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1. STUDIES ON THE HEDONIC VALUE OF FOOD

1.1. Aroma and taste (flavor) as parameters of food quality

1.1.1. Key odorants in hand-squeezed grapefruit juice

By application of the Aroma Extract Dilution Analysis on an extract prepared from fresh grapefruit juice, 37 odor-active compounds were detected in the Flavor Dilution (FD) factor range of 4 to 256, and subsequently identified. Among them the highest odor-activities (FD-factors) were determined for butanoic acid ethyl ester, p-1-menthene-8-thiol, (Z)-3-hexenal, 4,5-epoxy-(E)-2-decenal, 4-mercapto-4-methyl-pentane-2-one, 1-heptene-3-one and wine lactone. Besides the five last mentioned compounds, a total of 13 further odorants were identified for the first time as flavor constituents of grapefruit. The data confirm results of the literature on the significant contribution of 1-p-menthene-8-thiol in grapefruit aroma, but clearly show that a certain number of further odorants are necessary to elicit the typical grapefruit flavor.

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1.1.2. Key odorants in sweet bell pepper powders from Hungary and Morocco

By application of GC/Olfactometry on aroma extracts prepared from Hungarian sweet bell pepper powder (HBP) and Moroccan sweet bell pepper powder (MBP), 35 and 42 odor-active compounds, respectively, were detected in the HBP or the MBP. The identification experiments, in combination with the Flavor Dilution (FD) factors obtained by application of the Aroma Extract Dilution Analysis, revealed beta-ionone (violet-like), 4-hydroxy-2,5-dimethyl-3(2H)-furanone (Furaneol; caramel-like), 3-hydroxy-4,5-dimethyl-2(5H)-furanone (Sotolon; seasoning-like) and 2- and 3-methyl-butanoic acid with the highest odor activities (FD-factors of 8192 to 32768) among the 33 odorants which could be identified in the HBP. All odorants identified in the HBP were also characterized as odor-active volatiles in the MBP. The overall different aroma of the Moroccan sample could, however, be attributed to lower FD-factors of the five key odorants mentioned above and, in addition, to higher FD-factors of 10 odorants not present among the aroma compounds of the HBP, e.g., (Z)-1,5-

octadien-3-one. In total, 20 odor-active volatiles are reported here for the first time as volatile bell pepper constituents.

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1.1.3. Aroma compounds in dried hop cones (variety: Spalter Select) - Influence of drying

Application of the Aroma Extract Dilution Analysis on the volatiles obtained from dried cones of Spalter Select hops grown in the Hallertau revealed twenty-three odorants in the Flavor Dilution (FD) factor range of 16 to 4096, twenty of which could be identified. Based on high FD-factors, trans-4,5-epoxy-(E)-2-decenal, linalool and myrcene were identified as the most potent odorants, followed by 2-methyl-propanoic acid methyl ester, 2-methyl-butanoic acid methyl ester, (Z)-1,5-octadien-3-one, nonanal, (E,Z)-1,3,5-undecatriene, 1,3(E),5(Z),9-undecatetraene, 2-methylbutanoic acid propyl ester, 4-ethenyl-2-methoxyphenol and 1-octen-3-one. Ten of the high impact hop aroma compounds had previously not been identified as hop constituents and, in particular the 1,3(E),5(Z),9-undecatetraene has not yet been reported as a food odorant. In an extract obtained from fresh hop, in addition to the odorants found in the dry hop, (Z)-3-hexenal was characterized as a further key odorant rendering an additional green aroma note to the fresh material.

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1.1.4. Changes of potent odorants of raw Arabica coffee during roasting

Aroma extract dilution analysis of raw Arabica coffee revealed 3-isobutyl-2-methoxy-pyrazine (I), 2-methoxy-3,5-dimethyl-pyrazine (II), 2-methyl-butanoic acid ethyl ester (III), 3-methyl-butanoic acid ethyl ester (IV) and 3-isopropyl-2-methoxy-pyrazine (V) as potent odorants. The highest odor activity value was found for I followed by II, IV and V. It was concluded that I was responsible for the characteristic, peasy odor note of raw coffee. Twelve odorants occurring in raw coffee and (E)-beta-damascenone were also quantified after roasting. The concentration of I did not change, whereas methional, 3-hydroxy-4,5-dimethyl-2(5H)-furanone, vanillin, (E)-beta-damascenone, 4-vinyl- and 4-ethylguaiacol increased strongly during the roasting process. These compounds together with other odorants, which are exclusively formed by the roasting process (e.g. 2-furfurylthiol), mask the peasy odor of 3-isobutyl-2-methoxy-pyrazine.

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1.1.5. Aroma-simulation of a solid food on the basis of its odorant composition in the gas phase

The aroma-simulation for a solid food was investigated with roasted ground coffee as example. The concentrations of 22 potent odorants including acetaldehyde, methylpropanal, 2- and 3-methyl-butanal, 2,3-butanedione, 2,3-pentanedione, 2-furfurylthiol, 2-ethyl-3,5-dimethyl-pyrazine and 2,3-diethyl-5-methyl-pyrazine were quantified in the headspace above roasted coffee powder. A model mixture containing these odorants was prepared on the basis of the concentrations found in the headspace. When evaporated, the aroma of the model mixture matched that of the roasted coffee sample very well. Also after reduction of the model to the nine odorants mentioned above, the aroma was still near to that of the original coffee sample. By the determination of the headspace-concentrations of freshly ground coffee

and of coffee powder 15 min after grinding and by the preparation of the corresponding aroma models, the changes in the odor profile of a real coffee sample in dependence of the time past after grinding could be reproduced. The results of all experiments show that the new procedure is suitable to establish the composition of odorants which are perceived by the human nose in the air above a solid food.

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1.1.6. Studies on the crumb flavor of three-stage sourdough rye bread

Application of the Aroma Extract Dilution Analysis on an extract from the crumb of a fresh rye sourdough bread, the quantification of 22 of the most odor-active compounds identified by isotope dilution assays and, finally, the calculation of odor activity values (OAV's) revealed, in particular, 3-methyl-butanal, methional, phenylacetaldehyde, 2,3-butandione, hexanal, (E)-2-nonenal, (E,E)-2,4-decadienal, acetic acid, vanillin as well as 2- and 3-methyl-butanoic acid as key crumb odorants. These results were corroborated by aroma recombination studies. Quantitative measurements performed on selected odorants on line with the process from the flour to the ready-to-eat rye bread revealed that rye flour already contained significant amounts of some crumb odorants. Sourdough fermentation resulted in the formation of, in particular, acetic acid and 3-methyl-butanal, whereas, e.g., hexanal and methional decreased during the fermentation steps. The baking process finally led to losses of fermentation products by evaporation on the one hand, but formation of, e.g., methional by a thermally induced Strecker-degradation on the other hand.

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1.1.7. Model studies on the Strecker reaction - Influence of oxygen

Application of the Aroma Extract Dilution Analysis on the volatile compounds formed by reacting glucose and L-phenylalanine (30 min, 100 °C) revealed the "Strecker" aldehyde, phenylacetaldehyde (PA) and, in addition, phenylacetic acid (PAA) as the two key odorants among the volatiles formed. Quantitative measurements on four alpha-dicarbonyls generated in the glucose/L-phenylalanine mixture revealed the 3-desoxyosone and glyoxal as the first sugar degradation products, whereas 2-oxopropanal became the predominant alpha-dicarbonyl after about 4 h at 100 °C. Further model studies established 2-oxopropanal as the most effective alpha-dicarbonyl in generating PA as well as PAA from phenylalanine. However, the reaction parameters significantly influenced the ratio of both odorants. E.g., at pH 3.0 the ratio of PA to PAA was 3:1, whereas at pH 9.0 the ratio was 1:5. Furthermore, in the presence of oxygen and copper ions the formation of the acid was further increased. Compared to 2-oxopropanal and, also glyoxal, the 3-desoxyosone as well as the glucosone formed phenylacetaldehyde, but both were not very effective in acid generation. Based on the results, a new oxygen dependent formation pathway of the Strecker reaction leading to acid formation is discussed.

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1.1.8. Influence of L-cysteine on the formation of bitter-tasting amino-hexose-reductones from glucose and L-proline - identification of a novel furo[2,3-b]thiazine

Thermal treatment of a 1+1 mixture of glucose and L-proline led to the development of an intense bitter taste being reflected in high amounts of the bitter-tasting bispyrrolidino-hexose-

reductone formed. Heating the reaction mixture in the presence of L-cysteine drastically reduced the amounts of the amino-hexose-reductone and, thereby, the intensity of the bitter taste. Studies on the mechanism of the cysteine-induced reduction of the bitter taste revealed that the precursor of amino-hexose-reductones, the hexose-derived acetylformoin reacted more easily with L-cysteine to form the taste-less 7-hydroxy-4a,6-dimethyl-2H,3H,4aH-furo[2,3-b] thiazine, a previously unknown Maillard reaction product, than with L-proline to amino-hexose-reductone, thereby blocking the formation of bitter-tasting compounds.

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1.2. Color as parameter of food quality

1.2.1. The color activity concept - A novel approach to characterize key chromophores formed by non-enzymatic browning reactions

It is well accepted that the non-enzymatic browning of thermally processed foods originates mainly from the Maillard reaction between reducing carbohydrates and amino compounds. To evaluate the key chromophores amongst the multiplicity of reaction products formed, a screening method was developed which is based on the determination of the visual thresholds of colored fractions obtained after HPLC separation. This so called Color Dilution Analysis (CDA) is exemplified in the following paper which describes a browned aqueous xylose/furan-2-aldehyde/L-alanine solution. Twenty colored fractions were obtained, amongst which five fractions were evaluated with by far the highest color impacts. The identification experiments were, therefore, focused on the compounds evoking the intense color of these fractions. They revealed two orange colored 3(2H)-furanones, a red colored 3(2H)-pyrrolinone, an orange colored pyrano[2,3-b]pyranone and a yellow colored dione as the key chromophores. In order to evaluate the color impact of these color-active compounds more exactly, their absolute color contribution was measured by calculating their color activity values as the ratio of their concentrations to their color detection thresholds. By application of this novel analytical strategy, which we call the color activity concept, 13.5 % of the overall color of the reaction mixture was shown to be accounted for five colorants of known structures.

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1.2.1. Characterization of precursors and elucidation of the reaction pathway leading to a novel colored 2H,7H,8aH-Pyrano[2,3-b]pyran-3-one from pentoses by quantitative studies and 13C-labeling experiments

The intensely colored (1R,8aR)- and (1S,8aR)-4-(2-furyl)-7-[(2-furyl)methylidene]-2-hydroxy-2H,7H,8aH-pyrano[2,3-b]pyran-3-one has recently been identified as one of the main colored compounds formed in the presence of pentoses. To clarify its formation pathway, quantitative studies on the effectivity of certain carbohydrate degradation products as precursors of the colorant were performed indicating the 3-deoxypentos-2-ulose, furan-2-aldehyde and hydroxyacetaldehyd as the penultimate precursors. In addition, a labeling experiment with [13C1]-xylose was performed to elucidate, how these precursors are transformed into the 4-(2-furyl)-7-[(2-furyl)methylidene]-2-hydroxy-2H,7H,8aH-pyrano[2,3-b]pyran-3-one.

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2. DEVELOPMENT OF SPECIAL ANALYTICAL TECHNIQUES

2.1. Development of a stable isotope dilution assay for an accurate quantification of protein-bound N-(1-deoxy-D-fructos-1-yl)-L-lysine using a carbon-13 labeled internal standard

Syntheses of the labeled Amadori compound [$^{13}C_6$]-N-(1-deoxy-D-fructos-1-yl)-L-lysine ([$^{13}C_6$]-DFLys) and the labelled tetrapeptide Ala-[$^{13}C_6$]-DFLys-Leu-Gly are presented. The compounds were used in the development of stable isotope dilution assays for the quantification of the degree of glycosylation of bovine serum albumine treated for 20 min at 95 °C in the presence of glucose. The experiments revealed that the use of the labeled standards in combination with LC/MS allowed the exact quantification of protein bound DFLys with the high recovery rate of 95 % (at a spike level of 150 nmol/mg of protein) and a low detection limit of 5 nmol/mg of protein. The data revealed however, that DFLys is significantly degraded during the enzymic hydrolysis of the protein backbone generally needed in the quantification procedure and, furthermore, incomplete digestion of the protein was observed. Both sources of errors were clearly overcome by using in particular the labeled peptide as the internal standard.

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2.2. Model studies on the diffusion behaviour of the mycotoxin patulin in apples, tomatoes and wheat bread

Quantitative studies on the diffusion behaviour of the mycotoxin patulin (Pat) performed by stable isotope dilution assays using a carbon-13 labeled analogue as the internal standard revealed that Pat did not diffuse into apples affected by the fungus Penicillium expansum. In a distance of more than two centimeters from the infected zone the mycotoxin was not detectable. However, in a similar experiment with tomatoes the mycotoxin was found to penetrate into the whole fruit. These different characteristics were related to the physical laws of diffusion and attributed to differences in the texture of the foods. Like in apple tissue, the patulin content in molded wheat bread crumb fell sharply in a longer distance from the fungal mycelium. A comparison with aflatoxins revealed that these mycotoxins show much faster diffusion into the crumb compared to patulin.

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

3.1. Heat-induced thiol/disulphide exchange reactions in milk proteins: investigation of beta-lactoglobulin

Heating of milk induces the formation of aggregates of milk proteins by thiol/disulphide exchange reactions. Beta-Lactoglobulin and bovine serum albumin are responsible for these reactions as they are the only milk proteins containing a free thiol group. Because of its higher amount in milk, beta-lactoglobulin is assumed to be more important for thiol/disulphide exchange reactions than serum albumin. Aim of the present study was to establish thiol/disulphide exchange reactions in heat-treated beta-lactoglobulin solutions by identification, isolation and sequence analysis of cysteine and cystine containing peptides in tryptic digests of the protein. To enable a selective identification, free SH-groups were

alkylated with an SH-reagent containing a VIS-absorbing label immediately after heating. Cystine peptides in the tryptic beta-lactoglobulin hydrolysates were identified by differential HPLC prior to and after chemical reduction of the disulphide bonds. Relevant peptides were collected, sequenced with an automated protein sequencer and the sequences were assigned to the beta-lactoglobulin sequence. Heating of beta-lactoglobulin to 60 - 90 °C induced a shift of the free thiol group in position 121/119 to position 160 of the sequence, very close to the C-terminal end of the protein. For the investigation of the disulphide bonds isolated cystine containing peptides were sequenced directly without previous reduction. The positions of the disulphide bridges were identified by means of the peak generated by di-PTH cystine that was eluted very close to PTH tyrosine. The high reactivity of the free thiol group in native beta-lactoglobulin (position 121/119) during heating was demonstrated by the identification of an alternative disulphide bond from Cys121/119 to Cys160. The native linkage is Cys66-Cys160.

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3.2. Localisation of protein-bound thiol groups in wheat flour

The thiol/disulfide structure of gluten proteins strongly determines the rheological properties of wheat dough. About 5 % of cysteines in wheat flour occur in the reduced (thiol) form; 0.5 % are present in low-molecular-weight compounds like glutathione or cysteine, and 4.5 % in flour proteins. The distribution of protein-bound thiol groups on Osborne fractions and their localisation in gluten proteins are not known. Therefore, flours of the wheat cultivars "Rektor" and "Contra" were fractionated into water-soluble albumins and low-molecular-weight thiol compounds, salt-soluble globulins, alcohol-soluble gliadins and SDS-soluble glutenins. Free thiol groups were labelled with the fluorescent reagent DACM (N-(7-dimethylamino-4-methyl-2-oxo-3-chromenyl)maleinimide), and fluorescence was measured against a blank. The highest amounts of thiol groups were detected within the gliadins (about 60 % of total recovered fluorescence) followed by SDS-soluble glutenins (about 20 %). Both wheat cultivars did not significantly differ. In order to determine the position of thiol groups in single proteins, the labelled gliadin and reduced glutenin fractions of "Rektor" were separated by means of RP-HPLC. The measurement of fluorescence during elution indicated that major fluorescent components were located within the elution area of alpha- and gamma-gliadins (gliadin fraction) and of LMW subunits (glutenin fraction). N-terminal sequencing of the fluorescent proteins allowed the assignment to the protein type. Three peaks corresponded to alpha-gliadins, three peaks to gamma-gliadins and one peak to LMW subunits. The positions of the cysteine residues were determined by partial hydrolysis of the proteins with thermolysin and sequencing of fluorescent peptides separated by RP-HPLC. The LMW subunit contained one cysteine residue (Cx), the gamma-gliadin three residues (Cb*, Cc, Cz) and alpha-gliadin one residue (Cz) as binding site for DACM.

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3.3. Model studies on the reaction parameters governing the formation of disulphide bonds in LMW-type peptides by disulphide isomerase (DSI)

The formation of disulfides from the synthetic peptides LGQCV and FSQQQPCS in the presence of disulfide isomerase (ratio of thiol to enzyme: 10+1) was significantly accelerated in the pH range of 4 to 9, compared to a model without enzyme addition. However, a reshuffling experiment in which (LGQCV)2 and FSQQQPCS were used resulted in the formation of the mixed disulfide only at pH 7 to 9, but not at pH 5. Decreasing the enzyme

concentration by a factor of 200 also increased disulfide formation. However, because glutathione dimer had to be added to these models in order to re-activate the "reduced" enzyme, also mixed disulfides with glutathione were formed. Larger peptides (MW >2500 dalton) were not accepted by the enzyme thereby leading to an increase in glutathione attached to the shorter peptide used in the experiments.

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3.4. Contribution of *Aegilops tauschii* glutenin genes to the bread-making properties of wheat

The contribution of the diploid wild wheat species Aegilops tauschii (genome DD) to bread-making was studied investigating three synthetic hexaploid wheats (AABBDD) derived from a common Triticum turgidum var. durum (AABB) and three different Aegilops tauschii parental lines. The durum wheat had the HMW subunit composition 7+8, two Aegilops lines the composition 7+8 and 5+10 and one Aegilops line the composition 7+8 and 2+T1+T2. Bread-making properties of the flours were characterised by micro-scale extension tests of gluten and micro-baking tests. The durum wheat and the Aegilops wheat with HMW subunits 2+T1+T2 developed weak gluten and bread with low loaf volume, whereas the other Aegilops lines had relatively strong gluten and high loaf volume. Studies on the synthetic hexaploid lines indicated that HMW subunit alleles of durum and Aegilops parents were additively expressed. Bread loaf volumes, gluten maximum resistance and extensibility, dough surface and other quality characteristics of the hexaploid wheats were closely related with those of the Aegilops wheats. This clearly demonstrates that Aegilops lines determine the properties of the synthetic lines much more than durum wheat.

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3.5. Effects of HMW and LMW subunits of glutenin on the rheological dough properties and breadmaking quality of wheat

Previous studies on the effects of gluten proteins after addition to flours have been focussed on the HMW subsunits and on the rheological properties of gluten. These investigations were continued by studying the effects of HMW and LMW subunits ad gliadins on the rheological properties of dough and on bread volume. HMW and LMW subunit fractions and the gliadin fraction were produced from flour of the cultivar Rektor by a specific extraction/precipitation procedure. The protein fractions, either in a reduced form or reoxidised with $KBrO_3$ or KIO_3, were added in 1 % amounts to a base flour of the wheat cultivar Rektor and mixed with water. The corresponding doughs were then characterised by micro-scale extension tests and by micro-baking tests and were compared to doughs from the base flour without additives. The maximum resistance of dough was strongly increased by HMW subunits in a reduced state and by HMW subunits reoxidised with $KBrO_3$. A moderate increase of resistance was caused by HMW subunits reoxidised with KIO_3 and by LMW subunits reoxidised with $KBrO_3$ or KIO_3. LMW subunits in a reduced state and gliadins strongly lowered this resistance. The extensibility of dough was significantly increased only by gliadins and reduced HMW subunits; HMW subunits reoxidised with $KBrO_3$ had no effect, and all other fractions had a decreasing effect. In particular, glutenin subunits reoxidised with KIO_3 induced marked decrease of extensibility, resulting in bell-shape curved extensigrams, which were typical for plastic properties. The effect of reoxidised mixtures of HMW and LMW subunits (ratio = 2:1) on maximum resistance depended on the oxidising agent and on the conditions (reoxidation separated or together); extensibility was generally decreased. Bread volume was increased by

addition of HMW subunits reoxidised with $KBrO_3$ and decreased by LMW subunits reoxidised with $KBrO_3$ or KIO_3 and by a HMW/LMW subunit mixture reoxidised with $KBrO_3$.

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3.6. The influence of hot-air drying on the quality of dry wheat gluten

Dry wheat gluten, a by-product of starch production, is used by millers and bakers in order to improve the properties of baked products. The quality of commercial gluten, however, varies to a great extent and depends on the drying parameters. The influence of the flour quality and of the drying conditions on gluten quality was not known in detail. Therefore, drying experiments were carried out using a flash drier (Ultra Rotor) which allowed the variation of hot air temperature (230, 330 °C), solid content (60, 65 %) and number of drying steps (1, 2, 3). Two flours with different baking quality (A und C grade) were used as raw material. The dried products were used directly or in a rehydrated state to determine rheological properties (mixing and extension tests, measurements with stress rheometer and glutograph) and baking performance (baking tests on macro- and micro-scales). The results showed that the different drying parameters significantly influenced gluten quality. In particular, the number of drying steps was highly correlated with the decrease in quality, but also high temperature and low solid content led to undesirable gluten properties. The quality of gluten from flour A with a high baking quality was more influenced by processing parameters than that from flour C with a poor baking quality. Dough development (model based on starch and gelatine), resistance and extensibility (extension test) and shear time (Glutograph) of rehydrated gluten and the bread volume (model based on starch and gelatine) were most useful to judge the quality of gluten. In contrast, simple chemical methods like extraction and fluorescence measurement of gluten proteins did not allow a reliable estimation of gluten quality.

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3.7. Quantification of gluten proteins in wheat flour: application samples

In a previous work an extraction/HPLC procedure has been developed that allows the quantification of all gluten protein groups and types present in wheat flour. By means of this method the influence of varieties and growing conditions on the quantitative composition of gluten proteins have been demonstrated. Two further applications of the method to wheat flour - estimation of the grade of steaming and characterisation of varieties with unexpected baking quality - were tested in the present work. Previous studies have shown that the extractability of gliadins from bread with 60 % ethanol is strongly reduced in comparison to flour. Based on this result is was assumed that the extractability of gliadins could serve as an indicator for the grade of heat-treatment of flour. To corroborate this assumption differently treated wheat flours from industry (dried, steamed, chlorinated) were compared with non-treated flour and with bread. The samples were extracted stepwise with a salt solution, 60 % ethanol and a glutenin extraction solvent. Both gliadin and glutenin fraction were quantitatively analysed by RP-HPLC. The results demonstrated that the ratio of proteins extractable with 60 % ethanol (gliadins) to the non-extractable proteins reflected very well the grade of heat-treatment. This ratio was high for untreated, dried or chlorinated flours (1.70-2.19), low for steamed flours (0.57-0.83) and extremly low for fully heat-treated flour and bread (0.21, 0,28). The extractability of gliadins appears to be a better indicator for heat-treatment than enzyme activity. The combination of HMW subunits of glutenin encoded at the 1D chromosome is an important parameter for wheat quality. The combination 5+10 has been

correlated with high baking quality and the combination 2+12 with poor quality. Exceptions to this rule are, for example, the Austrian variety Achat (subunits 2+12) classified as a wheat with high bread-making quality and the French variety Tilburi (subunits 5+10) as a wheat with very poor quality. The quantification of gluten protein types and single HMW subunits by extraction/HPLC revealed that Achat contained high amounts of x-type HMW subunits typical for high quality varieties, which was caused by the presence of x-type subunit 1 and the over-production of x-type subunit 2. The poor variety Tilburi was also characterised by high amounts of x-type subunits, but the amounts of gliadins and LMW subunits of glutenin were extremely low, which strongly reduced total protein content of flour. These studies demonstrate again that, in order to predict flour quality, it is not sufficient to characterise HMW subunits in purely qualitative terms; the quantitative composition of gluten proteins has also to be considered.

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3.8. Development of a nephelometric method for the quantitative determination of small amounts of gliadin

Wheat starch is desired as an ingredient of gluten-free food, because it improves product quality, but is only permitted when the gliadin content is below 100 ppm. A reliable quantification of gliadin, however, is not possible because existing immunochemical assays are either not sensitive or specific enough and only partly available on a commercial basis. Therefore, a simple non-immunochemical method was developed based on a specific precipitation and nephelometric measurement of gliadin. As a reference a defined gliadin extract from cultivar "Rektor" (54.7 mg protein in 10 mL of 60 % ethanol) and a freeze-dried gliadin standard (84.1 % protein) were used. Aliquots of the extract (0.6-3.0 mg protein) were filled up with 60 % ethanol to 10 mL and mixed with 20 mL of 2-propanol. The turbidity was then measured by nephelometry over 60 min. The results demonstrated that nephelometry was at least 10fold more sensitive than turbidimetry. The values were strongly dependent on the time of measurement, and maxima were not reached within 60 min, when low concentrations (<1 mg/10 mL) were measured. Therefore, instead of 2-propanol the following organic solvents were tested for precipitation: ethanol, butanol, aceton, tetrahydrofuran, tert. butylmethylether (TBME) and mixtures of them. Mixtures of TBME with ethanol (1:1) and with 2-propanol (1:3) were the best. Experiments with a gliadin standard (15-300 ug) dissolved in 60 % ethanol/0.1 mol/L NaCl and precipitated with TMBE/2-Propanol showed again the dependence of nephelometric turbidity units on both gliadin concentration and measuring time. The time necessary to reach maximum values ranged from 8 min (300 µg) to 90 min (15 ug). When the maximum values were taken, a linear relation between turbidity units and gliadin concentration was obtained within a range of 0-300 µg. The detection limit was less than 15 ug corresponding to 15 ppm gliadin, when 1 g starch is extracted with 10 mL of solvent. The coefficient of variation was 1.8 % (12 determinations).

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3.9. Structure-function relationships of synthetic emulsifiers for the production of chocolate

As polar lipids can act as emulsifiers, some of them, e.g. lecithin or PGPR are used in the production of chocolate. Esters of polycondensated fatty acids of castor oil and polycondensated glycerol, briefly called PGPR, have a positive effect on the technical properties of chocolate mass as they decrease its viscosity and the yield value. However, up to

now, no information is available about the effect of individual components of PGPR. Aim of the present study was therefore the fractionation of a commercial PGPR-sample, the isolation of fractions or components and the determination of the structures of individual components. In this way, the effect of PGPR should be related to defined chemical structures. First, a commercial PGPR sample was characterised by the determination of physico-chemical parameters. The first step of the fractionation was an extraction of the sample with hexane/methanol. The methanol fraction was then subfractionated by preparative HPLC on a diol column. The subfractions were hydrolysed and fatty acids were determined quantitatively. Rechromatography of the subfractions by analytical HPLC or HPLC-GPC yielded individual components. Their molecular weights were determined by means of MALDI-TOF mass spectrometry and their structures were deduced from NMR spectroscopic data. These components were cyclic polyricinoleic acids with 2-10 ricinoleic acid residues per molecule. Because of the cyclic structure and the absence of glycerol, this class of compounds lacks a polar group as it is present in other PGPR components. Therefore it exhibits only a weak emulsifying activity in the chocolate mass.

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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 whole scientific data material and by means of the PC-data bank 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 "special bioactive compounds".

The 6. edition of the "Souci-Fachmann-Kraut Food Composition and Nutrition Table" has been published in June 2000.

The software of the SFKDB has been updated to guarantee its stability concerning the "millenium-problem". Adapted to the development of media, an on-line version of the Souci-Fachmann-Kraut Food Composition Table is in preparation, which offers different search functions (food items, nutrients and their concentrations, energy values) and the possibility to calculate the food composition data of mixed food.

The preparation of the 7. edition has been started, whereas the work on the 3. edition of the small Table "Der kleine Souci-Fachmann-Kraut: Lebensmitteltabelle für die Praxis" has been continued.

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