high-as-possible but correlated to a reasonable and explainable intake via usual food and cosmetics. The amount of carvone metabolized was 1 mg/kg. Urine extracts were analyzed by gas-chromatography-mass

spectrometry and the major metabolites were localized by mass trace comparison between 24h-control and 24h-test urine. From the mass spectra obtained the following metabolites were proposed: alpha,4-dimethyl-5-oxo-3-cyclohexene-1-acetic acid (dihydrocarvonic acid), alpha-methylene-4-methyl-5-oxo-3-cyclohexene-1-acetic acid (carvonic acid), and 5-(1,2-dihydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one (uroterpenolone). The identity was proven by syntheses and NMR-experiments. Minor metabolites were identified as reduction products of carvone, namely the alcohols carveol and dihydrocarveol. The major in vivo metabolite of carvone in rabbits, 10-hydroxy-carvone, was not detected. No differences in metabolism between S-(+)- and R-(-)-carvone were observed.

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1.2.3. Structure-function relationships of synthetic emulsifiers for the production of chocolate: synthesis of PGPR components

The emulsifier polyglycerol polyricinoleate (PGPR) is used in the production of chocolate decreasing the yield point of chocolate mass. PGPR is not a defined compound but a mixture of esters of polycondensated fatty acids of castor oil and polycondensated glycerol. However, up to now, no information is available about the effect of individual components of PGPR. Aim of the present study was therefore the synthesis of defined PGPR compounds. By adding defined components to the chocolate mass the relationship between structure and physical effects shall be discussed. Diglycerol was simply produced by reaction of allyl ether with peroxyformic acid and will be now an intermediate for the esterification with ricinoleic acid. Furthermore the synthesis of glyceryl 1-monoricinoleate is presented. After the introduction of triethylsilyl protecting groups it is now possible to add one ricinoleic acid unit after the other to glyceryl 1-monoricinoleate by using 12-hydroxy-9-(Z)-octadecenoic acid (2,2-dimethyl-1,3-dioxolan-4-yl) methyl ester as starting material.

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2. DEVELOPMENT OF SPECIAL ANALYTICAL TECHNIQUES

2.1. Exhaled Odorant Measurement (EXOM) - a new approach to quantify the degree of in-mouth release of food aroma compounds

Physiological factors influencing the transfer of volatiles from the oral cavity into the nose were studied. Special attention was paid to the act of swallowing and to effects caused by mouth or tongue movements. The investigations were carried out first with helium, then with aqueous odorant solutions using a novel approach called EXOM (exhaled odorant measurement)-concept. Therefore, the amounts of butanoic acid ethyl ester being exhaled through the nose during eating at distinct time intervals were quantified by application of stable isotope dilution assays after trapping of the odorants on Tenax.

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2.2. The Taste Dilution Analysis (TDA) - a novel bioassay for the identification of non-volatile, intensely tasting compounds in processed foods

Thermal treatment of aqueous solutions of xylose and primary amino acids led to a rapid development of bitter taste of the reaction mixture. To characterize the key compound causing this bitter taste, a novel bioassay, which is based on the determination of the taste threshold of

reaction products in serial dilutions of HPLC fractions, was developed to select the most intense taste compounds in the complex mixture of Maillard reaction products. By application of this so called Taste Dilution Analysis (TDA) twenty-one fractions were obtained, amongst which one fraction was evaluated with by far the highest taste impact. Carefully planned LC/MS as well as 1D- and 2D-NMR experiments were, therefore, focused on the compound contributing the most to the intense bitter taste of the Maillard mixture, and led to its unequivocal identification as the previously unknown 3-(2-furyl)-8-[(2-furyl)methyl]-4-hydroxymethyl-1-oxo-1H,4H-quinolizinium-7-olate. This novel compound, which we name Quinizolate, exhibited an intense bitter taste at an extraordinarily low detection threshold of 0.00025 mmol/kg water. As this novel taste compound was found to have a 2000- and 28-fold lower threshold concentration as the standard bitter compounds caffeine and quinine hydrochloride, respectively, Quinizolate might belong to one of the most intense bitter compounds reported so far.

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2.3. Studies on the mass spectrometric fragmentation of trimethylsilyl pantothenic acid

The characteristic fragment of trimethylsilylated pantothenic acid (TMS PA) at m/z 291 upon electron ionization was shown to originate from the molecular ion by a McLafferty rearrangement instead of resulting by ejection of 1,1,3,3-tetramethyl-1,3-disilacyclobutane. The verification consisted of labelling experiments as well as high-resolution mass spectrometry of the fragment and studies on it's isotopic distribution. The remaining fragmentation pathways of TMS PA were clarified by B/E-linked scans and collision-induced dissociation.

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3. RELATIONSHIP BETWEEN THE STRUCTURE OF BIOPOLYMERS AND THEIR TECHNOLOGICAL PROPERTIES

3.1. Modell studies on the influence of coffee melanoidins on the binding of flavour volatiles in coffee beverages

Addition of the total melanoidin fraction isolated by water extraction from medium roasted coffee powder to a model solution containing a set of 25 aroma compounds mimicking the aroma of a coffee brew reduced, in particular, the intensity of the roasty, sulfury aroma quality. Model studies performed by static headspace analysis revealed that especially three well-known coffee odorants, i.e. 2-furfurylthiol (FFT), 3-methyl-2-buten-1-thiol and formic acid 3-mercapto-3-methyl-butyl ester, were significantly reduced in the headspace above an aqueous model solution when melanoidins were added. In particular, the low molecular weight melanoidins (1500-3000 Da) led to the most significant decrease in FFT. In contrast, e.g., aldehydes remained unaffected by melanoidin addition.

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3.2. Heat-induced thiol-disulphide exchange reactions in milk proteins: studies on ß-lactoglobulin

Application of heat or high pressure to the major whey protein ß-lactoglobulin leads to the formation of gels that are elastic and stable only in the presence of intermolecular disulphide

bonds. Recently a free thiol group at the cysteine residue in position 160 and a disulphide bond between cysteine residues 121 and 160 were detected as a result of heat treatment of ß-lactoglobulin. Aim of further studies was to detect all heat-induced thiols and disulphide bonds of ß-lactoglobulin and to understand the course of the reactions. After heating of ß-lactoglobulin two free thiol groups at positions 66 and 160 and six different disulphide bonds have been detected. Amongst these, disulphide bonds from cysteine residues 66 to 121, 66 to 66 and 160 to 160 have not yet been detected, the last two of them being intermolecular. By using a mixture of different ß-lactoglobulins with amino acid modifications near the relevant cysteine residues it was demonstrated that the disulphide bonds of residues 121-160 and 66-121 were intramolecular and that the disulphide bond between residues 66 and 160 was intermolecular. From this it could be concluded that on heating the native thiol group of ß-lactoglobulin (position 119 or 121) is firstly shifted to positions 66 or 160. Next, these thiol groups take part in thiol-disulphide exchange reactions with other ß-lactoglobulin molecules leading to aggregates connected via intermolecular disulphide bonds. Direct formation of disulphide bonds by oxidation of thiol groups seems not to be likely, because the overall concentration of free thiols did not change during heating.

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3.3. Studies on the effects of microbial transglutaminase on gluten proteins of wheat

The enzyme transglutaminase (TG) catalyses the acyl transfer reaction between glutamine and lysine residues of protein chains thereby forming covalent cross-links. These cross-links can change the texture of proteins and for this reason, TG is applied by the food industry to improve product quality. For example, TG is known to have beneficial effects on breadmaking. However, only a few information is available on modifications of structure and texture in gluten proteins. Therefore, the effect of TG was systematically studied by means of model peptides, flour suspensions and doughs. Osborne fractionation, SDS-PAGE, GP-HPLC and RP-HPLC were used as analytical methods. The incubation of synthetic peptides mimicking sequences of HMW subunits in the presence of TG resulted in isopeptide bonds between glutamine and lysine residues; the N-terminal amino group was not involved in the reaction. Treatment of flour suspensions with TG decreased the extractability and increased the molecular weight of gluten proteins particularly mainly by cross-links of gliadins and HMW subunits. Dependent on the amount of TG used, dough development time and deformation, gluten extensibility and bread volume were decreased and gluten strength was increased. Based on these results the application of TG appears to be useful in the improvement of the baking quality of wheats having weak gluten.

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3.4. Ascorbic acid as regulator of redox reactions during dough mixing to control the quality of baked goods from flour with different baking performance

To get insight into the correlation between the concentration of low molecular weight thiols and the amount of ascorbic acid used for dough mixing, flour of the provenance CWRS was mixed by using different concentrations of ascorbic acid and the concentrations of low molecular thiols were determined. Compared to flour mixing of a dough decreased the concentration of reduced glutathione considerably. The concentration of reduced glutathione was minimal at a concentration of 125 mg ascorbic acid/kg of flour. A decrease of reduced glutathione to 0 nmol/kg of flour was not observed. The concentrations of free protein-bound thiols in glutenin were found to be in the range of 0,22-0,33 µmol/g of flour and 5,6-8,2

µmol/g of protein, respectively. These values are considerably lower than in whole flour. The addition of ascorbic acid led to an increase of the concentration of free thiols in glutenin. Finally, binding of oxidised glutathione to glutenin was investigated. It has been shown that those cysteine residues of glutenin that are able to form intermolecular disulphide bonds also reacted with oxidised glutathione. From this it could be concluded that a portion of these cysteine residues are free in dough. This result gives evidence that the postulated mechanism of action of ascorbic acid as a flour improver is true.

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3.5. Localisation protein-bound thiol groups in gliadins

Previous studies on two wheat cultivars ("Rektor", "Contra") have demonstrated that more than 60 % of thiol groups in wheat flour were located in the gliadin fractions. In order to determine the position of these thiol groups in the amino acid sequences and to study the influence of cultivar and oxygen, kernels of "Rektor" and "Contra" were milled under normal conditions and under nitrogen. Analysis of protein and thiol content indicated that the ratio thiol/protein in the four flours was similar. The flours were extracted under N2 according to Osborne and free thiol groups of the gliadin fractions were labelled with the fluorescent reagent DACM (N-(7-dimethylamino-4-methyl-2-oxo-3-chromenyl)maleinimide). The gliadin fractions were then preparatively separated by means of RP-HPLC. The measurement of fluorescence during elution indicated two labelled alpha- and two labelled gamma-gliadins. The positions of the free thiol groups were determined by partial hydrolysis of the proteins with thermolysin and sequencing of fluorescent peptides separated by RP-HPLC. Accordingly, alpha-gliadins contained one labelled cysteine residue in the C-terminal domain (Cz) and gamma-gliadins one labelled cysteine residue in the N-terminal domain (Cb*). These positions of free thiol groups were independent on wheat cultivar and the presence of oxygen during milling and flour storage.

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3.6. Influence of sulfur fertilisation on the quantitative composition of gluten protein types in wheat flour

Although different supplies of sulfur (S) during wheat growth are known to influence the quantitative composition of gluten proteins in flour, the effect on amount and proportions of single protein types have still not been determined. Therefore, the flours of the spring wheat "Star" grown on two different soils at four different levels of sulfur (0, 40, 80, 160 mg S per container) were analysed in detail using the extraction/HPLC procedure developed previously. The results demonstrated that the amount of total gluten proteins as well as the crude protein content of flour was not influenced, whereas amounts and proportions of single protein types were strongly influenced by different S-fertilisation. The changes were clearly dependent on the Cys- and Met-content of each protein type. The amount of S-free omega-gliadins was drastically and that of S-poor HMW subunits moderately increased by S-deficiency. In contrast, the amounts of S-rich gamma-gliadins and LMW subunits were significantly decreased, whereas the amount of alpha-gliadins was only slightly reduced. S-deficiency resulted in a remarkable shift of protein proportions. The gliadin/glutenin ratio was distinctly increased; omega-gliadins became major and gamma-gliadins minor components, whereas the ratio of HMW to LMW subunits was well-balanced.

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3.7. Relationship between the qualitative and quantitative compositions of gluten protein types and technological properties of hexaploid wheats derived from durum and Aegilops wheat

The contribution of the diploid wheat species Aegilops tauschii to the technological properties of hexaploid Triticum aestivum was previously studied by the investigation of synthetic hexaploid wheats derived from tetraploid durum wheat and three diploid Aegilops lines. The results indicated that bread volume, gluten index, SDS-sedimentation volume and maximum resistance of gluten were significantly influenced by the Aegilops lines. To determine the relationship between technological properties and qualitative and quantitative compositions of gluten proteins, the flours of parental and synthetic lines were extracted using a modified Osborne fractionation. Gliadin and glutenin fractions were then characterised by RP-HPLC on C8 silica gel. The HPLC patterns revealed typical differences between synthetic and parental lines. The gliadin patterns of all and the glutenin patterns of two synthetic lines were dominated by the Aegilops wheat. In one case of glutenin patterns, Aegilops and durum wheat had a similar influence. With respect to the amount of total gliadin and gliadin types, synthetic lines mostly lay between durum and Aegilops wheat. The amounts of total glutenin and glutenin types of the synthetic lines were generally higher than those of the parental lines. Strong correlations were found between the amount of total glutenin, HMW and LMW subunits and bread volume, maximum resistance of gluten, and SDS-sedimentation volume. The extensibility of glutenin was significantly correlated with the ratios of gliadins to glutenins and of gliadins to LMW subunits.

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3.8. Preparation and characterization of a European reference gliadin

The results of the immunochemical determination of gliadin in gluten-free foods are strongly dependent on the origin and type of the reference gliadin used for calibration. Therefore, the "European Working Group on Prolamin Analysis and Toxicity" decided to organise the preparation of a reference gliadin for collective use. Twenty-eight wheat varieties representative for France, the United Kingdom and Germany were selected as starting material. The kernels were milled, and after defatting the flour-mix (18 kg) was extracted with a salt solution to remove albumins and globulins and then with 60 % ethanol. The alcoholic extract was concentrated and desalted by ultrafiltration and lyophilised. The yield of gliadin was about 500 g, which corresponded to 58 % of the theoretical value. The product was homogenous in a high degree and completely soluble in 60 % ethanol. The crude protein content (N x 5.7) was 89.4 %. RP-HPLC revealed a composition with regular proportions of omega5- and omega1,2-gliadins, whereas those of alpha-gliadins were somewhat lower and those of gamma-gliadins were higher, respectively, compared with wheat varieties previously studied. HPLC patterns of the flour and the reference gliadin indicated that no essential protein was lost during the production procedure. According to the results of GP-HPLC, the reference gliadin contained 29 % oligomeric HMW gliadin and only 3 % albumins and globulins besides monomeric gliadins. Based on the properties determined, the product is a suitable reference material and can be recommended for common uses.

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3.9. Development of a common micro-baking test for wheat and rye flour

The efforts of breeders and genetic engineers to improve the properties of wheat and rye cultivars should be judged as early as possible. However, in such an early stage the available amounts of flour are too small to carry out standard baking tests. The existing micro-baking tests, differing in dough composition and dough treatment, can only be used for the assessment of either wheat or rye. The research objective was the development of a common micro-baking test suitable for the assessment of the baking quality of wheat, rye and mixtures of both, of wheat/rye hybrids and of rye that contains wheat proteins incorporated by genetic engineering. The kneading and baking properties of commercial wheat and rye flour and mixtures of them were determined for small samples (5 to 10 g of flour). 5 g of flour was found to be the lowest limit. With such an amount of flour, water absorption as well as the kneading requirements of a dough containing already sugar, fat, lactic acid and yeast necessary for baking could be determined in the 10 g micro-farinograph. The baking test itself was done with 7 g of dough. Resting times and rounding were similar to those used in the conventional micro-baking test for wheat. Loaf volume, shape and crumb properties determined were reproducible. Baking results were typical of pure wheat and rye. Wheat bread had a high volume with good crumb properties; the crumb of rye was dense and firm, the volume was low. The properties of flour mixtures lay between those of pure wheat and rye flours. Transgenic rye samples containing HMW subunits of wheat glutenin showed remarkable differences.

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3.10. Characterisation of gamma-secalins of rye

Rye is closely related with wheat according to plant taxonomy, but unable to form gluten. Structural differences of storage proteins have been proposed to be responsible. gamma-Secalins are major storage proteins of rye, but in contrast to the homologous gamma-gliadins of wheat only few information about their structures and amounts is available. In order to isolate and characterise gamma-secalins, flours of the rye cultivars "Danko" and "Halo" were extracted according to the Osborne procedure, and the fractions obtained were analysed by RP-HPLC and SDS-PAGE. The results of quantitation indicated that endosperm proteins of both flours consisted of about 26 % albumins and globulins, 65 % prolamins and 9 % glutelins. In comparison with wheat a much higher proportion of storage proteins was alcohol-soluble. The prolamin fractions contained all of the four storage protein types (HMW-, omega-, gamma-75k- and gamma-40k-secalins), whereas the glutelin fractions contained only HMW- and gamma-75k-secalins. Almost half the storage proteins consisted of gamma-75k-secalins, followed by gamma-40k-secalin (about 25 %); omega-secalins (16 %) and HMW-secalins (7 %) were minor components. Four major gamma-75k- and two gamma-40k-secalins of "Danko" were isolated from the prolamin and glutelin fractions by means of RP-HPLC. Amino acid compositions of gamma-40k-secalins corresponded to those of gamma-gliadins, whereas gamma-75k-secalins were characterised by higher contents of Gln and Pro. MALDI-TOF mass spectrometry indicated molecular masses of about 52,000 (gamma-75k) and 32,000 (gamma-40k), respectively. N-terminal amino acid sequences were homologous with those of gamma-gliadins with the exception of position 5 (Asn in gamma-75k- and Gly in gamma-40k-secalins) and of positon 12 (Cys in gamma-75k-secalins).

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4. FOOD COMPOSITION AND NUTRITION TABLES

The information about the composition of food adapted to the present scientific level is essential for administration, nutritional guidance and science. The "Souci-Fachmann-Kraut Food Composition and Nutrition Table" is actualized by evaluation of the international scientific publications available and by means of the PC database SFKDB. Selected data are transfered into the small table "Der kleine Souci-Fachmann-Kraut: Lebensmitteltabelle f¸r die Praxis", wich has been developed for the daily requirement of the consumer. The spectrum of food constituents covered in the large SFK-nutrition table also addresses preventive-medical aspects by the group of the "special bioactive compounds".

The Online-Version of the "Souci-Fachmann-Kraut Food Composition and Nutrition Table" is availiable on the WWW since January 2001.

The concept of the database with its different search and calculation tools enables the user to search for the specific food items, defined concentration and energy values, respectively. Additionally the calculation of the composition of raw food mixtures based on the data included in the database is realized by this electronic version.

The preparation of the 7. edition has been continued. A detailed evaluation of the database showed data gaps and old data especially in the case of the amino acids. Therefore the group of the amino acids, as an important aspect in the actual discussion about disease prevention and health the group of the bioactive compounds and due to the development of the analytical methodology iodine and folic acid data e.g. should be actualized and extended in the future.

The work on the 3rd edition of the small Table "Der kleine Souci-Fachmann-Kraut: Lebensmitteltabelle für die Praxis" has been continued.

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