

## Annual Report 1998

### Contents

#### Studies on the hedonic value of food - Aroma and taste (flavour) as parameters of food quality

- [Comparison of the key odorants of different virgin olive oils](#)
- [Key odorants in processed flavours](#)
  - [Odorants formed in mixtures of cysteine/carbohydrates treated under roasting conditions - comparison with aqueous systems](#)
  - [Characterization of important odour-active compounds formed in proline/glucose-mixtures - Influence of the reaction conditions](#)
  - [Model studies on the formation of 4 popcorn-like smelling odorants generated from the Maillard reaction of proline](#)
- [Odour and taste compounds of Camembert cheese](#)
- [Quantification of 2-methyl-3-furanthiol, 2-furfurylthiol, 3-mercapto-2-pentanone and 2-mercapto-3-pentanone in heated meat](#)
- [Hay-like off-flavour of dry parsley](#)
- [Aroma of orange juice](#)
  - [Aroma compounds in a freshly squeezed juice of Valencia late oranges](#)
  - [Release of orange volatiles during consumption of fruit and juice](#)
- [Studies on the development of selective chemosensor arrays for the evaluation of roasting degrees](#)
- [Studies on the non-enzymatic browning reaction in heated foods](#)
  - [Characterization of the chemical structure of novel coloured Maillard reaction products from furan-2-carboxaldehyde and amino acids](#)
  - [Studies on melanoidin-type colourants generated from the Maillard reaction of protein-bound lysine and furan-2-carboxaldehyde - chemical characterisation of a red coloured domain](#)
  - [Application of <sup>13</sup>C-labeling techniques for the elucidation of the formation pathway leading to a red coloured 1H-pyrrol-3\(2H\)-one during the Maillard reaction of furan-2-carboxaldehyde and L-alanine](#)

#### Studies non the relationship between the structure of biopolymers and their technological properties

- [Importance of amounts and proportions of HMW subunits for wheat quality](#)
- [Investigation of viscoelastic properties of dough and gluten from different wheat varieties by stress rheometry](#)
- [Reoxidation behaviour of wheat and rye glutelin subunits](#)
- [Study of the effect of DATEM](#)

- [Influence of variety and location on yield and quality of spelt grown under ecological conditions](#)

### **Characterisation of toxic structures in proteins**

- [Effect of single gliadin components on the fetal chick duodenum](#)
- [Studies of the affinity of single gliadin components in a commercial enzyme immunoassay](#)

### **Food composition and nutrition tables**

- [Actualisation of the tables](#)
  - [Scientific evaluation of the SFK-data](#)
- 

## **Summaries**

### **1. STUDIES ON THE HEDONIC VALUE OF FOOD - AROMA AND TASTE (FLAVOUR) AS PARAMETERS FOR FOOD QUALITY**

#### **1.1. Comparison of the key odorants of different virgin olive oils**

The potent odorants of virgin olive oils from Italy (I), Spain (S) and Morocco (M) were screened by aroma extract dilution analyses and gas chromatography olfactometry of headspace samples. After quantification odor activity values (OAVs) were calculated by dividing the concentrations of the odorants in the oil samples by their nasally and retronasally determined odor threshold values in sunflower oil. Basing on nasal thresholds the following compounds showed high OAVs in the oils given in brackets: acetaldehyde (I, S, M), acetic acid (I, S), propanal (I), 1-penten-3-one (I), (E,Z)-2,4-decadienal (I, M), trans-4,5-epoxy-(E)-2-decenal (I,S,M), (Z)-3-hexenal (I, M), (E)-2-hexenal (I), (Z)-3-hexenyl acetate (I), 4-methoxy-2-methyl-2-butanethiol (S), ethyl 2- and 3-methylbutyrate (S, M), 2- and 3-methylbutanal (S), ethyl cyclohexylcarboxylate (M), ethyl isobutyrate (M). Higher OAVs were additionally found for hexanal (I) and (Z)-2-nonenal (I, M) when retronasal odor thresholds were used as basis. The potent odorants were dissolved in a refined plant oil in the concentrations found in the three olive oil samples. The flavor profiles of the models obtained were very close to those of the real samples indicating that the different notes in the flavour profiles of these oils could be reproduced, e.g. green, fruity, black currant-like. Models missing one or several compounds with the same odor quality gave an insight into the importance of the odorants contributing to the flavour profiles of the oil samples. These results were confronted with those published recently by other groups.

### **Index**

#### **1.2. Key odorants in processed flavours**

##### **1.2.1. Odorants formed in mixtures of cysteine/carbohydrates treated under roasting conditions - comparison with aqueous systems**

Application of the Aroma Extract Dilution Analysis on volatile fractions obtained from dry-heated (180°C for 6 min on silica) mixtures of cysteine and ribose (I), glucose (II) or

rhamnose (III) revealed 2-furfurylthiol (FFT) and 2-acetyl-2-thiazoline with the highest Flavour Dilution (FD) factors in I, 2-acetyl-2-thiazoline, 2-propionyl-2-thiazoline and FFT in II and 5-methyl-2-furfurylthiol, 4-hydroxy-2,5-dimethyl-3(2H)-furanone, 2-acetyl-2-thiazoline, 2-propionyl-2-thiazoline and (Z)-2-propenyl-3,5-dimethylpyrazine in III. A comparison of the data with results of previous studies, in which the same mixtures had been reacted under aqueous conditions (145°C; 20 min) revealed that the dry-heating process favoured the formation of the roasty, popcorn-like smelling 2-acetyl- and 2-propionyl-2-thiazoline as well as the potato chip-like 2-ethyl-3,5-dimethylpyrazine and 2,3-diethyl-5-methylpyrazine in all three reaction systems. 2-Ethenyl- and (Z)-2-propenyl-3,5-dimethylpyrazine, both having an intense roast potato aroma were, however, selectively formed in the presence of ribose or rhamnose, respectively. Based on quantitative data, formation mechanisms generating the latter two pyrazines via their 1-desoxyosones as key intermediates are discussed.

## [Index](#)

### **1.2.2. Characterization of important odour-active compounds formed in proline/glucose-mixtures - Influence of the reaction conditions**

Application of the aroma extract dilution analysis on an aroma extract obtained by boiling a mixture of proline and glucose for 2 h revealed the two tautomers of 2-acetyltetrahydropyridine (ATHP; roasty, popcorn-like) as the most odour-active compounds among the 7 odorants detected in the FD-factor region of 16-4096. Contrary, in a proline/glucose mixture treated for 10 min at 160°C at a low water content, 2-acetyl-1-pyrroline (AP; roasty, popcorn-like) and 4-hydroxy-2,5-dimethyl-3(2H)-furanone showed the highest odour impact. Besides ATHP and AP, 2-propionyl-1-pyrroline and 2-propionyltetrahydropyridine were characterized for the first time in a proline/glucose Maillard system based on synthesized reference odorants.

## [Index](#)

### **1.2.3. Model studies on the formation of 4 popcorn-like smelling odorants generated from the Maillard reaction of proline**

Four popcorn-like smelling compounds have been shown to be generated from proline during Maillard-type reactions: 2-acetyltetrahydropyridine (ATHP), 2-acetyl-1-pyrroline (AP), 2-propionyltetrahydropyridine (PHTP) and 2-propionyl-1-pyrroline (PP). Based on labeling experiments with [<sup>13</sup>C<sub>6</sub>]-glucose and unlabeled proline as well as on quantitative data obtained in model studies using stable isotope dilution assays, 1-pyrroline and hydroxy-2-propanone were identified as very effective intermediates in generating ATHP. Synthesis of the key precursor 2-(1-hydroxy-2-oxo-propyl) pyrrolidine and studies on its degradation during thermal treatment confirmed its important role in ATHP formation. Boiling of this intermediate for 30 min in aqueous solution generated more than 30 % of ATHP on a molar basis. Experiments, in which hydroxypropanone was substituted by 1-hydroxy-2-butanone in the reaction with 1-pyrroline revealed that this reaction yields the homologous PHTP. Further results confirmed 1-pyrroline and 2-oxopropanal as important intermediates in the generation of 2-acetyl-1-pyrroline (AP). Based on the results of labeling experiments with [<sup>13</sup>C<sub>6</sub>]-glucose, 2 different mechanisms are proposed. One leads to AP via 2-(1,2-dioxopropyl) pyrrolidine as the precursor with elimination of carbon dioxide. The other suggests elimination of carbon-2 of the pyrroline ring. This mechanism was established by a result showing that from the reaction of 2-methyl-1-pyrroline with 2-oxopropanal the AP was also generated. Substitution

of 2-oxopropanal by 2-oxobutanal in the reaction with 1-pyrroline gave significant amounts of the homologous PP, confirming the important role of 1-pyrroline as the key intermediate in the formation of popcorn-like aromas.

## [Index](#)

### **1.3. Odour and taste compounds of Camembert cheese**

The potent odorants of two samples of Camembert (CAM) were screened by aroma extract dilution and concentration analyses and gas chromatography-olfactometry of headspace samples. After quantification, odour activity values (OAVs) were calculated by dividing the concentrations of the odorants in CAM by their odour thresholds values in sunflower oil (neutral compounds) and water (acids). In the class of the neutral odorants, the highest OAVs were found for methanethiol, methional and dimethyl sulfide all of which contributed to the sulfury, garlic-like note in the odour profile of Camembert. Although the OAV of 1-octen-3-ol was relatively low, this alcohol and the corresponding ketone were responsible for the mushroom-like note. In the acidic fraction, acetic, butyric and capric acid showed the highest OAVs.

The following substances were evaluated by the combined application of chemical and sensory analytical methods as the characteristic taste compounds of CAM: succinic acid, monosodium glutamate, ammonia and sodium chloride. It was also found that cadaverine, ornithine and citrulline may cause a bitter note. A flavour model based on an unripened, freeze-dried cheese of the Mozzarella type was prepared for CAM by the addition of the compounds which had been screened as important odour and taste contributors. Sensory evaluation indicated that the flavour profile of the model was close to that of the genuine CAM.

## [Index](#)

### **1.4. Quantification of 2-methyl-3-furanthiol, 2-furfurylthiol, 3-mercapto-2-pentanone and 2-mercapto-3-pentanone in heated meat**

A stable isotope dilution assay was developed for quantification of the potent odorants 2-methyl-3-furanthiol (MFT), 2-furfurylthiol (FFT), 2-mercapto-3-pentanone (2M3P) and 3-mercapto-2-pentanone (3M2P) in heated meat. The volatiles of meat were extracted with dichloromethane, which was spiked with definite amounts of stable isotopomers of MFT, FFT and 3M2P. The analytes and their labeled standards were enriched by reaction with p-hydroxymercuribenzoic acid and after liberation, the thiols were assayed by dynamic headspace gas chromatography in combination with mass spectrometry. The following amounts ( $\mu\text{g}/\text{kg}$ ) were found in meat samples boiled for 45 min: beef (MFT 7-28, FFT 13-42, 3M2P 55-73, 2M3P 20-44), pork (MFT 6-9, FFT 8-10, 3M2P 66-117, 2M3P 11-14), lamb (MFT 5-11, FFT 9-14, 3M2P 30, 2M3P 10). Chicken contained 4.5 of MFT, 2.4 of FFT, 100 of 3M2P and 13 of 2M3P after a boiling period of 60 min.

## [Index](#)

### **1.5. Hay-like off-flavour of dry parsley**

The flavour of parsley was changed during drying and storage. Quantification of 27 potent odorants, selected by dilution experiments and calculation of odour activity values, indicated

that 3-methyl-2,4-nonanedione (I) was mainly responsible for the hay-like off-flavour. Two furanoid fatty acids, known as precursors of I, were detected in dry parsley. The decrease in the intensities of the parsley-like, metallic and green notes in the odour profile during storage of dry parsley was due to losses of p-mentha-1,3,8-triene (II), myrcene (III) and (Z)-6-decenal (IV). Sulfurous, cabbage-like and malty notes were caused by dimethyl sulfide (V), methylpropanal (VI), 2- and 3-methylbutanal (VII/VIII). The effect of the water activity ( $a_w$  0.15, 0.25, 0.35) on the changes of I to VIII during storage of dry parsley was investigated.

## [Index](#)

### **1.6. Aroma of orange juice**

#### **1.6.1. Aroma compounds in a freshly squeezed juice of Valencia late oranges**

Application of the Aroma Extract Dilution Analysis (AEDA) on an extract of the volatiles isolated by solvent extraction of fresh orange juice followed by sublimation in vacuo at room temperature resulted in the detection of 43 odour-active compounds with Flavour Dilution (FD) factors between 4 and 1024. Among the 41 odorants identified, ethyl butanoate (fruity), followed by (Z)-3-hexenal (green) and 3a,4,5,7a-tetrahydro-3,6-dimethyl-2(3H)-benzofuranone (sweet, spicy) showed the highest FD factors. Further key odorants were ethyl 2-methylpropionate, S-ethyl 2-methylbutanoate and 4,5-epoxy-(E)-2-decenal (FD: 128). Application of the Static Headspace/Olfactometry (SHO) on a sample of the same juice revealed R-(-)-pinene, R-limonene, ethyl butanoate, S-ethyl 2-methylbutanoate and acetaldehyde as the most odour-active compounds in the headspace above the juice.

## [Index](#)

#### **1.6.2. Release of orange volatiles during consumption of fruit and juice**

Volatiles present in the human breath during consumption of a food can be analyzed by means of Atmospheric Pressure Chemical Ionization-Mass Spectrometry (APCI-MS) also called "nose space analysis". Using this method, the time intensity ( $I_{max}$ ) was determined for six volatiles during eating of orange segments or drinking of the juice thereof. For orange segments, ethyl butanoate and ethyl hexanoate had the lowest  $I_{max}$  value, whilst ethanol and acetaldehyde showed the highest value. Although ethanol was present at the highest concentration in the breath, based on odor activities, ethyl butanoate, ethyl hexanoate and acetaldehyde were the most important contributors to the overall "breath" aroma. In orange juice, limonene breath concentrations were lower compared to orange segments.

## [Index](#)

### **1.7. Studies on the development of selective chemosensor arrays for the evaluation of roasting degrees**

Previous studies had shown that 2-acetyl-1-pyrroline, 3-methylbutanal, methional, (E)-2-nonenal and 4-hydroxy-2,5-dimethyl-3(2H)-furanone are important contributors to the aromas of wheat bread crust and toasted wheat bread. Using the HRGC/SOMMSA-technique, previously developed by us, those sensor materials (commercial and selfmade sensors) were selected which were able to selectively detect the odorants under investigation. The results revealed that, for example, a ZnO/Pt sensor, when operated at 300°C, was able to selectively detect the crust odorant 2-acetyl-1-pyrroline. A copper phthalocyanine sensor selectively

detected (E)-2-nonenal in mixtures with several pyrazines. Based on the model studies, a portable sensor array was constructed which was able to detect the degree of roasting, e.g., of toasted bread slices. A combination of headspace-HRGC with the SOMMSA technique was shown to be a useful tool in the development of chemosensor arrays adapted to special challenges in flavour control, based on quantitative correlations of key odorants with indicator volatiles.

## [Index](#)

### **1.8. Studies on the non-enzymatic browning reaction in heated foods**

#### **1.8.1. Characterization of the chemical structure of novel coloured Maillard reaction products from furan-2-carboxaldehyde and amino acids**

Coloured compounds formed by Maillard-type reactions from furan-2-carboxaldehyde and primary and secondary amino acids including L-alanine and L-proline, respectively, have been identified. When furan-2-carboxaldehyde was heated with L-proline in aqueous solution at pH 7.0, an intense yellow coloured compound was generated, which was identified as an N-cyanine, namely 5-(S)-(2-carboxy-1-pyrrolidinyl)-2-hydroxy-(E,E)-2,4-pentadienal-(S)-(2-carboxypyrrolidine)imine, by application of several one- and two-dimensional NMR experiments and, in addition, by MS, UV and IR spectroscopy. Further thermal treatment of the cyanine resulted, upon a ring closure reaction, in the formation of (E)-4,5-bis-[(S)-2-carboxy-1-pyrrolidinyl]-2-cyclopenten-1-one, which has been, to our knowledge, as yet not reported in the literature. To confirm the proposed structures, L-proline was substituted by pyrrolidine and piperidine leading to analogous N-cyanines and cyclopentenones. On the other hand, thermal treatment of an aqueous solution of furan-2-carboxaldehyde and L-alanine led to the formation of two novel red coloured compounds, which were identified as (S)-4-[(E)-1-formyl-2-(2-furyl)ethenyl]-5-(2-furyl)-2-[(E)-(2-furyl) methylidene]-2,3-dihydro-(-amino-3-oxo-1H-pyrrole-6-acetic acid and the corresponding 2-[(Z)-(2-furyl)methylidene] isomer. This is the first time that chromophoric compounds comprising four linked rings with an amino acid moiety incorporated were identified in a Maillard reaction system.

## [Index](#)

#### **1.8.2. Studies on melanoidin-type colourants generated from the Maillard reaction of protein-bound lysine and furan-2-carboxaldehyde - chemical characterisation of a red coloured domain**

The identification of a coloured substructure of melanoidin-type colourants has been investigated. Brown-orange melanoidins with molecular weight >10000 Da were isolated from a thermally treated aqueous solution of casein and furan-2-carboxaldehyde using ultracentrifugation. After complete enzymatic digestion of the protein skeleton, two intense red coloured compounds were detected in the melanoidin hydrolysate by HPLC coupled to an DAD or an LC/MS. These compounds were identified as the previously unknown chromophoric amino acid (S)-2-amino-6-{4-[(E)-1-formyl-2-(2-furyl)ethenyl]-5-(2-furyl)-2-[(E)-(2-furyl) methylidene]-2,3-dihydro-3-oxo-1H-pyrrol-1-yl}hexanoic acid and its 2-[(Z)-(2-furyl)methylidene] isomer, by using 1D- and 2D-NMR techniques, by LC/MS, UV/VIS, and IR spectroscopy. The identification of these novel compounds verifies the idea that melanoidin-type colourants can be generated by a cross-linking reaction between a low molecular weight chromophore and a non-coloured high molecular biopolymer.

## [Index](#)

### **1.8.3. Application of $^{13}\text{C}$ -labeling techniques for the elucidation of the formation pathway leading to a red coloured 1H-pyrrol-3(2H)-one during the Maillard reaction of furan-2-carboxaldehyde and L-alanine**

The intensely red coloured compounds (S)-4-[(E)-1-formyl-2-(2-furyl)ethenyl]-5-(2-furyl)-2-[(E)-(2-furyl)methylidene]-2,3-dihydro-( $\alpha$ -amino-3-oxo-1H-pyrrole-6-acetic acid and the corresponding 2-[(Z)-(2-furyl)methylidene] isomer have recently been identified as the main coloured compounds formed upon thermal treatment of an aqueous solution of furan-2-carboxaldehyde and L-alanine. For clarification of their formation pathways, a labeling experiment with synthetic site specific [ $^{13}\text{C}$ ] enriched furan-2-carboxaldehyde was performed. The labeled carbon positions in the colourant were unequivocally assigned by  $^1\text{H}$  broad band decoupled  $^{13}\text{C}$  NMR spectroscopy. In contrast to conventional labeling experiments, prior to the reaction with L-alanine, the  $^{13}\text{C}$ -labeled furan-2-carboxaldehyde was diluted with the natural  $^{13}\text{C}$  abundant analogue to suppress the spectrum complexity due to homonuclear  $^{13}\text{C}$ - $^{13}\text{C}$  spin couplings. This powerful technique has been successfully used for the first time to clarify the formation route of a coloured Maillard reaction product.

## [Index](#)

## **2. STUDIES ON THE RELATIONSHIP BETWEEN THE STRUCTURE OF BIOPOLYMERS AND THEIR TECHNOLOGICAL PROPERTIES**

### **2.1. Importance of amounts and proportions of HMW subunits for wheat quality**

HMW subunits of wheat glutenin are generally considered to play a key role in gluten structure and to be closely related to wheat quality. The quantity of HMW subunits in flour has been proposed to be as important for wheat quality as their structure, but only few quantitative data are available in literature. Therefore, two assortments of wheat consisting of thirteen international and sixteen German cultivars were analysed for HMW subunit amounts and proportions by a combined extraction and HPLC procedure. The results demonstrate that the amounts varied in a broad range dependent on genotype and growing conditions. The proportions of subunits with a given subunit combination, however, varied only in small range. Generally, subunits nos. 2, 5, 7, 10 and 12 were major and subunits nos. 1, 2\*, 6, 8 and 9 were minor components. The amount of HMW subunits was highly correlated with dough development time, with maximum resistance of dough and gluten and with bread volume. Among HMW subunits the x-type (nos. 1-7) was much more important than the y-type (nos. 8-12). In particular, the presence of subunit no. 5 (additional Cys residue) and no. 7 (greatest amounts) influenced wheat quality.

## [Index](#)

### **2.2. Investigation of viscoelastic properties of dough and gluten from different wheat varieties by stress rheometry**

Two assortments of wheat flours containing 12 and 9 cultivars, respectively, were investigated for the viscoelastic properties of dough and gluten by oscillatory, creep-recovery and yield-point measurements using a stress rheometer. The results obtained were compared with the results from extension and baking tests and with gluten protein composition. Oscillatory measurements of dough showed no correlation of  $\tan \delta$  and  $G^*$  with dough

maximum resistance and with the ratio of gliadin to glutenin or to HMW and LMW subunits, whereas the results obtained for gluten were highly correlated. In contrast, creep-recovery and yield-point measurements were suitable for dough, but not for gluten. The ratio of viscosity to elasticity (V/E) and yield-point ( $\sigma$ ) of doughs were highly correlated with maximum resistance and with the ratio gliadin/glutenin and glutenin subunits, respectively. None of the methods tested by stress rheometry allowed an estimation of bread volumes determined by a micro-baking test.

## [Index](#)

### **2.3. Reoxidation behaviour of wheat and rye glutelin subunits**

HMW subunits of wheat are important for the aggregation of wheat glutelin and thus, for the rheological properties of dough and for breadmaking quality. Whereas the reoxidation behaviour of HMW subunits of wheat was already investigated, only a few informations are available for LMW subunits which are also integrated into glutenin polymers. There are also no informations about the reoxidation behaviour of HMW subunits of rye, which are homologous to wheat HMW subunits, but do not form a gluten-like material. For the investigation of reoxidation behaviour, HMW and LMW subunits were isolated from flours of the wheat cultivar Rektor (REK) and of the rye cultivar Danko (DAN) by a specific extraction/precipitation procedure. The fractions obtained (HMW-REK, HMW-DAN, LMW-REK) were then reoxidized with KBrO<sub>3</sub> and KIO<sub>3</sub> under different conditions. During reoxidation the thiol content of the fractions obtained was analysed with Ellman's reagent, and the molecular weight distribution of reoxidised proteins was determined by gel permeation chromatography. The results demonstrated that HMW-REK, HMW-DAN and LMW-REK were reoxidised much faster by KIO<sub>3</sub> than by KBrO<sub>3</sub>. The reoxidation behaviour of HMW-REK and HMW-DAN was similar. Both fractions produced more polymeric proteins during oxidation with KBrO<sub>3</sub> compared with KIO<sub>3</sub>, whereas LMW-REK formed higher amounts of polymeric proteins when was oxidised with KIO<sub>3</sub>.

## [Index](#)

### **2.4. Study of the effect of DATEM**

A commercial DATEM sample was separated by gel permeation chromatography (GPC) on Sephadex LH20 into 6 fractions which could be distinguished by their characteristic contents of acetic acid and tartaric acid. The different composition and polarity of the fractions was demonstrated by HPLC. The effect of the fractions on the baking performance and on gluten rheology was studied by micro-scale methods on the basis of 10 g of flour. Fractions F3, F4 and F5 out of the 6 GPC fractions had a good baking performance. F3 and F5 were then separated by preparative HPLC on a DIOL column into 20 fractions, respectively (F3-1 to F3-20 and F5-1 to F5-20), which were checked for activity by means of the micro-scale baking test. Only components with higher retention times exhibited a satisfactory baking performance. High loaf volumes were observed on addition of fractions F3-10, F5-8, F5-10 and F5-12 with F5-8 being the most abundant fraction of F5 (38 % by weight) and DATEM (16,4 % by peak area). Rechromatography of these fractions by analytical HPLC gave individual components. Their molecular masses were determined by electrospray ionisation mass spectrometry (ESI-MS) and were the basis for the deduction of the molecular structures. The structures of the components P5-8-1, P5-12-1 and P5-12-2 were confirmed by <sup>1</sup>H, <sup>13</sup>C and two-dimensional (HMQC, HMBC) NMR measurements.

## [Index](#)

### **2.5. Influence of variety and location on yield and quality of spelt grown under ecological conditions**

Spelt is known to be especially suitable for cultivation under ecological conditions because of its robustness and unpretentiousness with respect to nitrogen supply. In order to investigate the influence of genotype and location on cultivation characteristics, technological properties and gluten protein composition, three pure spelts, four spelts crossed with bread wheat and one bread wheat were ecologically cultivated at two locations. Further four spelt varieties were grown at a third location. With the exception of "Bauländer Spelz" (extreme tendency to lodging) pure spelts were characterised by increased plant height and tendency to lodging, and lower kernel yield. In contrast to bread wheat, spelt flours had a satisfactory protein content also under ecological conditions. The HPLC patterns of gliadins allowed the identification of genotype and, with one exception, of crossing with wheat. The amount of gliadin was strongly correlated with flour protein independent on location, whereas glutenin amounts were influenced by both genotype and location. In comparison with bread wheat, spelt varieties had a higher ratio of gliadin to glutenin; their doughs were softer and more extensible and need longer development times. Using a baking test optimised for spelt, spelt varieties even grown under ecological conditions showed high bread volumes, whereas bread wheat demonstrated a poor baking performance in both spelt and standard bread wheat test.

## [Index](#)

### **3. CHARACTERISATION OF TOXIC STRUCTURES IN PROTEINS**

#### **3.1. Effect of single gliadin components on the fetal chick duodenum**

Though gliadins are known for a long time to cause coeliac disease, the toxicity of different gliadin types is still uncertain. Therefore, the main components of (-, (- and (-type gliadins were produced from gliadin of the wheat variety Rektor by RP-HPLC. The purity and the type of the isolated components (1 (-, 8 (- and 4 (-gliadins) were confirmed by N-terminal amino acid sequencing. The isolated gliadins were then digested with immobilised pepsin and trypsin and 0.5 mg of the hydrolysates were tested by the fetal chicken test, which has been proven to be specific for the coeliac toxic effect of total gliadin. The reduction of sucrase activity compared with a control culture was taken as an indicator for toxicity. The results demonstrated that all gliadin components remarkably reduced sucrase activity. Important differences between the gliadin types could not be detected and only in a few cases, single components differed significantly. Based on these results, it seems impossible to remove the toxic factor of gliadins by breeding programs.

## [Index](#)

#### **3.2. Studies of the affinity of single gliadin components in a commercial enzyme immunoassay**

The only immunoassay developed for gliadin determination in gluten-free food, which has been ring-tested and is commercially available, is a test kit based on monoclonal antibodies against (-gliadins (Skerritt test). Previous studies have shown that different gliadin standards resulted in different calibration curves and it was proposed that the affinity of (-gliadins to the monoclonal antibodies varied amongst wheat varieties. In order to clarify this fundamental

problem, the main components of (-, (- and (-gliadins from winter wheat (Rektor) and the (-gliadins from a spring wheat (CWRS), from a wheat rye hybrid (Herzog) and from varieties of spelt, durum wheat, emmer and einkorn were isolated by RP-HPLC. The investigation by the Skerritt test revealed strong differences between both wheats and single (-gliadins. (-Gliadins from CWRS and Herzog showed the highest affinity, followed by spelt and emmer. (-Gliadins from durum wheat and einkorn had no detectable affinity. In the case of Rektor, only a minor (-component was strongly bound by the antibodies, and unspecific reactions of (-gliadins contributed more than the specific reaction with (-gliadins.

## [Index](#)

### **4. FOOD COMPOSITION AND NUTRITION TABLES**

#### **4.1. Actualisation of the 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 a continuous survey of the scientific literature and by means of the PC-data bank SFKDB. Selected data are transferred into the small table "Der kleine Souci, Fachmann, Kraut: Lebensmitteltabelle für die Praxis" which has been developed for the daily requirements of the consumer. In the future, the spectrum of food constituents covered in the large nutrition table will also address preventive-medical aspects. For the 6th edition of the SFK-table the following tasks have been carried out:

- Actualisation of the data addressing especially dietary fibre, a broad range of minerals and trace elements, the vitamin K and folic acid and cholesterol. For the compounds of the last two groups the new values are based on modern methods (predominant HPLC) and they replace in a few cases the old data which had been analysed by unspecific procedures (e.g. photometry, microbiological assays).
- Evaluation of a new shape of the nutrition table for the 6th SFK-edition and the development of the respective software for the SFKDB-data bank. The section "main ingredients" was enlarged by quoting the values for total nitrogen evaluated by the Kjeldahl method and by the values of total proteins evaluated according to the direction of the EU.
- Preparation of the 3rd edition of the "Kleiner Souci, Fachmann, Kraut: Lebensmitteltabelle für die Praxis".

## [Index](#)

#### **4.2. Scientific evaluation of the SFK-data**

The globalisation of our economy significantly influences the food market. Consequently, today many foods are imported from different regions of the earth. Exemplified by the zinc content of food raw products their differences are presented in dependence on their origin. A comparison of the data from European countries, such as Denmark, Sweden, Germany and England and from non-European countries, such as USA or South Africa showed only small variations for cow milk, wheat grains and potatoes. Greater variations were observed for leafy vegetables and fruits.

## [Index](#)

