Leibniz Institut
Deutsche Forschungsanstalt für Lebensmittelchemie

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Food composition and nutrition tables

Summaries

1. STRUCTURE AND FUNCTION OF LOW MOLECULAR WEIGHT FOOD COMPONENTS

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

1.1.1. Important Aroma Compounds in the peel oil Clementines (Citrus Reticulara Blanco cv. clementine)

In an extract prepared by solvent extraction of the peel from clementines, fourty-two odor-active compounds were detected by application of an Aroma Extract Dilution Analysis and subsequently identified by using the respective reference odorants. Among them, by far the highest Flavor Dilution (FD) factors were determined for the flowery smelling linalool, the fatty smelling (E,E)-deca-2,4-dienal and winelactone eliciting a sweet odor quality, followed by α-pinene, myrcene and octanal with pinetree-like, geranium leaf-like and citrus-like aromas. Among the thirty odor-active compounds identified, eleven aroma compounds are reported here for the first time as important contributors to clementine peel aroma, e.g. winelactone, (E,E)-nona-2,4-dienal, carvone, (Z)-hex-3-enal or tr-4,5-epoxy-(E)-dec-2-enal.

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1.1.2. Changes in roasted coffee aroma during storage - influence of the packaging

A sensory evaluation of roasted coffee that was stored in an inert packaging (can) and a commercial soft packaging revealed a significant difference in the overall aromas after 12 weeks of storage. The coffee having been stored in the soft packaging was clearly affected with an off-flavor. By application of comparative Aroma Extract Dilution Analysis and Headspace Dilution Analysis on both samples, distinct lower intensities of 8 odorants (e.g. 2-furfurylthiol, 3-methylbutanal, 2,3-butanedione) were detected in the off-flavor coffee. Quantitations by Stable Isotope Dilution Assays confirmed these odorants to be present in the negatively affected coffee in much lower concentrations and - in consequence - to cause the off-flavor. In model experiments, in which roasted coffee was stored under different conditions, oxygen was evaluated to play an important role by coffee staling.

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1.1.3. Comparison of key aroma compounds in cooked brown rice varieties

The aroma compounds present in cooked brown rice of the three varieties Improved Malagkit Sungsong (IMS), Basmati 370 (B 370), Khaskhani (KK) and of the variety Indica (German supermarket sample) were identified based on the application of Aroma Extract Dilution Analyses (AEDA). A total of 41 odor-active compounds were identified in the four samples, of which eleven are reported for the first time as rice constituents. 2-Amino acetophenone (medicinal, phenolic), which was up to now unknown in rice aroma, exhibited the highest FD-factor among the 30 to 39 odor-active compounds detected in all four varieties. 2-Acetyl-1-pyrroline, exhibiting an intense popcorn-like aroma-note, was confirmed as a further key

aroma constituent in IMS, B 370 and KK, but was not important in Indica. Differences in the FD-factors between the varieties were found for the previously unknown rice aroma compound 3-hydroxy-4,5-dimethyl-2(5H)-furanone (Sotolon; seasoning-like), which was higher in B 370 than in IMS and KK. In IMS, a yet unknown, spicy smelling component with a very high FD-factor could be detected, which also contributed with lower FD-factors to the overall aromas of B 370 and KK but was not present in Indica. The latter variety, which was available on the German market, differed most in its overall aroma from the three Asian brown rices.

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1.1.4. Comparison of odor-active compounds in rye flour and the corresponding rye sourdough

Application of the Aroma Extract Dilution Analysis on a flavor distillate prepared from freshly ground rye flour (type 1150) revealed 1-octen-3-one (mushroom-like), methional (cooked potato) and (E)-2-nonenal (fatty, green) with the highest Flavor Dilution (FD) factors among the 26 odor-active volatiles identified. Quantitative measurements performed by stable isotope dilution assays and a comparison to the odor thresholds of selected odorants in starch suggested methional, (E)-2-nonenal, and hexanal as contributors to the flour aroma, because their concentrations exceeded their odor threshold by factors >100. Application of the same approach on a rye sourdough prepared from the same batch of flour revealed 3-methylbutanal, vanillin, 3-methylbutanoic acid, methional, (E,E)-2,4-decadienal, 2,3-butandione and acetic acid as important odorants, since their concentrations exceeded their odor thresholds in water and starch by factors >100. A comparison of the concentrations of 20 odorants in rye flour and the sourdough made thereof indicated that flour, besides the fermentation process, is an important source of aroma compounds in dough. However, 3-methylbutanol, acetic acid and 2,3-butandione were much increased during fermentation, while (E,E)-2,4-decadienal or 2-methylbutanal were decreased. Similar results were obtained for five different flours and sourdoughs, respectively, although the amounts of some odorants in the flour and the sourdough differed significantly within batches.

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1.1.5. Characterisation of key aroma compounds formed in Maillard- type reactions of cysteamine and isothiaproline

Fructose was reacted in the presence of either cysteamine (model A) or isothiaproline (model B) in an aqueous buffer at 145°C and pH 7.0. Application of an Aroma Extract Dilution Analysis (AEDA) on the bulk of the volatile compounds formed in model A revealed 5-acetyl-3,4-dihydro-2H-1,4-thiazine (19), N-(2-mercaptoethyl)-1,3-thiazolidine (16), 4-hydroxy-2,5-dimethyl-3(2H)-furanone (15) and 2-acetyl-2-thiazoline (11) as the key aroma compounds among the 10 odorants detected. N-(2-Mercaptoethyl)-1,3-thiazolidine is reported for the first time among the volatiles generated in Maillard type reactions and exhibits the extremely low odor threshold of 0.005 ng/L in air.

A similar set of aroma compounds was formed when isothiaproline was reacted (model B), but the FD-factors were generally lower. Substitution of the buffer by silica gel/water (9+1 w/w) in both models and applying 150°C for 10 min also gave the same key odorants from both thio compounds, however, under these conditions isothiaproline was the better precursor of, in particular, 19 and 11. Quantitative measurements performed by means of stable isotope

dilution assays revealed a significant effect of the pH on odorant formation. E.g., in model A, formation of 19 as well as of 11 was suppressed at pH values below 5.0. A clear maximum was, however, found for 19 at pH 7.0 (about 1 mol % yield) while 11 increased with increasing the pH from 7.0 to 9.0.

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1.1.6. 13C-Labeling studies on structure and formation of the intensely bitter-tasting Maillard compounds quinizolate and homoquinizolate

Very recently, application of the taste dilution analysis on heated xylose/alanine solutions led to the isolation of two bitter tasting compounds exhibiting extraordinarily low detection thresholds of 0.00025 and 0.001 mmol/kg water, respectively. On the basis of LC/MS and NMR spectroscopy, the structures of these compounds, named quinizolate and homo-quinizolate, were proposed as 1-oxo-1H,4H-quinolizinium-7-olates (1a and 1b). Since recent experiments in our lab shed some doubt on the entire correctness of their structures, labeling experiments were performed in the present study to unequivocally determine the chemical structures and to elucidate the formation pathways of these key tastants. To achieve this, mixtures of multiply [13C] labeled and non-labeled pentoses were used as precursors to follow the joint transfer of several 13C atoms en bloc into the bitter compounds by LC/MS and NMR isotopomer diagnosis. Using this concept, addressed as "carbon modul labeling", the number of carbon atoms present in distinct carbohydrate fragments could be elucidated by means of LC-MS/MS techniques. 13C NMR spectroscopy has then been used to site-specifically visualize the mosaics assembled from [13C] labeled and [12C] labeled carbon modules in both bitter compounds, thus unequivocally demonstrating the structures of quinizolate and homoquinizolate to be the previously unknown (E)-2-[(2-furyl)methylidene]-7-[(2-furyl) methyl]-3-hydroxymethyl- (2a) and (E)-2-[(2-furyl)methylidene]-7-[(2-furyl)methyl]-3,8-bis(hydroxymethyl)-1-oxo-1H,2H,3H-indolizinium-6-olate (2b). Quantitative studies on their formation revealed pentoses and primary amino acids, in particular ribose and L-valine, as most efficient precursors, in particular when heated at low pH values. In addition, spiking the Maillard mixture with furan-2-aldehyde prior to heat treatment strongly favored the yields of both tastants. On the basis of these data as well as the informations provided by the NMR diagnostic isotopomer analysis, the pentose degradation products furan-2-aldehyde and 3,4-dideoxypentosulose were proposed as the key intermediates in the formation pathway leading to quinizolate and homoquinizolate.

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1.1.7. On the relationship between structure and "cooling" activity of cyclic α-keto enamines

3-Methyl- and 5-methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one were recently identified as intense cooling compounds in roasted dark malt. To gain more insights into the molecular requirements of these compounds for imparting a cooling sensation, 26 cyclic α-keto enamine derivatives were synthesized, and their physiological cooling activities were evaluated. Any modification of the amino moiety, the carbocyclic ring size, or incorporation of additional methyl groups led to a significant increase of the cooling threshold. Insertion of an oxygen atom into the 2-cyclopenten-1-one ring, however, increased the cooling activity, e.g. the cooling threshold of the 5-methyl-4-(1-pyrrolidinyl)-3(2H)-furanone was found to be 16-fold below the threshold concentration determined for the 3-methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one. Shifting the oxygen atom from the 4- into the 5-position of the

cyclopentenone ring resulted in a even more drastic increase in cooling activity, e.g. the 4-methyl-3-(1-pyrrolidinyl)-2(5H)-furanone exhibited the strongest cooling effect at the low oral threshold concentration of 0.02-0.06 mmol/L, which is 35-fold below the value determined for (-)-menthol. In contrast to the minty smelling (-)-menthol, most of the α-keto enamines were found to be virtually odorless, but impart a sensation of "cooling" to the oral cavity as well as to the skin, thus illustrating that there is no physiological link between cooling activity and mint-like odors.

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1.2. Physiology and techno-functional properties

1.2.1. Detection of a "non-aromatic" NIH shift during in vivo metabolism of the monoterpene carvone in humans

High resolution gas chromatography in combination with mass spectrometry and high resolution mass spectrometry was used to determine the positions and extent of labelling in the metabolites of carvone, namely in α,4-dimethyl-5-oxo-3-cyclohexene-1-acetic acid (dihydrocarvonic acid), α-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), after human ingestion of 9,9-dideutero- and 9-13C-carvone. Carvonic acid was formed by oxidation at the methyl carbon of the isopropenyl group of carvone whereas dihydrocarvonic acid was formed by oxidation at the methylene position, most probably via carvone epoxide. A "non-aromatic" NIH shift must occur during the subsequent reactions yielding dihydrocarvonic acid. Additionally, dehydrogenation of dihydrocarvonic acid and hydration of carvonic acid was observed, resulting in minor amounts of both acids owning a carboxy group of opposite origin. Uroterpenolone was found to be exclusively formed by oxidation at the methylene carbon of the isopropenyl group of carvone and thus, most probably by hydrolysis of carvone epoxide.

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1.2.2. Retronasal aroma stimulation during mastication and swallowing: a physiological-analytical study

The process of eating and drinking was observed in vivo by application of videofluoroscopy, a dynamic x-ray technique, as well as real-time magnetic resonance imaging. The study was aimed at elucidating chronologically the performances of the physiological organs involved in mastication and swallowing, mainly of the tongue, the pharynx and the soft palate (velum palatinum). Temporary physiological barriers during food consumption were visualized which are capable of retaining volatiles within the oral cavity. These barriers allow the access of odorants to the nasal cavity only at certain times during the eating process. Their effectiveness is related to the texture of the food as well as the amount of food material present in the oral cavity and, thereby, directly influences retronasal aroma perception. Together with the application of the SOOM (spit-off odorant measurement)-technique, the exact timing of odorant transfer to the nose as well as the phenomenon of odorant adsorption to oral mucosa were studied. This investigation revealed a new understanding of flavor perception as it is caused during the eating process.

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2. DEVELOPMENT OF SPECIAL ANALYTICAL TECHNIQUES

2.1. Syntheses of labeled vitamers of folic acid to be used as internal standards in stable isotope dilution assays

[$^{2}H_{4}$]-folic acid was synthesized by deuterating p-aminobenzoic acid, which was then coupled to glutamic acid and 6-formylpterin. Using [2H4]- folic acid as starting component enabled the preparation of labeled vitamers tetrahydrofolate, 5-formyltetrahydrofolate, 5-methyltetrahydrofolate and 10-formylfolate which were characterized by electrospray mass spectrometry and collision-induced dissociation. The mass spectrometric studies confirmed that the compounds could be used as internal standards in stable isotope dilution assays.

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2.2. Simple and quantitative determination of phospholipids by thin layer chromatography

Because of common structural elements phospholipids can act as emulsifiers and can influence the baking performance of wheat doughs. Therefore, those polar lipids, e.g. lecithin, which can be isolated in an industrial scale from plant sources (soybean, rapeseed), are used as part of improvers for breadmaking. Lecithin improves the fermentation behaviour of yeasted doughs, the loaf volume of bread and the structure of bread crumb. Commercial lecithin contains several fractions that can be subdivided into numerous individual components. Aim of the first part of the study presented here, was the determination of the phospholipid composition of eight different commercial lecithin samples. A method was developed which can be easily carried out even if no expensive laboratory equipment is present. The method implies separation of the samples by thin layer chromatography, detection with copper sulphate/o-phosphoric acid, documentation of the chromatogram with a commercial flat bed scanner, transformation of the image into a x/y-chromatogram, integration of the peaks and calculation of the amounts. Nine phospholipid classes were quantified in the samples with detection limits of 200-1400 ng and variation coefficients from 2-9 % for the major components. The results were in accordance with data provided by the producers of the lecithin samples.

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2.3. Development of a method based on gel chromatography for the determination of gliadin and gluten in wheat starch

Wheat starch is desired as an ingredient of gluten-free food but only permitted when the gliadin content is below 100 ppm. A reliable quantification of gliadin, however, has not been possible, because the immunoassays developed are not sufficiently sensitive, accurate or specific. Therefore, a relatively simple method based on gel chromatography (GP-HPCL) was developed. GP-HPLC enables the separation of gliadin from low-molecular-weight components (e.g. albumins and globulins) and gliadin quantification by UV absorbance, which is highly correlated with protein content. Unfortunately, UV measurement is not sensitive enough to detect gliadin concentrations <25 ppm, therefore the ethanol extract obtained from starch has to be concentrated. GP-HPLC was performed under the following condition: column: Superdex 200 (Mr = 10,000-600,000) - elution solvent: 1.5 % SDS + 62.5 mmol/L Tris-HCl (pH 7.0) - flow rate: 0.6 mL/min - injection volume: 100 µL - detection: 206 nm. The calibration curve for a gliadin standard (PWG-gliadin) was linear within a range

of 0-30 µg and the detection limit was about 0.5 µg. In preliminary experiments, extraction procedure, concentration of extracts and filtration were optimised. The analysis of starch samples included the following steps: extraction of 1 g with 10 mL 60 % ethanol under shaking, centrifugation, drying of 4 mL supernatant with a vacuum centrifuge, dissolving in 500 µL elution solvent, filtration and injection of 100 µL. According to this procedure the detection limit corresponded to about 10 ppm gliadin. Besides gliadin total gluten (gliadin + glutenin) could be determined, when a reducing agent was added to the extraction solvent and an increased temperature (60°C) was applied. By use of the developed method and the calibration curve for PWG-gliadin 23 starch samples from different producers were analysed for their gliadin and, in parts, gluten content. The values for gliadin were between 15 and 574 ppm and the average coefficient of variation was (2.6 %. The determination of gluten indicated that the ratio of gliadin to gluten can very in a broad range depending on the starch sample. Moreover, the results demonstrated that the crude protein content (N x 5.7) did not allow an estimation of the gliadin or gluten content. In addition to starch other raw material used for the production of gluten-free food was tested by the GP-HPLC method. Gliadin determination was, in principle, possible for apple fiber, buckwheat groats, spice mixture and chestnut flour. In the case of millet and rice flours, only the content of gluten could be determined. Because of large peaks in the region of gliadins the extract of skim milk powder and maize flour could not be analysed for gliadin or gluten content.

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

3.1. Model studies on the water and gas-holding capacity of remix-dough for micro baking tests

A micro baking test originally developed to compare volume performance of dried gluten has been optimized in order to yield typical wheat bread crumb. Starting with freeze dried gluten and commercial wheat starch, then adding step by step polysaccharides, gelatine and natural fibers, the functional properties of these fractions have been monitored by scanning electron microscopy, baking tests and rheological investigations. Temperature ramp measurements with a stress rheometer have been adapted for quality control of the dough components and to study their rheological interactions during baking. Soluble substances in the free water phase have been found to be important for gas holding in the oven rise of remix dough. Gelatine is able to substitute for the wheat flour soluble fraction as can be visualised by SEM. Water holding capacity can be risen by natural fibers. The enhanced baking test yields crumb properties similar to wheat bread. Changes of crumb firmness during aging have been monitored by micro compression tests.

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3.2. Characterization of γ-75k-secalins from rye - I. Amino acid sequences

γ-75k-Secalins are typical for the storage proteins of rye and contribute more than 30 % of flour proteins. In contrast to gluten proteins, however, information of amino acid sequences of (-75k-secalins are scarcely available. Therefore, two major components were isolated from rye flour and analysed for partial amino acid sequences. The alcohol-soluble prolamin fraction, which contained most of the γ-75k-secalins, was isolated from flour of the rye cultivar "Danko" using a modified Osborne fractionation and was separated by preparative

RP-HPLC. The two major components P1 and P2 were digested with (-chymotrypsin, trypsin and thermolysin. The different partial hydrolysates were preparatively separated by two steps of RP-HPLC and the resulting peptides were characterised by sequences analysis and, in parts, by mass spectrometry. By means of overlapping peptides and by comparison with known complete sequences of a γ-75k-secalin (gSec2A) derived from a wheat translocation line and of γ-gliadins, the sequence of the C-terminal domain of P1 was completely determined except that one of 148 amino acid residues could not be identified. The results demonstrated a close relationship to gSec2A and a high degree of homology to (-gliadins including eight cysteine residues in homologous positions. The C-terminal domain of γ-75k-secalin P2 was characterised by the determination of about 70 % of the sequences and showed a close relationship with P1. The N-terminal domain of P1 was obtained after tryptic digestion and HPLC separation. The molecular mass was about 36,000 and, thus, much higher than that of γ-gliadins. Sequence analysis of peptides from the enzymatic digests revealed that the N-terminal domain of P1 was closely related to gSec2A; it was characterised by repetitive sequences rich in Gln and Pro similar to corresponding sequences of (-gliadins, but including more modifications. In contrast to (-gliadins, one Cys residue was present in the C-terminal domain explaining the aggregative character of γ-75k-secalins. The partial sequences of the N-terminal domain of P2 was similar to those of P1, except that P2 had an additional Cys residues. In summary γ-75k-secalins are homologous with γ-gliadins in the C-terminal domain, but different in the N-terminal domain due to the increased length and the presence of cysteine residues.

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3.3. Characterization of γ-75k-secalins from rye - II. Disulfide bonds

γ-75k-Secalins, the major components of storage proteins of rye are partially homologous with γ-gliadins of wheat, but in contrast to γ-gliadins, they occur not in a monomeric, but in an aggregated state. It has been proposed that γ-75k-secalins form intermolecular disulfide bonds, but the experimental proof is missing until now. Therefore, the disulfide bonds of aggregated γ-75k-secalins were studied in the present work. They were isolated from the prolamin fraction of the rye flour "Danko" by preparative RP-HPLC and digested with thermolysin. The resulting peptides were pre-separated by gel chromatography into eight fractions (G1-G8). By means of differential chromatography (RP-HPLC before and after reduction of disulfide bonds), cystine containing peptides were identified. Numerous cystine peptides were then isolated from the fractions G3-G7 by preparative RP-HPLC and analysed by sequencing and mass spectrometry. The results indicated that the eight cysteines of the C-terminal domain were linked in the same positions as the intramolecular disulfide bonds of γ-gliadins (Cd/Ce, Cc/Cf1, Cf2/Cy, Cw/Cz). Cysteine Ca, characteristic for the N-terminal domain of γ-75k-secalins, was shown to be linked by an intermolecular disulfide bond with the corresponding residue of the same protein type (Ca/Ca). Disulfide bonds including Cb of γ-75k-secalins or cysteines of HMW secalins were not detected obviously due to the low amount in the prolamin fraction. In summary, disulfide bonds within the C-terminal domain of γ-75k-secalins are homologous with those of monomeric γ-gliadins and aggregated LMW subunits of wheat. The presence of a cysteine in the N-terminal domain is responsible for the aggregative nature of γ-75k-secalins. They are different from LMW subunits due to a missing cysteine in the C-terminal that forms an intermolecular disulfide bond. Therefore, aggregation of γ-75k-secalins is limited.

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3.4. Studies on flour proteins from transgenic rye stably expressing HMW subunits of wheat

The two transgenic rye lines L26 and L8 stably expressing HMW subunits 10 and 5+10 from wheat, respectively, were compared with the corresponding non-transgenic rye line L22. Flour proteins were separated into albumins/globulins, prolamins and glutelin subunits by a modified Osborne fractionation. Portions of the prolamin fractions were reduced in the same manner as glutelins. The different fractions were then characterised and quantified by RP-HPLC on C8 silica gel and, in parts, by gel chromatography on Superdex 200. The crude protein content of flours, the amount of total extractable proteins and the proportion of albumins/globulins did not significantly differ between transgenic and non-transgenic rye. The amount of transgenic HMW subunits was 6 % (subunit 10) or 17 % (subunits 5+10) of the total extractable proteins. The proportions of alcohol-soluble storage proteins (prolamins) were drastically reduced in transgenic rye and, as a consequence, the proportions of alchohol-insoluble proteins (glutelins) were increase due to a shift of HMW- and γ-75k-secalins. Gel chromatography of the prolamin fractions revealed that the transgenic rye flours contained a significantly lower proportions of alcohol-soluble oligomeric proteins compared with the non-transgenic flour. The quantitative data demonstrate that the HMW subunits of wheat lead to a higher degree of polymerisation of storage proteins in rye flour. The HMW subunit combination 5+10 showed stronger effects than subunit 10 alone. Because a considerable amount of γ-40k-secalins was present in the glutelin fraction of L8, it can be concluded that HMW subunit 5 caused changes in the disulfide structure of this protein type.

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3.5. Investigation of the in-vivo toxicity of a putative immunodominant peptide from α-gliadins

Peptides corresponding to amino acid residues 57-68 and 62-75, respectively, have been shown to stimulate specifically small intestinal T-cell clones from coeliac patients. However, in-vivo toxicity of such peptides has not been proven. Therefore, in-vivo experiments with a positive control (peptic tryptic digest of gliadin, PTG), with gliadin peptide G8 (residues 56-75 (-gliadins) and with a negative control (peptide C1 corresponding to residues 53-72 of β-casein) were performed. The peptides were synthesised by means of a peptide synthesiser. The crude peptides were purified by two steps of RP-HPLC. Both peptides were chromatographically pure (>99 %) and their masses determined by mass spectrometry corresponded to the theoretical values. Four adults with coeliac disease, all of whom were on a gluten-free diet, underwent three challenges. The aqueous solutions of PTG and peptides G8 and C1 were infused into the duodenum and biopsies were taken before infusion and at 2, 4 and 6 h after the start of infusion. Biopsies were then analysed for the height of enterocytes, the villus height to crypt ratio and the number of intra-epithelial lymphocytes. PTG (1 g) was given first to confirm a positive reaction and to prime the small intestinal T-cells. All four subjects developed significant changes in the relevant parameters. After a regeneration period of a few weeks, 100 mg of peptide G8 was given to the first patient, however, this patient developed diarrhoea and faecal incontinence on the following days; thus, the dose was reduced to 20 mg for the subsequent patients. Similar to PTG, peptide G8 caused significant effects on enterocytes and lymphocytes. In contrast the negative control peptide C1 did not affect any of those variables typical for mucosa damage. Thus, it was shown that the putative immunodominant peptide G8 corresponding to 56-75 of α-gliadins exacerbates coeliac disease in-vivo.

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3.6. Studies on the coeliac activity of avenin, the prolamin fraction of oats

It is well established that the wheat protein gliadin triggers inflammation in coeliac patients. However, the potential toxicity of avenin, the equivalent protein in oats, is debated. The aim of the study was, therefore, to investigate the immunogeneity of avenin in comparison with gliadin using the cytokines (-interferon (IFN) and interleukin-2 (IL2) as markers of immunological activity. Four rolled oat samples, which had been available as source for the isolation of avenins, were analysed for the avenin content by an extraction/HPLC procedure and for wheat contamination by PCR. The defatted flour of the sample which was free of wheat and had the highest avenin content was extracted stepwise with a salt solution and 60 % ethanol. Avenin was isolated from the ethanol extract and digested with agarose-bound pepsin and trypsin. The effects of both peptic tryptic digests of gliadin (PTG) and avenin (PTA) were then studied in an organ-culture-test system. Duodenal biopsies from 17 treated coeliac patients were cultured with 5 mg/mL of PTG or PTA at 37°C for 4 hours. Biopsies cultured with medium alone served as a control. Biopsies of 16 non-coeliac persons were also cultured with PTG or PTA. Total RNA was extracted from the tissue after culture and cytokine RNA was quantified by PCR. Cytokine protein secreted into the medium was measured by ELISA. After culture with PTG, an increase in IFN/RNA was observed in all 9 patients with treated coeliac disease. Increased IFN protein was also found in four of these patients. Smaller increases in IL2/RNA were detected in 6 subjects with increased IL2 protein found in 2 patients. In contrast to PTG, there was no significant IFN or IL2 response when coeliac biopsies were cultured with PTA. Similarly, biopsies from normal controls did not respond to PTG or PTA. The finding of this study suggests that the immunogenic sequences in gliadin are not present in avenin. Moreover, they are in keeping with in vivo studies, which report that oats are safe for consumption by coeliac patients.

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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 für die Praxis", which 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 work on the 3. edition of the small Table "Der kleine Souci-Fachmann-Kraut: Lebensmitteltabelle für die Praxis" has been continued, the publication is planed for autumn this year.

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 data of this group partly has been revised and as an important aspect in the actual discussion about disease prevention and health, data of the group of the bioactive compounds has been extended. Due to the development of the analytical methodology some data should be actualized in the future (e.g. iodine and folic acid data).

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. In order to document the data quality and to give the user informations about the scientific background of the SFK-database, the publication of the following parameters: source of literature, analytical methodology and number of samples is planed for the next update of the online-version.

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