PROGRAM & BOOK OF ABSTRACTS

International conference on new knowledge on chemical reactions during food processing and storage

CHEMICAL REACTIONS IN FOODS VIII

February 15-17 • 2017
Prague • Czech Republic

Jana Pulkabová, Monika Tomániová, Jana Hajšlová and Marco Arlorio
Editors
International conference on new knowledge on chemical reactions during food processing and storage

CHEMICAL REACTIONS IN FOODS VIII

February 15-17 • 2017
Prague • Czech Republic

Vienna House Diplomat Prague

Organized by

University of Chemistry and Technology, Prague,
Department of Food Analysis and Nutrition, Prague, Czech Republic

&

Universitá del Piemonte Orientale "A. Avogadro",
Dip. di Scienze del Farmaco, Novara, Italy

Conference is held under auspices of minister of agriculture of the Czech Republic
Marian Jurecka, and under auspices of Food Chemistry Division, EuCheMS.
**Scientific committee:**

Prof. Jana Hajslova *(chair)* (University of Chemistry and Technology, Prague, Czech Republic)

Prof. Marco Arlorio *(co-chair)* (Università del Piemonte Orientale A. Avogadro, Italy)

Prof. Lanfranco Conte (University of Udine, Italy)

Prof. Vincenzo Fogliano (Wageningen UR, Netherlands)

Prof. Marina Heinonen (University of Helsinki, Finland)

Prof. Thomas Henle (Technische Universitaet Dresden, Germany)

Prof. Rudi Krska (University of Natural Resources and Life Sciences, Vienna, IFA-Tulln, Austria)

Prof. Michael Murkovic (Graz University of Technology, Austria)

Prof. Livia Simon Sarkadi (Budapest University of Technology and Economics, Hungary)

Prof. Peter Schieberle (Technische Universitat Munchen, Germany)

**Local organizers:**

Dr. Monika Tomaniova *(chair)*

Prof. Jana Hajslova

Assoc. Prof. Jana Pulkrabova

Staff of the University of Chemistry and Technology, Prague, Czech Republic

PhD students of the University of Chemistry and Technology, Prague, Czech Republic
CRF2017 Media partners

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PROGRAM

8th International Conference on Chemical Reactions in Foods

February 15-17, 2017

Vienna House Diplomat Prague • PRAGUE • CZECH REPUBLIC

Conference is held under auspices of the minister of agriculture of the Czech Republic Marian Jurecka, and under auspices of Food Chemistry Division, EuCheMS.
Area bounded by red line is devoted to the CRF 2017 conference (lecture hall and poster area).

1: Registration desk
2: Conference hall (oral sessions and interactive course)
3: Poster area & Coffee breaks & Welcome drink
4: Conference restaurant (lunch)
5: Lifts to the hotel rooms
**CRF 2017 – PROGRAM AT A GLANCE**

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<th>WEDNESDAY February 15, 2017</th>
<th>THURSDAY February 16, 2017</th>
<th>FRIDAY February 17, 2017</th>
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<tr>
<td>8:00–9:00</td>
<td>Registration desk open</td>
<td>Registration desk open</td>
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<tr>
<td>9:00–10:00</td>
<td>Interactive course for young scientists</td>
<td>Oral session 3 CHEMICAL REACTIONS IN PROCESSED / STORED FOODS I</td>
<td>Oral session 6 CHEMICAL REACTIONS IN PROCESSED / STORED FOODS III</td>
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<tr>
<td>10:00–10:30</td>
<td>Coffee Break</td>
<td>Coffee Break</td>
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<tr>
<td>10:30–11:00</td>
<td>Oral session 4 RECENT STRATEGIES FOR HIGH FOOD QUALITY, INCREASED SHELF LIFE AND SAFETY</td>
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<tr>
<td>11:00–12:00</td>
<td>Oral session 1 STRATEGIES TO IMPROVE FOOD QUALITY AND CHEMICAL SAFETY</td>
<td>Lunch</td>
<td>Oral session 7 CHEMICAL REACTIONS IN PROCESSED / STORED FOODS IV</td>
</tr>
<tr>
<td>12:00–12:30</td>
<td>Opening of the conference &amp; Welcome to the CRF 2017</td>
<td></td>
<td>Final discussion panel &amp; CRF 2017 poster award &amp; Closing address</td>
</tr>
<tr>
<td>12:30–13:30</td>
<td>Oral session 2 CHEMICAL REACTIONS ASSOCIATED WITH FOOD FLAVOURS</td>
<td>Lunch</td>
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<tr>
<td>13:30–15:00</td>
<td>Coffee Break</td>
<td>Poster session</td>
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<tr>
<td>15:00–15:30</td>
<td>Oral session 5 CHEMICAL REACTIONS IN PROCESSED / STORED FOODS II</td>
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<tr>
<td>15:30–18:00</td>
<td>Welcome Drink</td>
<td>Conference Dinner</td>
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<tr>
<td>18:30–19:30</td>
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</table>

Coffee breaks and Welcome drink will be served in the conference area; lunch will be served in the hotel restaurant Loreta.
### WEDNESDAY, February 15, 2017

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<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>8:00–12:00</td>
<td>Registration for the CRF 2017 conference</td>
</tr>
<tr>
<td>9:00–11:00</td>
<td>INTERACTIVE COURSE FOR YOUNG SCIENTISTS</td>
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<tr>
<td></td>
<td>FOOD CHEMISTRY: LET’S ADDRESS JOINTLY CHALLENGES FOR FUTURE</td>
</tr>
<tr>
<td></td>
<td>Moderators: Milena Stranka (University of Chemistry and Technology, Prague, Czech Republic) &amp; Tomas Davidek (Nestlé Product Technology Centre Orbe, Nestec Ltd., Orbe, Switzerland)</td>
</tr>
<tr>
<td>12:00–12:30</td>
<td>OPENING of the conference and WELCOME</td>
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<tr>
<td></td>
<td>Jana Hajslova &amp; Marco Arlorio, Chairs of the CRF 2017 Scientific Committee</td>
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<td></td>
<td>Tomas Ruml, Dean of Faculty of Food and Biochemical Technology, UCT Prague</td>
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<td></td>
<td>Marco Arlorio, Chair of the Division of Food Chemistry, EuCheMS</td>
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<tr>
<td></td>
<td>Representative of Ministry, Ministry of Agriculture of the Czech Republic</td>
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<tr>
<td></td>
<td>MUSIC WELCOME</td>
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<tr>
<td>12:30–15:00</td>
<td>ORAL SESSION 1: STRATEGIES TO IMPROVE FOOD QUALITY AND CHEMICAL SAFETY</td>
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<td></td>
<td>Chairpersons: Jana Hajslova and Marco Arlorio</td>
</tr>
<tr>
<td>12:30–12:55</td>
<td>L1 TECHNICAL REGULATORY DEVELOPMENTS: ACRYLAMIDE, 3-MCPD, 2-MCPD AND GLYCIDYL FATTY ACID ESTERS AS WELL AS FURAN - AN INDUSTRY PERSPECTIVE</td>
</tr>
<tr>
<td></td>
<td>Beate Kettlitz, FoodDrinkEurope, Brussels, Belgium</td>
</tr>
<tr>
<td>12:55–13:15</td>
<td>L2 FORMATION AND METABOLIZATION OF GLYCATED AMINO ACIDS IN THE BREWING PROCESS</td>
</tr>
<tr>
<td></td>
<td>Michael Hellwig, Technische Universität Dresden, Dresden, Germany</td>
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<tr>
<td></td>
<td>Henning Sören Schmidt, Westfälische Wilhelms-Universität Münster, Münster, Germany</td>
</tr>
<tr>
<td>13:35–13:55</td>
<td>L4 HYDROLYSIS OF VICINE AND CONVICINE IN FABA BEAN SUSPENSIONS AND SOURDOUGHS</td>
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<tr>
<td></td>
<td>Marjo Pulkkinen, University of Helsinki, Helsinki, Finland</td>
</tr>
<tr>
<td>13:55–14:05</td>
<td>L5* THE RELATIONSHIP BETWEEN DOUGH COMPOSITION AND 3-MCPD ESTERS CONTENT IN COOKIES</td>
</tr>
<tr>
<td></td>
<td>Beverly Belkova, University of Chemistry and Technology, Prague, Czech Republic</td>
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<tr>
<td>14:05–14:15</td>
<td>L6* NEW NATURAL SEASONINGS FROM WINE POMACE TO INHIBIT LIPID AND PROTEIN OXIDATION DURING STORAGE OF BEEF PATTIES</td>
</tr>
<tr>
<td></td>
<td>Javier García-Lomillo, University of Burgos, Burgos, Spain</td>
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<tr>
<td>14:15–14:40</td>
<td>L7 FORMATION AND ANALYSIS OF DESIRED AROMA-ACTIVE AND UNDESIGNED FOOD-BORNE TOXICANTS DURING FOOD PROCESSING</td>
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<td></td>
<td>Michael Granvogl, Technical University of Munich, Freising, Germany</td>
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<tr>
<td>14:40–15:00</td>
<td>L8 MITIGATION OF AFLATOXINS CONTENT: IN SILICO ANALYSIS AS THE FIRST STEP IN THE ENZYMES-BASED STRATEGIES</td>
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<tr>
<td></td>
<td>Luca Dellaflora, University of Parma, Parma, Italy</td>
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<tr>
<td>Time</td>
<td>Session</td>
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<tr>
<td>15:00–15:30</td>
<td>Coffee Break</td>
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<tr>
<td>15:30–18:05</td>
<td>ORAL SESSION 2:</td>
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<td>15:30–15:55</td>
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<td>15:55–16:20</td>
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<td>16:20–16:45</td>
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<td>16:45–17:05</td>
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<td>17:05–17:25</td>
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<td>17:25–17:35</td>
<td>L14*</td>
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<td>17:35–17:45</td>
<td>L15*</td>
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<td>17:45–18:05</td>
<td>L16</td>
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<tr>
<td>18:30–19:30</td>
<td>Conference Welcome Drink</td>
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## ORAL SESSION 3: CHEMICAL REACTIONS IN PROCESSED / STORED FOODS I

**Chairpersons:** Hans-Gerd Janssen and Lanfranco Conte

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<th>Time</th>
<th>Session</th>
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<th>Speaker</th>
<th>Institution</th>
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<tr>
<td>9:00–9:25</td>
<td>L17</td>
<td>CASEIN AND CASEIN MICELLES: STRUCTURES, FUNCTIONS, FUNCTIONALIZATION</td>
<td>Thomas Henle</td>
<td>Technische Universität Dresden, Dresden, Germany</td>
</tr>
<tr>
<td>9:25–9:50</td>
<td>L18</td>
<td>TRANSGLYCOSYLATION REACTIONS, A MAIN MECHANISM OF PHENOLICS INCORPORATION IN COFFEE MELANOIDINS AND THEIR INHIBITION BY MAILLARD REACTION</td>
<td>Manuel A. Coimbra</td>
<td>University of Aveiro, Aveiro, Portugal</td>
</tr>
<tr>
<td>9:50–10:10</td>
<td>L19</td>
<td>RELATIONSHIPS BETWEEN ANTIOXIDANT EFFICIENCIES IN EMULSIONS AND THEIR INTERFACIAL ANTIOXIDANT CONCENTRATIONS. APPLICATION OF THE PSEUDOPHASE KINETIC MODEL</td>
<td>Carlos Bravo-Díaz</td>
<td>Universidad de Vigo, Vigo, Spain</td>
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<td></td>
<td>L20</td>
<td>cancelled</td>
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<tr>
<td>10:10–10:30</td>
<td>L21</td>
<td>REACTIVITY OF FREE MALONDIALDEHYDE IN OIL-IN-WATER EMULSIONS DURING IN VITRO DIGESTION</td>
<td>Angelique Vandemoortele</td>
<td>Ghent University, Ghent, Belgium</td>
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### Lunch

12:35–13:30

Conference restaurant

**Lunch**
### THURSDAY, February 16, 2017

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<tr>
<th>Time</th>
<th>Session/Activity</th>
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<tr>
<td>13:30–15:00</td>
<td>POSTER SESSION&lt;br&gt;Authors’ presentation slot. Posters are displayed during the whole conference.</td>
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<td>15:00–15:30</td>
<td>Coffee Break</td>
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<tr>
<td>15:30–17:50</td>
<td>ORAL SESSION 5: CHEMICAL REACTIONS IN PROCESSED / STORED FOODS II&lt;br&gt;Chairpersons: Thomas Henle and Marina Heinonen</td>
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<tr>
<td>15:30–15:55</td>
<td><strong>L26</strong> CHEMICAL REACTIONS IN COOKED FOODS: THE CONSEQUENCES ON DIGESTIBILITY&lt;br&gt;<strong>Vincenzo Fogliano</strong>, University of Wageningen, Wageningen, The Netherlands</td>
</tr>
<tr>
<td>15:55–16:20</td>
<td><strong>L27</strong> PROTEIN OXIDATION IN FOODS&lt;br&gt;<strong>Marina Heinonen</strong>, University of Helsinki, Helsinki, Finland</td>
</tr>
<tr>
<td>16:20–16:40</td>
<td><strong>L28</strong> THE QUALITY OF LOW LACTOSE MILK IS AFFECTED BY THE SIDE PROTEOLYTIC ACTIVITY OF THE LACTASE USED IN THE PRODUCTION PROCESS&lt;br&gt;<strong>Antonio Dario Troise</strong>, University of Naples Federico II, Napoli, Italy</td>
</tr>
<tr>
<td>16:40–17:00</td>
<td><strong>L29</strong> NOVEL AND HIGHLY SENSITIVE MARKER PEPTIDES TO PREDICT THE INDUSTRIAL HEAT TREATMENT OF MILK&lt;br&gt;<strong>Sevim Dalabasmaz</strong>, Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany</td>
</tr>
<tr>
<td>17:00–17:10</td>
<td><strong>L30</strong> OHMIC HEATING: A PROMISING TECHNOLOGY FOR MINIMIZATION OF FURAN FORMATION IN STERILIZED VEGETABLE / MEAT BABY FOOD&lt;br&gt;<strong>Jaromir Hradecky</strong>, University of Chemistry and Technology, Prague, Czech Republic</td>
</tr>
<tr>
<td>17:10–17:30</td>
<td><strong>L31</strong> ADDITION OF SODIUM ASCORBATE, CITRIC AND ASCORBIC ACIDS TO EXTEND THE SHELF-LIFE OF TUNA MEAT FISH IS A RISK OR A BENEFIT FOR CONSUMERS?&lt;br&gt;<strong>Mila Nocentini</strong>, Istituto Zooprofilattico Sperimentale del Lazio E Della Toscana (IZSLT), Florence, Italy</td>
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<tr>
<td>17:30–17:50</td>
<td><strong>L32</strong> USE OF PECTIC POLYSACCHARIDES AS AN ACRYLAMIDE MITIGATION STRATEGY - COMPETITION BETWEEN SUGAR ALDEHYDE AND CARBOXYLIC GROUPS&lt;br&gt;<strong>Claudia Passos</strong>, University of Aveiro, Aveiro, Portugal</td>
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* Young scientists’ presentation

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8th International conference on Chemical Reactions in Foods (CRF 2017)<br>February 15-17, 2017, Prague, Czech Republic
### ORAL SESSIONS

**FRIDAY, February 17, 2017**

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<th>Session</th>
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<td>9:00-10:25</td>
<td><strong>ORAL SESSION 6:</strong></td>
<td>CHEMICAL REACTIONS IN PROCESSED / STORED FOODS III</td>
<td>Manuel A. Coimbra and Nadia Mulinacci</td>
</tr>
<tr>
<td>9:00-9:25</td>
<td>L33</td>
<td>BIOACTIVE COMPOUNDS FROM MARINE SOURCES</td>
<td>Klara Stensvåg, The UiT The Arctic University of Norway, Tromsø, Norway</td>
</tr>
<tr>
<td>9:25-9:55</td>
<td>L34</td>
<td>REVEALING POLYPHENOL-PROFILE AND ANTIMICROBIAL ACTIVITY OF SELECTED PROPOLIS SAMPLES, UNDERPINNING PLAUSIBLE IMPLICATIONS IN HEALTH-PROMOTING FOOD PRODUCTS</td>
<td>Attila Kiss, Kaposvár University, Kaposvár, Hungary</td>
</tr>
<tr>
<td>9:55-10:05</td>
<td>L35*</td>
<td>CHINESE HAWTHORN (CRATAEGUS PINNATIFIDA) FRUIT: A POTENTIAL NOVEL FOOD?</td>
<td>Kamila Hurkova, University of Chemistry and Technology, Prague, Czech Republic</td>
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<tr>
<td>10:05-10:25</td>
<td>L36</td>
<td>DETERMINATION OF THE ORIGIN FOR ANTHRAQUINONE IN ORGANIC TEA PRODUCTION</td>
<td>Anna Romanotto, PiCA GmbH Berlin, Berlin, Germany</td>
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<tr>
<td>10:25-11:00</td>
<td>Conference area</td>
<td>Coffee Break</td>
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<tr>
<td>11:00-13:00</td>
<td><strong>ORAL SESSION 7:</strong></td>
<td>CHEMICAL REACTIONS IN PROCESSED / STORED FOODS IV</td>
<td>Jana Hajslova and Marco Arlorio</td>
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<tr>
<td>11:00-11:20</td>
<td>L37</td>
<td>LIGNANS IN VIRGIN OLIVE OILS: EFFECT OF REFINING PROCESS AND FRAUDS</td>
<td>Nadia Mulinacci, Università degli Studi di Firenze, Firenze, Italy</td>
</tr>
<tr>
<td>11:20-11:40</td>
<td>L38</td>
<td>FORMATION OF EPOXY FATTY ACIDS DURING PHOTO-OXIDATION IN OIL IN WATER EMULSIONS</td>
<td>Phuong Pham, Ghent University, Ghent, Belgium</td>
</tr>
<tr>
<td>11:40-11:50</td>
<td>L39*</td>
<td>METABOLIC CHANGES DURING STORAGE OF RAPESEEDS AND CONSEQUENCES FOR THE QUALITY OF THE RESULTING VIRGIN, COLD-PRESSED OIL</td>
<td>Anja Bonte, Max Rubner-Institut, Detmold, Germany</td>
</tr>
<tr>
<td>11:50-12:10</td>
<td>L40</td>
<td>OXIDATION OF FATTY ACIDS IN BULK TRIGLICERIDES PHASES</td>
<td>Marini Damanik, Graz University of Technology, Graz, Austria</td>
</tr>
<tr>
<td>12:10-12:30</td>
<td>L41</td>
<td>THE UNIQUE CHEMISTRY OF MANUKA HONEY (LEPTOSPERMUM SCOPARIUM)</td>
<td>Jana Rückriemen, Technische Universitaet Dresden, Dresden, Germany</td>
</tr>
<tr>
<td>12:30-13:00</td>
<td>Conference hall</td>
<td>FINAL DISCUSSION PANEL</td>
<td>Panellists: CRF 2017 Scientific Committee</td>
</tr>
<tr>
<td>13:00-13:30</td>
<td>Conference hall</td>
<td>CLOSING ADDRESS</td>
<td>Jana Hajslova &amp; Marco Arlorio, Chairs of the CRF 2017 conference</td>
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* Young scientists’ presentation
### POSTER SESSION

**WEDNESDAY - FRIDAY, February 15-17, 2017**

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<tr>
<td>13:30–15:00</td>
<td>POSTER SESSION (Thursday, February 16, 2017 - authors´ presentation slot)</td>
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- **CHEMICAL REACTIONS IN PROCESSED / STORED FOODS**
- **RECENT STRATEGIES FOR HIGH FOOD QUALITY, INCREASED SHELF LIFE AND SAFETY**
- **CHEMICAL REACTIONS INVOLVING FOOD IMPROVEMENT AGENTS (ADDITIVES, ENZYMES, FLAVORINGS), MITIGATION FOOD CONTAMINANTS AND RESIDUES**
- **BIOLOGICALLY-ACTIVE CONSTITUENTS IN FOOD CROPS AND PRODUCTS THEREOF**
- **CHEMISTRY BEHIND NOVEL FOODS, BOTANICALS AND DERIVED PREPARATIONS, FOOD SUPPLEMENTS**

*Posters are displayed during the whole conference.*
POSTER SESSION

**P1** EFFECT OF VARIOUS COOKING TECHNOLOGIES ON QUALITY AND STARCH NUTRITIONAL PROPERTIES OF PULSES
Sanaa Ragaee, El-Sayed Abdel-Aal

**P2** VOLATILE COMPOUNDS PROFILE OF MICROWAVE TREATED TART CHERRY PUREES WITH ADDITION OF SUGARS DURING STORAGE
Anita Pichler, Ivana Ivić, Josip Šimunović, Mirela Kopjar

**P3** TEXTURE AND AROMA PROFILE OF SOUR CHERRY FILLINGS
Anita Pichler, Ivana Ivić, Mirela Kopjar

**P4** AROMATIC PROFILE OF RASPBERRY CREAM FILLINGS WITH SUGARS, MODIFIED STARCHES AND HYDROCOLLOIDS
Anita Pichler, Anita Kerekeš, Tijana Pinkle, Mirela Kopjar

**P5** TEXTURAL PROPERTIES OF MODEL SYSTEMS OF HYDROCOLLOIDS AND SUGARS
Mirela Kopjar, Anita Pichler

**P6** FREE MCPDS, THEIR ESTERS AND GLYCIDYL-ESTERS IN FOOD: PRECISION AND ACCURACY FOR MONITORING FOOD PRODUCTS AND MITIGATION PROCESSES
Emiliano De Dominicis, Alberto Stocco, Elena Barolo, Claudia Piazza, Jean-Baptiste Gay

**P7** PROMOTION OF MAILLARD REACTIONS BY CHITOSAN-GENIPIN FILMS IN MODEL WINE SOLUTIONS
M. Angélica M. Rocha, Cláudia Nunes, Manuel A. Coimbra

**P8** PESTICIDES HOUSEHOLD PROCESSING FACTORS OF NATURALY CONTAMINATED FRESH TOMATOES AND APPLES
Maria Rosa Repetti, Vanesa La Barba, Dario Maggioni, Melina Michlig, Florencia Magni, Horacio Beldoménico

**P9** REDUCTION AND TRANSFORMATION OF DEOXYNIVALENOL DURING THERMAL PROCESSING
David Stadler, Alexandra Malachova, Franz Berthiller, Rainer Schuhmacher, Christoph Büschl, Michele Suman, Francesca Lambertini, Rudolf Krksa

**P10** AUTHENTICATION OF MEAT AND MEAT PRODUCTS USING LC-MS/MS - TARGET PROTEOMIC ANALYSIS APPROACH
Štěpán Czornyj, Eva Forejtová, Soňa Baršová

**P11** ANALYSIS OF CHEMICAL COMPOSITIONS AND CORDYCEPIN IN TOCHUKASO MUSHROOM
Hyo-Nam Song, Tae-Young Kim

**P12** GELATION OF FUNCTIONALIZED CASEIN - INFLUENCE OF MAILLARD REACTION AND ENZYME-CATALYZED PROTEIN CROSS-LINKING
Thomas Henle, Mariella Hannb, Natalie Hubbe

**P13** INFLUENCE OF CYCLODEXTRINS ON ACE-INHIBITORY DIPEPTIDES PRESENT IN PROTEIN HYDROLYSATES
Thomas Henle, Steffi Rudolph, Edris Riedel

**P14** FREE MAILLARD REACTION PRODUCTS IN MILK FROM “ORGANIC” AND “CONVENTIONAL” FARMING
Thomas Hofmann, Uwe Schwarzenbolz, Nina Sparmann, Thomas Henle

**P15** NEW SEASONING FROM WINE POMACE PROMOTES THE FORMATION OF PYRAZINES IN BARBECUED BEEF PATTIES
Javier García-Lomillo, Mª Luisa González-SanJosé, Miriam Ortegas-Heras, Raquel Del Pino-García, Mª Dolores Rivero-Pérez, Pilar Muñíz-Rodríguez

**P16** PHYSICOCHEMICAL PROPERTIES OF DRIED ARONIA FRUIT BY DECOMPRESSED HEAT PUMP DRYER (DHPD)
Hyun-Chol Jung, Sang-Yeol Kim, Sang-Ro Lee, Hyo-Nam Song

**P17** IDENTIFICATION OF BIPHENYLS - CONTAMINANTS RESPONSIBLE FOR OFF-FLAVOUR IN SOFT DRINKS
Helena Cizkova, Vojtech Kruzik, Iveta Sistkova
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<th>Authors</th>
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Food processing, in particular thermally driven processes, induce chemical changes to food materials that may lead to the adventitious formation of certain compounds, so-called process contaminants, which in some cases could be harmful to human health. These contaminants - such as acrylamide or furan - are often formed together with flavour substances which are of the great importance for food quality and food taste, or - as in the case of chloroesters and glycidyl esters - are generated during the refining process of food raw materials such as vegetable oils. In practice, it is difficult to completely avoid the formation of heat-induced contaminants while at the same time still ensuring the product properties in such a way so that the food continues to meet quality and safety requirements.

Intensive scientific studies on these compounds have been conducted over the past decades by researchers in academia and the food industry. Increasing insight in understanding the presence, formation, and potential risks to public health posed by the compounds formed during food processing has been gained and where possible mitigation strategies have been developed.

This contribution will focus on technical and regulatory developments, as well as possible mitigation strategies to lower their occurrence in food (i.e. acrylamide, furan, 3-MCPD, 2-MCPD and glycidyl fatty acid esters).

Acrylamide
Since acrylamide was first identified in food in 2002, the food industry has been committed to mitigating acrylamide formation. In its 2015 opinion, the European Food Safety Authority (EFSA) acknowledged that FoodDrinkEurope’s ‘acrylamide toolbox’, which is also supported by the Commission and Member States, is an important initiative to reduce acrylamide across the relevant food categories. FoodDrinkEurope coordinates the efforts of individual food manufacturers and their associations.

Despite all these efforts, several food business operators (FBOs) have not yet fully embraced the tools stipulated in the Toolbox, and progress in the implementation of the tools can be significantly improved. Therefore, FoodDrinkEurope welcomes the European Commission’s draft Regulation, which introduces mandatory measures for consumer protection and will result in the further progressive reduction of acrylamide in the European food supply. The Commission proposes to implement the ALARA principle, to be met through the implementation by food business operators of process controls and other measures established in sector-specific Codes of Practice. The implementation of the Codes of Practice will be enforced and monitored by competent national authorities. Benchmark values for acrylamide in different food categories will be included in the Regulation.

3-MCPD, 2-MCPD and glycidyl fatty acid esters
Fatty acid esters of monochloropropanols (termed MCPD esters or ‘bound’ MCPD) have been identified in a wide range of processed foods. Most of the bound MCPD in the human diet stems from refined vegetable oils.

MCPD esters, that include the isomers 3-MCPD and 2-MCPD, and glycidyl esters are two independent classes of process contaminants known to form during the refining of fats and oils. Most of the focus of research so far has been on 3-MCPD esters, and only very little data are available on the levels of 2-MCPD esters in foods.
The food industry has conducted extensive research into the formation of MCPD esters and glycidyl esters. Based on this research, the oil and fat manufacturers have developed a catalogue of mitigation strategies, that are being applied to lower the levels of MCPD esters and glycidyl esters to as low as reasonably achievable, whilst maintaining the safety and important organoleptic properties of fats and oils.

Health Authorities have expressed concerns about possible health risks linked to the intake of 3-MCPD esters and glycidyl esters. The European Food Safety Authority (EFSA) issued its latest opinion on the presence of process contaminants in vegetable oils and foods in May 2016. EFSA concludes that potential health concerns for consumers exist for certain processed foods such as vegetable oils and margarines, and for infants consuming infant formula which contain palm oils and other vegetable derived fats.

A draft regulation is now on the table which focuses on measures related to baby and infant food as well as vegetable oils.

FoodDrinkEurope will not develop a toolbox for the mitigation of these substances in processed food, since its formation during food processing has not been confirmed for most foods. FoodDrinkEurope does, however, endorse the toolbox developed by its member BLL, the German Bund für Lebensmittelrecht und Lebensmittelkunde. This toolbox was developed by a group of representatives from the German food industry sector, research institutes and private laboratories under coordination of the BLL. It contains tested “tools” across the entire food chain. It will enable the individual user to profit from the knowledge and experience available in research and practice in order to reduce the levels of 3-MCPD esters and Glycidyl esters accordingly.

Furan
The chemical furan is present in a variety of cooked and/or heat processed foods, including canned and jarred foods (soups, sauces, gravies, pasta) as well as baby food in jars, baked bread, breakfast cereals and coffee. First detected in the 1960s, furan is likely to have been part of the human diet for thousands of years, as it can be formed through traditional cooking methods. In high doses, it can cause cancer in animals and could be a potential carcinogen to humans. The European Commission (EC) has asked the European Food Safety Agency (EFSA) to provide a scientific opinion on the health risks associated with furan and the more recently the closely related alkylfurans 2- and 3-methylfuran (2-MeF and 3-MeF) in food. This opinion is expected by end 2017.

The food industry has conducted intensive research on the analysis, chemical formation and possible mitigation of furan in foods. The overall approach is to apply the ALARA concept, which essentially means that FBOs should take every reasonable measure to reduce the presence of furan in the final product, taking into consideration Quality and other Food Safety requirements. However, it is important to remember that interventions or changes to thermal processing steps cannot be done without thorough analysis, as lowering thermal treatment may have serious microbiological effects and possibly result in an unsafe product.

FoodDrinkEurope is working on the preparation of a furan “Toolbox”, analogous to the well know “acrylamide toolbox”.

The FoodDrinkEurope furan “Toolbox” would provide possible avenues of mitigation of furan for Food Business Operators, being aware that most of the measures at this stage are based mainly on laboratory or pilot scale trials.

Keywords: acrylamide, 3-MCPD, 2-MCPD and glycidyl fatty acid esters, furan, food processing, mitigation strategies
FORMATION AND METABOLIZATION OF GLYCATED AMINO ACIDS IN THE BREWING PROCESS

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The occurrence of amino acids and reducing sugars in green malt allows for the formation of significant amounts of Maillard reaction products (MRPs) during kilning [2]. These products are decisive for the color and aroma of beer. However, only little information is available in the literature on the extent of lysine modification in different types of beer [3]. Moreover, there are no investigations on the metabolic fate of individual glycated amino acids in the presence of brewer’s yeast (Saccharomyces cerevisiae). Individual MRPs (fructosyllysine, maltosyllysine, pyrraline, formyline, maltosine, MG-H1, and argpyrimidine) were quantitated by HPLC–ESI–MS/MS in the MRM mode. Free MRPs were analyzed directly. A high-molecular weight fraction was isolated by dialysis (MWCO, 14 kDa) and hydrolyzed enzymatically for the analysis of protein-bound MRPs. Free amino acids were quantitated by amino acid analysis. Moreover, a study on the transformation of glycated amino acids (e.g., fructosyllysine, pyrraline, formyline) in the presence of S. cerevisiae was performed. Based on this study, the respective metabolites were synthesized and quantitated in beers by HPLC-MS/MS. Fructosyllysine and maltosyllysine are the most important free and protein-bound glycated amino acids in beer, followed by pyrraline, MG-H1 and formyline. Experiments using S. cerevisiae proved that free glycated amino acids are not utilized by this yeast, while in dipeptide-bound form, these products can enter yeast cells and undergo metabolism by the Ehrlich pathway [1] (amino acid fermentation) under formation mainly of the respective Ehrlich alcohols (“fusel alcohols”) and amino acid-derived α-hydroxy acids. Along with tyrosol and tryptophol (each up to 30 mg/L), the novel fusel alcohols pyrralinol (up to 0.22 mg/L) and formylinol (up to 0.14 mg/L) were quantitated in beer for the first time. In conclusion, the consumption of beer contributes significantly to the dietary intake of MRPs. Moreover, the metabolism of glycated amino acids by brewer’s yeast is a novel physiological performance, whose influence on the brewing process is completely unknown. Knowledge on the physiology of the novel fusel alcohols pyrralinol and formylinol, which could represent new bioactive constituents in beer, is also lacking. The mechanisms of formation of these compounds are currently evaluated in a study covering the whole brewing process.


Keywords: Maillard reaction, beer, Saccharomyces cerevisiae, metabolism, Ehrlich pathway
The secondary fungal metabolites T-2 toxin (T2) and HT-2 toxin (HT2) are *Fusarium* mycotoxins that are classified into the group of type A-trichothecenes with T2 being the most acute cytotoxic member amongst the group of trichothecene mycotoxins. The main route of exposure for humans is the consumption of contaminated cereals or cereal products that undergo a series of physical and thermal treatments along the chain of food production. Studies on the effects of food processing on the mycotoxin content revealed that processing has indeed an effect on mycotoxin-levels in food which is considered in threshold values that have been established for some mycotoxins by the European Commission. Until today no such maximum levels for T2 and HT2 have been set by the EU legislative authorities which is of concern due to their toxic potential. One question of interest that is coming more into the focus of researchers is the fate of mycotoxins during food processing. While physical treatments, e.g. cleaning and sorting usually go hand in hand with a toxin-redistribution, thermal treatments were shown to induce chemical degradation reactions. The elucidation of the degradation products and their toxic potential is crucial to distinguish whether the processing conditions contribute to an increased food safety or not. Using extrusion cooking and baking two typical food processing techniques were carried out in order to determine the degradation rates of T2 and HT2 that occur under industrial-like conditions. These experiments were assisted by model heating experiments to trace the reaction products of T2 and HT2 formed during heat treatment by HPLC-MS/MS and HPLC-HRMS.

**Keywords:** T-2 toxin, mycotoxins, thermal food processing, extrusion cooking

**Acknowledgement:** This research project (AiF 18319 N) was supported by the German Ministry of Economics and Technology (via AiF) and the FEI (Forschungskreis der Ernährungsindustrie e.V., Bonn)
HYDROLYSIS OF VICINE AND CONVICINE IN FABA BEAN SUSPENSIONS AND SOURDOUGHS

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Faba bean (Vicia faba) is a versatile legume crop that can be used in ingredients and foods as a protein source. The antinutritive compounds occurring solely in faba bean, vicine and convicine, are hydrolyzed to their corresponding aglycones, divicine and isouramil, that have strong oxidative capacity. In case of genetic deficiency of glucose-6-phosphate dehydrogenase (G6PD)-enzyme, the aglycones can cause lysis of the red blood cells leading to hemolytic anemia called favism. Attempts to remove vicine and convicine via plant breeding and processing have not yet been successful enough. Enzymatic treatment of faba beans with added beta-glucosidase or fermentation using lactic acid bacteria with beta-glucosidase activity seem promising to remove vicine, convicine and their aglycones. Faba bean have also been suggested to have endogenous beta-glucosidase activity in ripened seeds. The aims of the study were to investigate beta-glucosidase activity of faba beans and that of selected microbes used in fermentation. In addition, effect of acidity (low pH) to hydrolyze the glycosidic bond was also studied. Endogenic enzyme activity and effect of acidity were tested in suspensions of two flours at selected pH values at 37°C. Incubation times were 4 and 24 hours. Sourdoughs were inoculated with selected microbes that were Pediococcus pentosaceus (S1), and two Lactobacillus plantarum strains (S2, S3). Fermentation was carried out at 20°C and 25°C for 24 h. Extraction of samples and analysis conditions of reversed phase HPLC-UV- method are given in Pulkkinen et al (2015). Hydrolysis of vicine and convicine was rather low without external enzyme source in faba bean suspensions. In a short incubation at pH values 4.5 and 5 at 37°C, only ≤ 10% of vicine and convicine was hydrolyzed. In longer incubation, 20-25% of vicine and 15-30% of convicine was lost in both flours. In acidic conditions loss of vicine was rather low as being ≤ 10% at pH 1 and 2. Loss of convicine was 65-70 % at pH 1 and 10-20 % at pH 2 for both flours. Fermentation temperature had an effect on ability to hydrolyze vicine and convicine. Hydrolysis was rather minimal during the first hours of fermentation. After 24 h fermentation, vicine and convicine contents were reduced at 25 °C in sourdoughs inoculated with S1 and S3, when at 20 C hydrolysis did not occur. Sourdoughs fermented at 25°C were more acidic than the ones fermented at 20°C. The whole pH range was 4.6-5.2 for sourdoughs fermented at 25°C and 4.9-5.8 at 20°C, respectively. Low fermentation temperatures were used to achieve consumer acceptance. Specific Lactobacillus plantarum strains are thus able to produce beta-glucosidase. However, marked differences between strains were found.

Keywords: vicine, convicine, hydrolysis, fermentation, HPLC
THE RELATIONSHIP BETWEEN DOUGH COMPOSITION AND 3-MCPD ESTERS CONTENT IN COOKIES

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A number of flavor-significant compounds together with a typical color are formed during baking. Unfortunately, under some conditions, hazardous processing contaminants such as acrylamide, 5-hydroxymethylfurfural, or 3-monochloro-1,2-propandiol esters (3-MCPD esters) may also originate. The latter group of compounds was first found in refined vegetable oils (mainly in palm oil) and then also in various thermally processed foodstuff. Since there is a suspicion, that free 3-MCPD (classified as possible human carcinogen) may be released from its bound form by action of gastrointestinal lipases, EFSA CONTAM panel established the tolerable daily intake (TDI) up to 0.8 μg/kg body weight per day for 3-MCPD. As cookies are one of the major contributors to 3-MCPD esters dietary intake, especially for infants and toddlers, the objective of this study was to focus on the relationship of various cookies recipes and baking conditions (baking time and temperature) on the formation of these processing contaminants. Except of the type of fat, emulsifiers may also play a role of precursors of 3-MCPD esters, as they contain mono- and diacylglycerols or, in case of lecithin, phospholipids. In addition to 3-MCPD esters formation, to assess the sensory value of these cookies prepared under various conditions, the aromatic profile was investigated. Finally, the quality of infant and toddler cookies available on the market was monitored, too.

Keywords: 3-MCPD esters, emulsifier, cookies, aromatic compounds, baking

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L6
CANCELLED
FORMATION AND ANALYSIS OF DESIRED AROMA-ACTIVE AND UNDESIRED FOOD-BORNE TOXICANTS DURING FOOD PROCESSING

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In the past, many studies have been undertaken to elucidate the key odorants of food and to identify formation pathways of the so-called “food-borne toxicants”. But, up to now, analytical approaches including the quantitation of desirable aroma-active compounds in combination with undesirable toxicologically relevant substances by sensitive methods are scarcely available. The lecture will present recent studies, which were combining the analysis of important aroma compounds and of selected food-borne toxicants (e.g., acrylamide, acrolein, crotonaldehyde, styrene, etc.) formed during food-processing, e.g., brewing of beer or deep-frying of potato chips and donuts in different edible oils. Odorants were identified by gas chromatography-olfactometry as well as GC-MS and quantitated by stable isotope dilution analysis (SIDA). For the toxicants, new quantitation methods using stable isotopically labeled standards (e.g., [13C3]-acrolein or synthesized [13C4]-crotonaldehyde) were developed and formation pathways were proven by labeling experiments. In summary, it will be shown that lowering the amounts of undesirable compounds in combination with the maintenance of an overall aroma well accepted by the consumers is a challenging task.

Keywords: food-borne toxicants, aroma-active compounds, gas chromatography-mass spectrometry, stable isotope dilution analysis
MITIGATION OF AFLATOXINS CONTENT: IN SILICO ANALYSIS AS THE FIRST STEP IN THE ENZYMES-BASED STRATEGIES

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Mycotoxins are low-molecular weight molecules produced as secondary metabolites by various species of filamentous fungi. They can be found in food and feed, and the dietary intake may cause severe illnesses and disorders in humans and animals. Therefore, the development of cost-effective strategies for mitigating mycotoxins content is definitely a major task for the scientific research to ensure more safe food and feed, and to address the forthcoming issues in the view of global trade and sustainability. The mitigation of mycotoxins content via enzymatic degradation is accounted among the most promising strategies, also on the account of the fact that it can be used on low- or non-compliant food batches to reduce and/or reuse wastes and offers a straightforward strategy for the mitigation in situ. Nevertheless, the search of effective enzymes is still challenging and time-consuming, especially in the first stages, dealing with a coarse-grained filtering of query enzymes that is drastically affected by the realistic affordability of proteins. The in silico analysis may strongly support the research in the early stage by providing evidence-based hierarchization of enzymes libraries for the rational design of further experimental trials. As a proof of concept, the present work dealt with the degradation of aflatoxin B1 and M1 mycotoxins by laccase enzymes from Trametes versicolor, which are promising enzymes to control aflatoxins contamination. In particular, the enzymes-substrate affinity of the various enzyme isoforms was investigated through 3D molecular modeling techniques, ranking enzymes for substrate affinity and pinpointing structural differences among the isoforms that are relevant for the substrate-enzyme recognition. The possible formation of different products of degradation between aflatoxin B1 and M1 has been hypothesized as well. Overall, 3D modeling has proved to be an effective analytical tool to assess the enzyme-substrate affinity and may effectively support the search of degrading enzyme at the early stage.

Keywords: aflatoxin, enzymatic mitigation, maize
WHEN FLAVOR TURNS INTO COLOR: NEW INSIGHTS ON (ETHYL)VANILLIN CHEMISTRY IN FOODS

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The Maillard Reactions (MRs), a complex group of reactions allowing the formation of aroma, color and, sometimes, potentially toxic compounds in foods, were deeply studied in the past. The appearance of brown color triggered by the formation/accumulation of melanoidins in food is correlated with the chemical profile of foods, mainly at sensorial level. Beside MRs, caramelization of sugar can contribute to the browning of some foods (e.g. baked products), but other chemical reactions involving ingredients are still under-investigated. Natural or synthetic vanillin (4-hydroxy-3-methoxybenzaldehyde), with the more aromatic and stable synthetic analog ethyl vanillin (4-hydroxy-3-ethoxybenzaldehyde), is broadly used as flavoring agent, especially in bakery products. Previous data suggested loss of intensity of the sweet/flavored aroma of vanillin during baking – in addition to the simple volatilization in oven - supporting the idea that “vanillin aroma” is affected by food components, especially proteins and amino acids [1]. Moreover, old data suggest the reaction of vanillin in alkaline medium with carbonyl-bearing compounds, yielding yellow, orange or red colorations (particularly aliphatic ketones containing a methyl group) [2]. Starting from these highlights, this oral communication will present a deep investigation on the reactions occurring between (ethyl)vanillin and secondary amines/amino acids, showing its ability to participate to “colored” chemical reactions and highlighting the prompt and efficient formation of benzoquinone derivatives, which color may contribute, together with the MRs, to the overall browning process. Colored derivatives (moving from brown/brilliant red to orange) were produced in laboratory as result of the reaction between (ethyl)vanillin and secondary amino groups in aerobic (hydro)alcoholic conditions. The 2,5-diamino-1,4-benzoquinones were produced with high yields (70-80%), then characterized by NMR, and the mechanism of their formation was elucidated. A model food (biscuit) was used to study the formation of these “new pigments”, further evaluated by HPLC-MS, bringing new information about the influence of food additives in biscuit formulas. Information about the uniformity of the color on the food surface, as well as new toxicological data (cyto- and genotoxicity) will be also provided. Interaction with proteins, hydrolyzed protein and amino acids will be also discussed, finally showing the coloring/solubility properties of diaminobenzoquinone-like molecules. Concluding, the reactions triggering loss of (ethyl)vanillin flavoring capacity, thus leading to new colored molecules in foods, were elucidated, opening a new scenario for food chemists involved in color development-based studies.


Keywords: (ethyl)vanillin, diaminobenzoquinones, orange-red colors, food color
L10
NEW INSIGHTS INTO FRUIT CULTIVATION AND PROCESSING BASED ON PRODUCT FLAVOUR

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Fruit cultivation plays a very important role in the Southern parts of Austria. Besides the cultivation of grapes for the wine production, enormous amounts of apples, elderberries, peaches and other crop have been traditionally cultivated. Due to the developments on the European fruit market (e.g. developments after the start of the Russian embargo), the price for apples from the local production decreased significantly. In addition, new agricultural problems arose due to the occurrence of new parasites like drosophila suzukii as well as due to extreme climatic conditions like the very late onset of winter in April 2016 leading to enormous crop failure in the harvest 2016. All these issues trigger a rethinking process within the local agriculture as for many farmers the cultivation of international apple varieties like Golden Delicious or Gala is not further economically viable under the existing conditions. As a consequence, there is - on the one hand a change in crop and on the other hand a recall on old fruit varieties that have been traditionally grown in this geographic region for many decades. The production of high quality products from not traditionally grown crop as well as from old fruit varieties require a deep understanding of the flavour properties and the flavour changes that occur in course of the production cycle. In this lecture, it will be demonstrated at the examples of selected fruit varieties like apples or black chokeberry (Aronia melanocarpa) how the use of flavour analysis (by means of mainly gas chromatographic techniques) as well as sensory evaluation (by the use of traditional as well as new and rapid techniques) is used to support the production of high quality products in order to strengthen the position of local farmers on the market.

Keywords: fruit processing, flavour chemistry, sensory evaluation
Flavour of foods is without doubts one of the key consumer preference drivers and consequently its optimization is of a crucial importance for food manufacturers. Thermal processing, such as roasting, baking, toasting, extrusion, cooking, frying, etc. trigger significant changes in key product attributes, including color, flavor and texture. From the chemical point of view these thermal processes are very complex as many reactions happen in parallel and compete for precursors and intermediates. A careful control of the process parameters based on deep understanding of reaction pathways is required to enhance generation of beneficial compounds (aroma, taste, bioactives) while mitigating undesirable ones (e.g. acrylamide) and thus to ensure high product quality. The complexity of the real food systems makes it difficult to study the reaction pathways directly in the food matrix, therefore simplified model systems are often used instead. The results of such studies provide some useful information, but may not always reflect the reality of a complex food system. Consequently, findings obtained from model studies should be validated in a real food environment. Using new as well as already published data on coffee roasting and cereal extrusion (1-3), the lecture will illustrate different approaches that are used in our laboratories to elucidate the flavor generation pathways in complex food systems. Special attention will be paid to the labelling experiments employing sugars or amino acids including the CAMOLA method (carbohydrate module labelling) (4).


Keywords: Maillard reaction, flavor, reaction pathways, labelling studie, CAMOLA
FACTORS INFLUENCING THE KEY AROMA COMPOUNDS OF RUM

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Rum, an alcoholic beverage, is either produced from molasses or sugar cane juice by fermentation, distillation, and ageing. To check the influence of each processing step on the final aroma, the sensomics approach was applied and 43 aroma compounds were quantitated in molasses, mash, distillate, and the final rum using stable isotope dilution analysis (SIDA). (E)-β-Damascenone was determined already in molasses and its concentration significantly increased during distillation resulting in the highest odor activity value (OAV; ratio of concentration divided by the respective odor threshold) in the rum. Vanillin, 4-ethylphenol, and 2-methoxyphenol are compounds mainly stemming from the wood barrels used for ageing and showed all an OAV >1 in the rum. Altogether, the concentrations of 68% of aroma-active compounds increased during the whole process, demonstrating the influence of manufacturing on the overall rum aroma. Besides technology, the raw materials are well-known to influence the aroma of the final spirit. Thus, rums produced either from molasses or sugar cane juice were analyzed by means of the sensomics approach indicating clear differences in the concentrations of key odorants. Finally, a non-targeted analysis for authentication based on the whole set of volatiles was successfully developed enabling the discrimination of high quality sugar cane rums and the molasses.

Keywords: rum, sensomics concept, production process
HOW TO PRODUCE FLAVORS AND FRAGRANCES FROM ALPHA-PINENE - DESIGN THE LIPASE-BASED CATALYST FOR SELECTIVE BIOCATALYTIC OXIDATION OF ALPHA-PINENE

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α-Alpha-pinene is the main component of the monoterpene fraction, especially for turpentine (i.e. paper and pulp industry residue available in bulk quantities at a low price). Commonly, its applicability is limited to fuel of the recovery boilers. However, alpha-pinene is considered a platform molecule with a great potential for the production of pharmaceuticals, agrochemicals and fine chemicals. In this context, we developed several biocatalytic model-systems for the conversion of alpha-pinene into value-added derivatives (e.g. alpha-pinene oxide, campholenal, camphene, carveol, verbenol, verbenone, etc) with many applications in food industry (e.g. flavors and fragrances). Indirect biocatalytic oxidation of alpha-pinene is proposed using lipase, H2O2 and ethyl acetate as biocatalyst, oxidation reagent and co-reagent/organic solvent, respectively. Different biocatalyst designs have been tested. One of the models involved the lipase-based cross-linked aggregates design (cross-linked enzyme aggregates (CLEA) and cross-linked enzyme aggregates onto magnetic particles (CLEMPA)), which were compared to covalent design (e.g. covalent immobilized enzyme (CIE) on magnetic particles (MP) supports). Both CLEA and CLEMPA designs afforded better oxidation yields of alpha-pinene (around 30% for both biocatalysts) compared to CIE (14%). Also, the investigated biocatalysts allowed the production of alpha-pinene oxide (40%) and derivatives such as camphene (15%) and campholenal (20%). Second model investigated the biotransformation α-pinene using bifunctional biocatalysts designed as carbohydrate biopolymers entrapping lipase enzyme. Lipase assisted the oxidation of α-pinene using H2O2 as oxidation reagent and ethyl acetate as both acetate-supplier and solvent affording α-pinene oxide as the main product. Further, the biopolymer promoted the isomerization of α-pinene oxide to campholenic aldehyde and trans-carenol. The presence of biopolymers enhanced the catalytic activity of the biocomposites as compared to the free enzyme (ie 13.39x10³, 19.76x10³ and 26.46x10³ for the free lipase, lipase-carrageenan and lipase-alginate, respectively). The biocatalysts stability and reusability were confirmed in six consecutively reaction runs. Thus, we offer different alternatives for α-pinene valorization into value-added products related to the biocatalyst design involved in the biochemical process. In this way, the selectivity of the biocatalytic transformation of α-pinene was guided to the production of different terpenoidic compounds with flavors and fragrances properties.

Keywords: flavors/fragrances, biocatalysis, alpha-pinene, selectivity, lipase

Acknowledgement: This work was financially supported by UEFISCDI, Romania (PCCA 105/2014 and Bridge 27-BG/2016) and the COST Action CM1303.
ELUCIDATION OF THE FUSTY/MUSTY OFF-FLAVOR IN NATIVE COLD-PRESSED RAPESEED OILS FOR THE DEVELOPMENT OF A QUICK METHOD FOR QUALITY CONTROL

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The sensomics approach was used to clarify the formation of the fusty/musty off-flavor of native cold-pressed rapeseed oil using a “positive control” (PC) showing the desired sensory attributes and an oil eliciting a fusty/musty off-flavor (OF). Sixteen compounds increased significantly in OF. Investigation of the corresponding rapeseeds (OFS), from which OF was pressed, showed the same compounds above their respective odor thresholds in oil as found in OF, only differing in their respective concentrations. Thus, not the pressing process but a poor quality of the seeds does cause the off-flavor formation. Most of the products responsible for the off-flavor are caused by microorganisms, such as the Ehrlich degradation products 2- and 3-methylbutanoic acid and 2-phenylethanol, 2-methoxyphenol, or 4-methylphenol. Their formation is favored by inappropriate storage conditions including elevated temperatures and/or moisture. Analysis of 7 further oils with the identical sensory defect (OF1-7) and 5 further oils eliciting the desired sensory attributes confirmed these odorants as general marker compounds for the fusty/musty “off-flavor”. The analytical data were statistically evaluated via principal component analysis (PCA) showing a clear separation of both oil groups. Finally, a new quick method for quality control of rapeseeds via headspace GC-FID was developed using 2- and 3-methylbutanoic acid as aroma-active marker compounds.

Keywords: sensomics concept, rapeseed oil, “off-flavor"
**L15**

**FURFURYL ALCOHOL FORMATION DURING ROASTING OF COFFEE**

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The Maillard reaction is a major chemical interaction that takes place during processing of food products. It is extremely important to understand this particular network of reactions since it results in a wide range of compounds affecting color, flavor and/or aroma [1]. One of these compounds is furfuryl alcohol, a characteristic aroma compound in roasted coffee (widely consumed beverage around the globe). What makes furfuryl alcohol noteworthy amid coffee components is not only the fact that coffee is considered the major source for human exposure to FA [2], but it was also proven in several animal models that furfuryl alcohol can form DNA adducts which might lead to mutations [3, 4]. Even though several papers have already suggested reaction pathways for the formation of furfuryl alcohol [5], still no study has investigated the actual FA precursor in food samples. Dry model systems of coffee, coffee constituents and presumed furfuryl alcohol precursors were examined for furfuryl alcohol production upon roasting at temperatures ranging from 180–260°C. A fully validated reversed phase HPLC method was used for furfuryl alcohol determination, utilizing a C8 column as solid phase and water with methanol as mobile phase eluents. During these experiments, no single green coffee constituent produced furfuryl alcohol, while mixtures of mono or oligo carbohydrates (as in sucrose, the major sugar found in green coffee) with most amino acids led to the formation of furfuryl alcohol in varying quantities. 5-carbon sugars model systems (especially deoxy ribose) were capable of furfuryl alcohol production without the presence of amino acids. The addition of organic acids naturally present in green coffee to the model system affected furfuryl alcohol production differently. Additionally, the influence of the degree of green coffee’s moisture on furfuryl alcohol formation was investigated. In this work we introduce a comprehensive study of the potential precursors and reaction mechanisms leading to the formation of furfuryl alcohol. The main objective is to propose an explanation for the very high concentrations of furfuryl alcohol in coffee compared to other food products.

(3) B. Monien et al., Carcinogenesis (2011) 32: 1533–1539.

**Keywords:** furfuryl alcohol, coffee, Maillard reaction, model systems

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ADDITION OF ANTIOXIDANTS IN COOKED MEAT: MITIGATION OF HETEROCYCLIC AROMATIC AMINES AND SENSORY EFFECTS

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Heterocyclic aromatic amines (HAAs) are potent mutagens that are formed during heating process in meat. Studies have shown that the addition of specific antioxidants can significantly reduce their formation [Meurillon, M. and Engel, E. (2016). Trends in Food Science & Technology, 50, pp.70-84]. However, antioxidant choice remains empirical and there is no information regarding the sensory impact and consumer preference on the antioxidant treated meat. In the present research, the aim was to study different mitigating ingredients to reduce the formation of HAAs in cooked meat while preserving the sensory quality of the product and the consumer acceptability. The first part of this research concerned the choice of antioxidants to be studied. Different molecular modeling approaches were used to target pertinent antioxidants of polyphenol family. Then, these antioxidants (quercetin, epicatechin, resveratrol, carvacrol) as well as natural products known to be rich in the se antioxidants (capers, green tea, red Pinot wine, oregano) were injected in ground beef patties at different concentration (0.1%, 0.25% or 0.5%) or marinade time (2, 4 or 6h) and the resulting meat products were pan-fried following WHO’s recommendation to reach an internal temperature of 70°C. The amount of HAAs was then assessed with LC–APCI–MS/MS to determine which formulations have the major inhibiting effect on their formation. In the following part of the work, the formulations based on polyphenol-rich natural ingredients were studied using sensory evaluation and GC–Olfactometer (GC-O) to evaluate the flavor impact of the additives. Accordingly, ground beef patties were treated with red Pinot wine, green organic tea, whole capers or dried oregano at different concentration or marinade time. The samples were then pan-fried on medium heat for 14min to the recommended temperature of 70°C, before being served. A hedonic assessment was first performed on 59 meat consumers by u sing a 9-point scale, resulting in high dissimilarities preferences amongst concentrations and antioxidants. The flavour dissimilarities between samples were characterized and quantified through descriptive quantitative analysis and non-verbal profiling with a panel (n=15) familiarized with the procedures. Dissimilarities amongst products were highly correlated to their olfactory profile. Hence, the use of GC-O enabled to determine the origin and nature of the odor-active compounds responsible for the segmentation that will further be discussed in this paper. Further research on the mechanism of action of the antioxidants on HAAs would allow us to control the formation of undesirable odor-active off-product and enhance consumer acceptance. This work focused on formulation with polyphenolic antioxidants for HAA mitigation could be subsequently generalized to other families of antioxidants and later applied to other process-induced toxicants of meat products such as polycyclic aromatic hydrocarbons.

Keywords: heterocyclic aromatic amines, mitigation, antioxidants, sensory evaluation, olfactometry

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CASEIN AND CASEIN MICELLES: STRUCTURES, FUNCTIONS, FUNCTIONALIZATION

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Caseins, main proteins in the milk of nearly all mammals, undergo a process of self-association during lactation to form micelles ranging between 50 and 300 nm. The detailed structure of casein micelles as well as the mechanisms underlying the structure formation are only partly understood. Within our research, we attempt to clarify the interactions that are responsible for the organization of the micellar structure and to investigate strategies for the directed modification of natural and artificial micelles which can serve as carriers (“nanocapsules”) of biologically relevant compounds. Process-induced chemical reactions during heating or storage have a significant impact on the protein and micelle structure. Glycation reactions (also referred to a Maillard reactions) can be applied to prepare glycoconjugates in the early stage of the complex reaction and to achieve non-enzymatic protein crosslinking in advanced stages. Corresponding reactions significantly affect the functional properties such as gelling and flavour binding. The presentation will focus on our recent studies concerning interactions between casein micelles from the milk of various mammals and bioactive guest molecules. Furthermore, studies dealing with the impact of glycation on the functional properties of milk proteins will be reported, which may demonstrate the potential of a controlled functionalization for practical applications.

Keywords: casein, casein micelles, milk, glycation reactions, functional properties of milk proteins
TRANSGLYCOSYLATION REACTIONS, A MAIN MECHANISM OF PHENOLICS INCORPORATION IN COFFEE MELANOIDINS AND THEIR INHIBITION BY MAILLARD REACTION

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Melanoidins are brown compounds and a main component of coffee brews [1]. Although their detailed structure is not yet known, some important structural features have been elucidated in recent years, as the presence of covalently-linked polysaccharides, proteins and phenolic compounds. Although polysaccharides depolymerize under roasting conditions, they are also able to polymerize, forming new polysaccharides through non-enzymatic transglycosylation reactions (TGRs) [2,3]. TGRs can also occur between carbohydrates and aglycones containing hydroxyl groups, such as chlorogenic acids present in daily used consumed foods like coffee [4]. The dry environments at high temperatures, as those occurring when foods are roasted, are able to promote new acetal and ketal groups between carbohydrates, phenolic compounds, organic acids, and amino acids. Because proteins are very reactive with reducing sugars through Maillard reaction, their presence plays a regulatory role concerning TGRs extension. Although some specific reactions are more favorable than others, they occur randomly, leading to the formation of highly complex polysaccharide-based polymeric brown compounds. Because food is very heterogeneous in its composition, it is not possible to have a unique melanoidin structure. However, it is possible to predict the major patterns promoted by the carbohydrate and phenolic moieties.


Keywords: roasted foods, melanoidins, polysaccharides, phenolic compounds, Maillard reaction

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L19

RELATIONSHIPS BETWEEN ANTIOXIDANT EFFICIENCIES IN EMULSIONS AND THEIR INTERFACIAL ANTIOXIDANT CONCENTRATIONS. APPLICATION OF THE PSEUDOPHASE KINETIC MODEL

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Predicting antioxidant, AO, efficiency is of primary interest in the food industry in the quest to minimize oxidation of polyunsaturated lipid-based foods in particular applications. The efficiency of antioxidants depends on both the rates of reaction with the radicals and on their concentrations at the reaction site. However, key aspects relating the structural features of AOs to their activities are not fully understood because structural similarities of AOs do not always mean similarities in their activity. For example, increasing the number of C atoms in the alkyl chains of AOs not only changes their hydrophilic-lipophilic balance (HLB) but also affects their relative solubilities in the oil, water, and interfacial regions of the emulsion or AO oxidation/reduction potentials. To get insights into the complex relationships governing the efficiency of antioxidants and their chemical nature, we determined the effects of the HLB of series of homologous AOs derived from phenolic acids (gallic and caffeic) and hydroxytyrosol with alkyl chains of 1-16 carbon atoms on the oxidative stability of olive oil-in-water emulsions by monitoring the formation of conjugated dienes (CDs) at early stages of oxidation.[1,2] To correlate their efficiency with their molecular structure, we also determined, in the same intact emulsions, their distributions between the oil, interfacial and aqueous regions by employing a chemical kinetic method. The interpretation of the experimental results is grounded on the pseudophase kinetic models widely employed to interpret reactivity in colloidal systems and permits determining the concentration of the antioxidants in the interfacial region of the emulsions.[1,2] Results provide physical evidence that the variations in the efficiency of homologous series of antioxidants in emulsions are due to differences in their interfacial concentrations, confirming that - other things being equal - there is a direct relationship between the percentage of AO in the interfacial region of the emulsions and their efficiency. Application of the pseudophase kinetic model furnishes, therefore, a natural explanation, based on molecular properties, to the cut-off effect.


Keywords: antioxidant interfacial concentration, antioxidant efficiency, antioxidant distribution, pseudophase kinetic model
L20
CANCELLED
Malondialdehyde (MDA), a typical aldehyde resulting from the oxidation of ω-3 and ω-6 fatty acids, has been widely used as a marker to measure the extent of oxidative deterioration of lipids in foods and biological systems. When MDA is generated endogenously in cells and tissues as a result of oxidative processes, it is considered to be a potential causal agent of numerous human diseases, such as different types of cancer, diabetes, etc. The interaction of various proteins with MDA under physiological conditions has been shown to generate various potential toxic adducts and to cause cross-linking of proteins due to its reactivity towards reactive amino groups. Moreover, MDA is prone to an aldol type self-condensation and hydrolytic cleavage under physiological conditions leading to the formation of a dimer and trimer, and acetaldehyde (AA) respectively which are highly toxic and mutagenic as well. The reactivity of MDA during digestion, especially its behavior in food matrices under gastric and duodenal conditions, has scarcely been studied. Besides, the presence and potential absorption of its aldol self-condensation and cleavage products in foods is not taken into consideration. In this study, the influence of in vitro digestion on MDA, its cleavage products, and aldol self-condensation products in fully hydrogenated coconut oil-in-water (O/W) emulsions stabilized by Tween 20 was evaluated, using an in vitro gastrointestinal digestion method simulating gastric and small intestinal phases. Initially the behavior of MDA in various model systems, i.e. aqueous buffer, saturated oil and Tween 20 stabilized O/W emulsions, after 24h incubation at 4 and 40°C was elucidated. After 24h incubation, these model systems were subjected to an in vitro digestion whereby the amount of free MDA was examined. Furthermore, the concentration of AA was determined in order to assess the dominant reaction pathway of MDA. The recoveries of MDA before digestion of the model systems were compared after incubation at 4 and 40°C. At both temperatures, the reactivity of MDA in aqueous buffer was the same. Surprisingly, MDA was very reactive in saturated oil. However, the degradation in oil proved to be strongly temperature dependent which mainly affected the aldol self-condensation of MDA. The reactivity of MDA in O/W emulsions also depended on the temperature which influenced the partitioning of MDA in both phases of the emulsion. Nevertheless, at both temperatures, the aldol self-condensation was the dominant reaction in O/W emulsions. However, during in vitro digestion of the model systems, the free MDA content altered depending on the degree of hydrolytic cleavage and aldol self-condensation of MDA before digestion. In conclusion, this study revealed that MDA is a very reactive molecule whose reactivity does not stop at the point of ingestion. Consequently, the exposure of MDA to the human body cannot be estimated based on the determination of free MDA in foods.

Keywords: malondialdehyde, oil-in-water emulsion, in vitro digestion, oxidation marker
L22

LIPID OXIDATION REACTIONS IN FAT-RICH FOODS: IS THE CURRENT ANALYTICAL TOOLBOX SUFFICIENT

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Improving the shelf life of oil-based food products by delaying the onset of lipid oxidation is a challenge that the Food Industry has been facing already for decades. Despite that, the understanding of the complex multitude of reactions that occur simultaneously over the shelf life of the products is still rather limited. For the development of new products this means large numbers of time consuming (accelerated) shelf-life studies are needed, which unfortunately not always are good indicators for actual product stability. A better understanding of the lipid reactions occurring is needed. Analytical chemistry can help here. Good progress has been made as will be shown, but more work remains needed. In the current presentation, we will discuss the wide range of analytical methods we have developed over the years to monitor chemical changes in fatty foods over time. Our toolbox includes sensor technology to monitor oxygen consumption, NMR based methods for rapid assessment of hydroperoxides, LC-MS methods for measuring non-volatile intermediates and end-products, size exclusion chromatography to monitor partial glyceride formation and polymerisation, GC for monitoring disappearance of unsaturated acids and volatiles release etc. Through joint deployment of this vast array of methods combined with advanced data reduction and -processing methods we can study lipid oxidation simultaneously from many different chemical perspectives. The application of this approach will be exemplified using the specific case of lipid oxidation in an important food emulsion: mayonnaise.

Keywords: lipid oxidation, food emulsions, mayonnaise, analytical methods

Acknowledgement: All people who contributed to the analytical work are kindfully acknowledged.
The study of minor compounds in edible fats and oils is an evergreen topic of this branch of scientific research, that had greatly benefited of improvement of analytical equipment. Some of these minor compounds can be used as markers of quality like in the case of health claims, while other compounds can be used as markers of purity, like is in the case of sterols. Both the above mentioned cases are rather old, but nowadays, even sterols can be considered in a different point of view, thanks to the improvement in separation techniques: recent researches by Mariani demonstrated that campesterol peak is indeed formed by the contribute of two epimers, whose distribution is different in different fats and oils, in the meantime, the presence of ergosterol can be related to poor technology of fruit storage before oil extraction. Sterols had traditionally been analysed after saponification that makes them all free, however, in fats and oils, sterols can be free as well as esters with fatty acids, nowadays, the evaluation of free and esterified form can be useful to assess several oil characteristics, like, e.g. the ageing of the oil, as the equilibrium between the two form can depend also on storage. Not only sterols, but also other hydroxylated compounds (e.g. tocopherols) can occur in free and esterified form and these two, too, can give interesting information. Phenolics (also called polyphenols or biophenols) are compounds that are peculiar of virgin olive oils: the Reg (EU)432/2012 establish that they can be cited in the “health claim” of extra virgin olive oils, but only in the case that the concentration of hydroxytyrosol and tyrosol and some related compounds is more than 5 mg/5g of oil. The expression is rather ambiguous, in fresh extracted oils free hydroxytyrosol and tyrosol concentration is rather low, while it increase after some times, as a result of hydrolysis of other molecules that contain them (oleuropein and ligstroside). Some analytical proposal deal with the possibility to carry out and hydrolysis and measure the total amount of these two compounds. Last but not least, very minor compound are the volatiles ones that can be related to sensory evaluation: some details dealing with the possibility to built up a mathematical model to describe selected defetcs of olive oils will be described, as well as some similar approaches useful to evaluate the oxidative conditions of fats used as ingredients in food.

Keywords: edible fats and oils, minor compounds, analytical techniques, aging of fats and oils
Cold-pressed oils have become very popular commodity since they are believed to contain compounds associated with health benefits that are transferred in high quantities from a raw material from which they are prepared. Minimal losses of bioactive compounds are expected thanks to mild processing condition used for their production. Currently, a wide range of oily seeds is used for cold-pressing; some of them were not traditionally used for plant oils preparation. With regards to a relatively high cost of cold-pressed oils, various fraudulent practices might be encountered. In our study, in which altogether 12 kinds of freshly-pressed oils (prepared from various seeds of flax, pumpkin, hemp, poppy, argania, milk thistle and black cumin) and those after oxidation were involved (to accelerate oxidation process, oils were held 10 days in closed jars at 60°C). In experimental work, we focused not only on the oils authentication, but also on assessment their stability and identification of oxidation markers. In addition to conventional tests commonly performed when evaluating oils oxidation, polar fraction of oils (isolated by aqueous methanol) in which most of bioactive compounds is present, was in depth investigated using UHPLC/ SFC- HRMS/MS techniques for non-targeted screening. Employing advanced chemometric methods for data processing, clustering of cold-pressed oils, regardless their degree of oxidation, was observed, moreover, a number of characteristic markers enabling their classification was identified. Interestingly, transformation of these compounds, as the result of oxidation process, was observed, this was, for instance, the case of cyclolinopeptides characteristic for linseed oil. In the follow-up study, the assessment of bioactivity of these oils based on employing an array of biochemical and cell test will be performed.

**Keywords:** cold-pressed oils, authentication, stability, oxidation markers

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HEAT LOAD OF EXTENDED SHELF LIFE (ESL) MILK AND CREAM
IN AUSTRIA

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The recent trend towards a longer keeping ability of pasteurized milk, without the negative flavour change normally associated with ultra-high temperature (UHT) treatment, has resulted in the development of extended shelf life (ESL) milk. However, heating causes a significant loss of organoleptic and nutritional quality (e.g., cooked flavour; vitamin destruction). Therefore, different Time-Temperature Integrators (TTIs) have been used to evaluate the heat load of ESL milk products. The objective of this study was to investigate the actual heat load of liquid milk (n=200) and whipping cream (n=58) samples at retail in Austria, either raw, pasteurized, ESL or UHT, respectively. The established RP–HPLC method enabled the separation of whey proteins within 21 minutes and was used for determination of acid-soluble ß-Lg. Furosine was analysed by ion-pair chromatography RP–HPLC within 7 minutes. Referring to liquid milk, half of the analysed samples designated as ESL milk showed acid-soluble ß-Lg contents lower than 1.800 mg/L milk, which had been proposed as threshold level in Austria. Most of these ESL milk samples with excessive heat-load had a surprisingly low amount of native ß-lactoglobulin (< 500 mg/L) and a high furosine content (> 40 mg/100 g protein), which was almost comparable to that of UHT milk. Concerning whipping cream, furosine levels increased with higher heat load of cream in the logical order pasteurized < ESL << UHT, and allowed a significant discrimination of heat load of these products. Thus, furosine content of 70 mg/100 g protein was suggested as an upper heating limit for pasteurized cream, whereas 100 mg/100 g protein could be accepted as obligatory limit for tolerable heat load of ESL cream. In conclusion, acid-soluble ß-Lg is definitely most suitable for heat load evaluation of liquid milk, whereas furosine proved to be a reliable indicator to assess the heat load of whipping cream.

Keywords: extended shelf life (ESL) milk, extended shelf life (ESL) cream, heat load, time-temperature integrators (TTIs), HPLC
Sometime between two millions and 250,000 years ago humans domesticated the fire and begun to eat cooked foods. This was a turning point influencing human evolution and its sensory preferences. There are many good reasons for humans to prefer cooked foods: cooking strongly decreases the risk of eating foods contaminated by pathogens; cooking inactivate many heat labile toxins: many potential poisoned plant foods become edible after cooking; cooking is a social matter and cooking practices are part of knowledge to be transmitted to our fellows. From the digestion point of view it has been clearly demonstrated that cooked foods provide much more energy than the corresponding raw ones. So it is not surprising that flavours and coloured compounds formed by cooking turned into “signals of trust” for humans. The cooking flavours became potent signals of attraction to our ancestors and we still experience the same sensation when inha ling the smells of foods being prepared in the kitchen flavour or when passing by a bakery shop. In this lecture the details of the mechanisms influencing the digestibility of lipid, protein and carbohydrates present in processed foods will be provided. About lipid the physical accessibility of the fat globules is the most important parameter. Digestibility is enhanced as consequence of the physical damage of the original food structure. This has been showed, for instance, upon cooking of peanuts. When fed to mouse, cooked peanuts significantly increased the amount of energy gain compared to raw peanuts. Mild thermal treatments increase protein digestibility due to protein denaturation, inactivation of the protease inhibitors and modification of cell wall integrity. On the other hand, severe thermal treatments, especially those occurring in low moisture foods, decrease protein digestibility because of protein aggregation and blockage of trypsin preferred hydrolysis sites. Finally, all treatments promoting starch gelatinization enormously increase its digestibility. However industrial treatments can be much more effective than simple boiling. For instance, in extrusion cooking heat, pressure and mechanical sheering to produce plasticized, expanded and cooked products are used. The moist heating combined with the mechanical shearing result in starch gelatinization but also disruption of molecular interactions between starch molecules within the granule which further increase starch digestibility.

Keywords: digestibility, lipid, protein and carbohydrates, processed foods, chemical reactions
Protein oxidation is one of the key causes of food deterioration. The mechanisms of protein oxidation include amino-acid side chain modification, protein cross-linking, and protein fragmentation (1). We have investigated the oxidative stability of both dairy and meat proteins as well as oxidative reactions of proteins isolated from various plant sources such as oats, fababeans, quinoa, and amaranth. In these studies, versatile tools including both conventional spectrometric and fluorometric tools as well as newly developed LC–MS methods have been applied. It is well understood that protein oxidation pathways are complex and cannot be explained by any universal method of monitoring a single type of oxidation product, such as protein carbonyls. Lipid oxidation products such as hydroperoxides and carbonyls are known to interact with amino acids, peptides and proteins. Recently, it was shown by using LC-MS tools that malondialdehyde does form protein-lipid adducts with peptides isolated from whey protein, lactalbumin (2). However, oxidation of food proteins is not only catalyzed by lipid oxidation products, but also proteins in fat-free food products or in foods with reduced fat content undergo oxidative changes. Depending on the amino acid composition, tryptic isolates of whey proteins produce methionine sulfoxide and sulfone, formylkynurenine, and dityrosine when oxidized in a metal catalyzed reaction in a non-lipid environment (3, 4). Lysine oxidation in for example meat products may be monitored by following semialdehyde formation using LC–MS (1). Oxidation of essential amino acids such as methionine, lysine, tyrosine and tryptophan may be of concern due to processing and storage. In addition to decrease in nutritional value, protein oxidation products may be of health concern such as formylkynurenine resulting from oxidation of tryptophan. Food proteins also have many functional properties including stabilizing of emulsions, gels and foams, and water binding properties. In our recent studies, the impact of plant derived proteins on the oxidative stability of food emulsions has been investigated (5).


Keywords: protein, oxidation, mechanisms
THE QUALITY OF LOW LACTOSE MILK IS AFFECTED BY THE SIDE PROTEOLYTIC ACTIVITY OF THE LACTASE USED IN THE PRODUCTION PROCESS

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Lactose intolerance syndrome can be efficiently tackled consuming low lactose products. Lactase is the key tool to manufacture low lactose milk (LLM); its addition can be done “in batch” before thermal treatment, or directly “in pack” after sterilization. Both technologies lead to a final concentration of lactose lower than 0.1% resulting in an increase of reducing sugars, glucose and galactose. Data on sensory properties, bound Maillard Reaction products (MRPs), free Amadori products (APs) formation and total lysine and free amino acids release were obtained on six commercial Italian LLMs over six months storage. The survey showed that the side proteolytic activity of lactase caused the release of amino acids with a significant higher MRPs, APs and off-flavors formation in 80% of samples produced by adding the enzyme in the pack after thermal treatment, while the samples produced with in batch technology guaranteed the control of Maillard reaction. These trends were particularly evident for the release of hydrophobic and aromatic side chain amino acids; for furosine formation; acetic acid, one of the markers of 2,3-enolization; for the release of leucine and the consequent formation of the intermediate N-(1-deoxy-D-fructos-1-yl)-L-leucine and its Strecker degradation, 3-methylbutanal; for methionine and the formation of methional upon the degradation of N-(1-deoxy-D-fructos-1-yl)-L-methionine. It was concluded that the in pack addition of lactase after milk sterilization can have negative sensorial and nutritional consequences mainly related to the enzyme side proteolytic activity especially for prolonged storage time. In the case of in pack addition of the enzyme the purity of lactase became a challenging prerequisite for the final quality of low lactose milk.

Keywords: low lactose milk, maillard reaction, amino acids, amadori products, off flavors
Milk is heated to ensure microbial safety and to reduce enzyme activity in order to prolong its shelf life. In dairy industry, there are several ways of heating which result in different milk types, such as pasteurized milk, ESL-milk and UHT milk. Since heating also reduces the quality and nutritional value, it is very important for food industry and food authorities to be able to differentiate between the various milk types by sophisticated analytical techniques to ensure food authenticity. In previous studies, it was shown that milk contains more than 250 peptides and the peptide profile of milk changes according to applied heating procedure. The goal of the present project was therefore to identify milk peptides, which can be used as highly sensitive markers for industrial heating of milk. As a training set; commercially available pasteurized (n=20), extended shelf life (n=29) and Ultra Heat Treated (n=29) milk samples, produced by dairies located all over Germany and also neighbouring countries like Austria, Belgium and the Netherlands were collected. After a quick peptide purification by StageTip, peptide profiling by MALDI–TOF mass spectrometry was performed. The results showed that peptide profile of milk was heavily influenced by the industrial heat processing. With the help of multivariate statistical analyses (PCA and AHC), 13 peptides for UHT milk and 6 peptides for mildly heated milk (pasteurised and ESL) were selected as markers to predict the heating application. Afterwards, cut-off levels of these marker peptides were defined using receiver operating characteristic (ROC) analysis. Feasibility of the cut-off levels was performed with a blind test samples which consisted of 10 samples from each type of milk. Thus the peptide $m/z$ 1701.01 was identified as a marker which could ideally differentiate between UHT and mildly heated products. Additionally, the peptides $m/z$ 2055.10 and $m/z$ 2216.13 were able to differentiate between pasteurized/microfiltrated ESL milk from higher heated ESL milk with an accuracy of 81%. Due to their high reliability and validity, these 3 marker peptides are now suitable for routine analysis to control the thermal processing conditions of commercially available milk samples. Furthermore, it was observed that the peptide profile of milk is not only dependent on the heating applications, but also on other parameters such as storage duration, season or the regional differences. Thus, the peptide profile could serve as a “fingerprint” of the milk samples, ensuring food authentication.

Keywords: marker peptide, peptide profile of milk, industrial heating, PCA, MALDI-TOF MS

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OHMIC HEATING: A PROMISING TECHNOLOGY FOR MINIMIZATION OF FURAN FORMATION IN STERILIZED VEGETABLE / MEAT BABY FOOD

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Occurrence of furan in heat-treated foods is of health concern because of its carcinogenic potential (class 2B according to IARC). In this context, the search for processing practices ensuring not only microbial safety and acceptable sensorial features, but also, at the same time, reducing or even eliminating furan formation represents a current challenge. In this study, a novel technology, ohmic heating, used for baby food (vegetable / vegetable-meat) sterilization was investigated. For furan and other volatiles analysis, head-space solid-phase microextraction coupled to gas chromatography - mass spectrometry (HS-SPME/GC-MS) was used. When compared to classic thermal sterilization (F0 3-8 min), significant reduction of furan was achieved by ohmic heating. To assess the impact of these two sterilization procedures on formation of volatiles, chemometric tools were used for chromatographic fingerprints assessment. The results showed that differences existed not only in the extent of furan formation but also in other volatiles, obviously due to differing extent of heat-induced reactions.

Keywords: furan, SPME-GC-MS, baby food production, ohmic heating

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ADDITION OF SODIUM ASCORBATE, CITRIC AND ASCORBIC ACIDS TO EXTEND THE SHELF-LIFE OF TUNA MEAT FISH IS A RISK OR A BENEFIT FOR CONSUMERS?

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Consumers rely heavily on fresh meat color which is a prime sensory parameter determining consumer acceptance of a meat. Deviations from the bright red color of fresh meat lead to product rejection and revenue loss. As a consequence, market pressure has lead to the implementation of shelf-life of fish products, without changing its nutritional and sensory characteristics, by the use of different methods, which range from freezing and frozen storage to the use of chemical substances for preserving foodstuffs. The red color of tuna flesh is primarily due to the presence of relatively large amounts of myoglobin (Mb), a protein that in the presence of oxygen forms the red oxy-myoglobin. This derivative degrades during storage, ultimately forming brown metmyoglobin. The reaction products of lipid oxidation compromise further the meat color by accelerating Mb oxidation. Many strategies have been developed to inhibit lipid oxidation, not only to minimize rancidity but also to improve color stability. In general, additives useful for food preservation against damage and deterioration caused by chemical reactions, biological, and microbiological processes are commonly used. In regard to the inhibition of lipid oxidation, citric acid has been shown to play a synergic role with primary antioxidants during minced fish processing (1). In the same way, ascorbic acid (E300) and sodium ascorbate (E301) are commonly used in food production to prevent the oxidation of food, and, therefore, to maintain the color of the food. In present work, the effect of aqueous solutions of sodium ascorbate, citric and ascorbic acids on tuna meat fish has been investigated by the analysis of electronic absorption spectra in their normal and second derivative modes, comparing the results with those obtained on purified myoglobin with the same experimental conditions. The treatment of fish with the mixture of permitted preservatives (E300, E301 and E331) leads to the appearance with time of a broad electronic absorption band near 420 nm, different from that of oxy-myoglobin adduct, but very similar to the carbon monoxide-myoglobin complex (2). This band interferes with the spectrophotometric determination of the presence of carbon monoxide in fish products (3). As for the CO complex, in the presence of the additives, a very stable compound characterized by bright red color is formed which might mask aging of the products and increase the toxicological risk associated with the extended shelf-life of the products.


Keywords: shelf life, tuna meat fish, myoglobin, electronc absorption spectra
USE OF PECTIC POLYSACCHARIDES AS AN ACRYLAMIDE MITIGATION STRATEGY – COMPETITION BETWEEN SUGAR ALDEHYDE AND CARBOXYLIC GROUPS

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Food heating adds taste and color, improving consumers’ acceptance of the products. Both, colored and flavored compounds are generated during thermal processing mainly due to Maillard reactions. This process produces also some toxic compounds, such as acrylamide [1]. The main route for acrylamide formation is the reaction between reducing sugars and the amino acid asparagine. As foods pH modulates acrylamide formation, a mitigation strategy is to roast foods will the lowest possible pH value. For example, tartaric acid, a grapes component, or citric acid, from citrus fruits, can be used as food additives. However, their sour taste prevents their use in a large number of applications, namely in biscuits. In this work, it is shown that pectic polysaccharides provide the required acidity to biscuits dough to minimize the formation of acrylamide without interfering in the biscuits taste. Pectic polysaccharides are polymers of alpha-(1,4)-linked galacturonic acid repeating residues (ca. 300-1000), with a variable number of methyl ester groups or free carboxylic groups, with acid properties. Because the component sugars are polymerized, they do not behave as reducing sugars and, consequently, do not promote the formation of acrylamide. In this work, biscuits were prepared with addition of a polymeric commercial pectic polysaccharide obtained from citrus (CP) and their acrylamide content was evaluated. Also, biscuits were prepared using tartaric acid as control to the acidity effect. When compared to control biscuits, a statistically significant reduction in pH of the dough was observed. The amount of acrylamide determined in biscuits without supplementation was 139–181 μg/kg. A statistically significant acrylamide decrease of 67% was observed with supplementation of pectic polysaccharides. This result is comparable to the 52% decrease observed when using tartaric acid. Because reducing sugars are precursors of acrylamide, the use of galacturonic acid, which contains both a free aldehyde group and a free carboxylic group, lead to a significant acrylamide increase. This result shows the advantage of using acidic polysaccharides due to their negligible amount of free aldehyde groups available. The quality attributes of the pectic polysaccharides supplemented biscuits were all considered acceptable by a non-trained sensory panel, and did not present the characteristic sour taste of tartaric acid. The results presented show that acrylamide mitigation can be successfully overcome using pectic polysaccharides, while maintaining biscuits sensorial characteristics.


Keywords: acrylamide, pectic polysaccharides, galacturonic acid, tartaric acid, cookies

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BIOACTIVE COMPOUNDS IN MARINE SOURCES

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Marine fish is an important source for food in the world, but there is also unused marine resources that we know less about in terms of the biomass and basic knowledge of bioactive molecules that might be usable for different purposes. Many of the drugs approved today is based on knowledge from natural products (over 60%) from terrestrial sources. During the last decades, however, there has been a growing interest for bioprospecting of marine resources for their unique bioactive properties in addition for being usable as food or food products. Marine organisms like animals and bacteria together with other biological material of marine origin, are a source of huge potential for exploring novel bioactive components with activities that can be exploited. In this context, marine proteins and peptides are very interesting. The wide repertoire of biological functions that such natural peptides have, make them exciting for bioprospecting and drug discovery. Among them, antimicrobial peptides (AMPs) are interesting since the increased spreading of bacterial resistance in humans and other pathogenic bacteria worldwide against commercial available antibiotics, have stimulated the search for novel antimicrobials. We have characterized several new classes of marine AMPs and explored their mode of action. The organisms that produce these bioactives have been collected from the Arctic or/and sub-Arctic region and can be very diverse covering biological resources from microalgae to invertebrates. Different approaches and examples in bioprospecting will be looked into. This will include characterizations of mechanisms of action, SAR studies and designed new marine mimicking molecules that might be candidates for novel lead compounds.

Keywords: marine organisms, bioactive components, marine proteins and peptides, bioprospecting

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CANCELLED
Chinese Hawthorn (Crataegus Pinnatifida) Fruit: A Potential Novel Food?

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Hawthorn is a traditional medicinal plant representing Crataegus genus, which is widely distributed in the temperate regions in Asia, Europe, and North America. It has long history in traditional medicine; various clinical investigations and other research suggest that extracts of hawthorn fruits and leaves have multiple health effects including hypolipidemic, anti-atherosclerotic, hypotensive, cardioprotective and blood vessel relaxing activities. Besides of richness in vitamin C content, hawthorn beneficial effects are mainly attributed to the high content of specific phenolic compounds. The phenolics composition in hawthorn fruits varies among species and cultivars, but most of these compounds belong to B-type procyanidins, flavonol glycosides, anthocyanins and phenolic acids. The predominant species today in China is Crataegus pinnatifida. Unlike European hawthorn (Crataegus laevigata), Chinese hawthorn is planted for its edible fruit, which is bigger and tastes better than its European relative. This, in China very popular fruit, is utilized as a fresh, dried fruit, in jams, juices, and tinned foods, and is a basic ingredient for making wines and for various sweet foods, moreover, it is also often used in food supplements. With regards to the above fact, a large scale cultivation of Crataegus pinnatifida in the Czech Republic has been considered. The aim of the current study was to perform a comprehensive evaluation of Crataegus pinnatifida fruits as a candidate for classification as ‘novel food’ according to Regulation (EC) No 258/97. For this purpose, various analytical platforms were used to evaluate antioxidant activity, vitamin C, polyphenols profile and metabolomic fingerprint of fruits. The results were compared with those obtained on fruits from two cultivars of Crataegus laevigata, traditionally grown in the Czech Republic. According to our results, fruits of Crataegus laevigata contain 41 ± 3.3 and 93 ± 7.4 mg/kg of fresh weight (FW) of vitamin C and 4.8 ± 0.5 and 6.0 ± 0.6 g/kg FW of total polyphenols. In comparison, four times higher content of vitamin C and twice the amount of total polyphenols was found in fruits of Crataegus pinnatifida. A strong correlation was observed between the quantity of vitamin C and total polyphenols and antioxidant activity, which was 25% higher for fruits of Crataegus pinnatifida compared to Crataegus laevigata. Metabolomic fingerprints did not show any significant qualitative differences in both ionization polarities between the two hawthorn species, in other words, the similarity was confirmed. All of the monitored substances (organic acids, sugars, lipids and phenolic compounds) were tentatively identified in both hawthorn species and varied only in their intensities. As regards bioactivity, the comparative tests are ongoing.

Keywords: hawthorn, Crataegus laevigata, Crataegus pinnatifida, novel food, polyphenols

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DETERMINATION OF THE ORIGIN FOR ANTHRAQUINONE IN ORGANIC TEA PRODUCTION

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In recent years, tea (camelia sinensis, camelia assamica) has been viewed more and more critically because the problematic substance anthraquinone (9,10-anthraquinone, AQ) have been found in it worldwide. The origin of AQ cannot be precisely located, so in spite of the optimizing and inspection of growth and production processes from planting to packaging, many final products are not marketable. At the moment AQ is regulated in the Regulation (EC) No 396/2005 for pesticides. the current MRL is 0.02 mg/kg in tea. The goal of this study is to locate the sources of AQ on the basis of extensive testing and analysis of the teas and their environment, including different parts of the plants, soil and dust, as well as fertilizers and fortifiers. The study began with planting and went through all the production steps to determine when and where there is a significant growth in the amounts of AQ. From October 2015 to October 2016 more than 300 different samples were taken and analyzed. The results have shown, that in growing as well as in production there are inputs of AQ present. In the environment the factors such as the distance to cities, roads, railway play an important role and built together so called AQ initial finding. AQ source in production is clearly the contact with the hot air produced through coal or wood burning. The AQ findings in additional samples like moss shown, that AQ is also present in it. Consequential the old hypothesis that AQ is endogenously produced has been refuted. It was proved, that AQ is developed form PAH (Anthracene), other oxy PAHs are also present. Summarized, anthraquinone is - contaminant in production (fossil fuels and wood) - contaminant in the environment (present in fine dust, air) - known contaminant from the paper industry - it is definitely not a pesticide in tea cultivation (in the past bird repellent, in tea irrelevant-> no use, counterproductively) As a result of this study is the necessity of regulation of Anthraquinone in tea through the contaminants regulation, The Commission Regulation (EC) No 1881/2006 with a higher level than 0.02 mg/kg.

Keywords: anthraquinone, contaminant, burning of fossil fuels, origin from the PAHs

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LIGNANS IN VIRGIN OLIVE OILS: EFFECT OF REFINING PROCESS AND FRAUDS

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The research was focused to study the lignans, (+)-1-acetoxypinoresinol and (+)-pinoresinol, in olive oils. These molecules are the most abundant phenolic compounds after secoiridoids in virgin olive oil, their concentration mainly depends on the cultivar and the milling process does not affect their amount in a significant manner. The main goals of this study were to investigate on the influence of the olive oil refining process on the phenolic profile and to propose the detection of new isobaric lignans as chemical markers of undeclared presence of refined virgin olive oils in commercial Extra Virgin Olive Oils. The refining process usually leads to elimination, through degradation, of all the phenolic substances, whose presence is highly coveted today in virgin olive oils, especially derivatives of oleuropein. Nevertheless, after this process lignans are not fully removed and remain in very small quantities in refined oils. We analyzed some commercial olive oils and three series of partially and fully-refined olive oils from Italian, Tunisian and Spanish industrial production. The lignan content was evaluated by HPLC–DAD–TOF/MS and some isobaric forms of natural (+)-pinoresinol and (+)-1-acetoxypinoresinol were detected for the first time. It was assessed that the isobaric forms occur only after the bleaching step of the refining process and remain unaltered after the final deodorizing step. We confirmed their presence in three series of olive oils of different origin and derived by an industrial refining process. The proposed mechanism of rearrangement of the natural precursors, (+)-1-acetoxypinoresinol and (+)-pinoresinol, inducing the formation of the isobaric forms, was confirmed by a dynamic molecular simulation study, which provided results in agreement with the chromatographic findings obtained in this research. To the best of our knowledge, isobaric forms of lignans have never been described in olive oils before our research. The detection of these molecules was possible by HPLC–DAD without the need of more expensive mass spectrometric detectors. This aspect will facilitate the application of this method as a routine control for the olive oil quality in the next future. Due to their higher price, virgin olive oils are very attractive targets for fraudsters, consequently, there is a continuous search for new markers to detect adulterations and to guarantee the quality and safety of these products. Detection of these new lignans can be proposed to reveal undeclared presence of refined olive oils in commercial extra-virgin and/or virgin olive oils.

Keywords: (+)-pinoresinol; (+)-1-acetoxypinoresinol, lampante virgin olive oil, HPLC-DAD-MS-TOF, bleaching, olive oil fraud
FORMATION OF EPOXY FATTY ACIDS DURING PHOTO-OXIDATION IN OIL IN WATER EMULSIONS

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Lipids in foods are prone to various oxidation processes. As a result of lipid oxidation various compounds are produced, of which short chain aldehydes are studied most intensively due to their sensorial impact. Also other oxygenated compounds like epoxy-, o xo- and hydroxy fatty acids are formed. Epoxy fatty acids are pro-toxins which become toxic after they are altered during metabolism. The presence of epoxy fatty acids in the human body is related to different diseases such as acute inflammation or adult respiration distress syndrome. Previously we showed that epoxy fatty acids were present in significant quantities in fresh market oils having a low peroxide value. This was remarkable as typically the presence of epoxy fatty acids in foods was associated with heat treated or fried products. This discrepancy indicates that our knowledge on the formation of epoxy fatty acids is still scarce. In addition, limited data on their stability in foods are available, which in view of the presence of a reactive electrophilic epoxide group is quite relevant if nucleophilic food components such proteins are present. Therefore, in this study the formation of epoxy fatty acids in casein stabilized O/W emulsions during photo-oxidation was investigated using riboflavin as a photosensitizer and using respectively sunflower, linseed or olive oil. In parallel, samples were stored in the dark as a control. Epoxy fatty acids were determined after extraction of the lipids from the emulsions followed by base-catalyzed-methylation, a three step solid phase extraction (SPE) to separate polar fatty acids, and gas-chromatographic analysis. The stability of methyl cis-9,10-epoxy-octadecanoate (methyl cis-9,10-epoxy stearate) in casein based O/W emulsions, and in protein solutions was studied in phosphate and citrate buffers at different pH levels (pH 5.0 to pH 12), with C7:0-triglyceride as oil component. Results showed that methyl cis-9,10-epoxy-stearate was stable for 4 weeks in the emulsions using phosphate buffer at pH 7.4, while at pH 12 there was a significant reduction after 2 weeks of storage in the dark, probably due to saponification of the methyl esters. In citrate buffers, the spiked epoxy FAME remained unchanged until 3 weeks of storage at pH 5. Remarkably, a decrease was already observed after 2 weeks at pH 7. Based on these results, casein stabilized O/W emulsion system using phosphate buffer at pH 7.4 was selected to study the formation of epoxy fatty acids in selected O/W emulsions using riboflavin as a photosensitizer. Their formations in samples in light and in dark conditions (the controls) were compared. In sunflower O/W emulsions, total epoxy fatty acid increased from 26.24 to 36.95 μg/mL after 21 days of incubation in samples stored in dark, while it was raised to 45.93 μg/mL in samples stored in light. Epoxy fatty acids, mainly the trans isomer, was formed in higher quantity in photo-oxidized samples compared to samples stored in the dark.

Keywords: Epoxy fatty acids, oil-in-water emulsions, riboflavin, photo-oxidation, methyl cis-9,10-epoxy-octadecanoate
METABOLIC CHANGES DURING STORAGE OF RAPESEEDS AND CONSEQUENCES FOR THE QUALITY OF THE RESULTING VIRGIN, COLD-PRESSED OIL

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Rapeseed oil is the most famous edible oil in Germany and a very popular product in the European Union. Virgin, cold-pressed rapeseed oils have a market share of about 5% of the German rapeseed oil market. As low processed products, these oils enjoy a good reputation among consumers. The quality of virgin, cold-pressed rapeseed oils mostly depends on harvest and storage conditions of the rapeseeds. Quality control of these oils is performed by sensory evaluation with a panel of 3-5 trained persons. As this method is a time consuming, personal intensive and sometimes inconsistent procedure there is a need for an analytical support of the quality control. Hence many different of virgin, cold-pressed rapeseed oils were analyzed via dynamic headspace GC–MS to obtain information about the distribution and differences of volatile compounds between sensory good and bad rapeseed oils from the market. Moreover, in two laboratory experiments, rapeseeds were stored under different humidity and temperature conditions to see which changes occur in seed metabolites and in the volatile compounds of the resulting rapeseed oil. These experiments gave additional information about those factors influencing rapeseed oil quality. In the first approach, seeds were stored on tablets for four days at room temperature under humid conditions. The seeds were spread on tablets and held moistly over the whole day. Germination was visible after one day of storage. The amino acid and glucosinolate composition of the seeds was determined daily using subsamples of the seeds via UHPLC–FLD and HPLC–DAD, respectively. Rapeseed oils were pressed daily and the oil volatile composition was determined via dynamic headspace GC–MS. The amino acid concentrations in seeds rapidly increased over storage time. There was also a clear correlation between raising indole glucosinolates concentrations in the stored rapeseeds and the “germinated” sensory impression as well as volatile glucosinolate degradation products in the resulting rapeseed oils from the 3rd day of storage on. The second approach was performed with increased seed moisture up to 15%. Seeds were stored in closed plastic boxes over 17 days, one part at room temperature and one part at 30°C. PCA shows a clear shift in volatile compounds of resulting rapeseed oils already at the first day of storage, whereas a decreasing sensory quality was detected at the 3rd day (30°C) and 7th day (room temperature), respectively. Sensory evaluation as well as analytic results show accelerated changes in the rapeseed oil quality and volatile compound concentrations at 30°C-storage. Volatile glucosinolate degradation products rose up clearly to the 3rd storage day, were not influenced by temperature and seem to have no impact on the sensory quality of the oils. Some compounds could be products of bacterial metabolism, as they also were detected in volatile compounds of bacteria extracted from rapeseeds.

Keywords: rapeseed storage, metabolites, volatile compounds, sensory evaluation, virgin, cold-pressed rapeseed oil

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Triolein is heated in the Ranzimat 679 for 10 hours. The formation of secondary oxidation products was analyzed using the gradient RP-HPLC coupled to MS via an atmospheric pressure chemical ionization (APCI) source for fast screening and identification of aldehydes which were formed during oxidation of triolein. The secondary oxidation products with low molecular weight were derivatized with dinitro-phenylhydrazine (DNPH) to produce DNP-hydrazones. The kinetex EVO, C18 (150 x 3 mm²) column is used for separation with detection at 400 nm with a gradient elution using a mixture of 60 % methanol in water changing to 100% acetonitrile. Identification with the Qtrap LC--MS brings extreme full-scan sensitivity to produce a good separation of secondary oxidation products analysis. Using this method for secondary oxidation products gives some benefits. Not only the sample used in the small amount but also the method was simple and needed a short time for analysis which was 13 minutes. Some of the peaks obtained shows a maximum with a reduction after 6 hours. The fifth substances of the selected peaks which are A (7.14), B (8.40), C (10.31), D (11.23), and E (12.50) showed that in the 6 h produced the highest value of area and it decreased significantly at the 6.5 h. Further identification was done by LC–MS, we have identified the compounds at the specified retention times. The highest peak of oxidation product was decanal with 2.8 μmol/g, followed by nonanal 2.3 μmol/g, octanal 1.9 μmol/g, heptanal 1.5 μmol/g and hexanal 1.5 μmol/g in 10 h oxidation of triolein. All values are based on a calibration with hexanal. Regarding to some studies, the destruction of essential fatty acids and lipid soluble vitamins such as vitamins A, D, E, and K effected not only the nutritional value but also the caloric content. Moreover, free radicals and metabolites formed during oxidation may exert adverse effects on human health. The oxidized oils are absorbed in the intestine, transported to the liver via chylomicrons, and may affect unaltered hepatic cells as well as the process of hepatocarcinogenesis. Considering the disadvantages of aldehydes in the oxidized oil, α-tocopherol and β-carotene were added in order to reduce the rate of aldehydes formation in the oil.

(5) Tao, L. (2015) Advances in food technology and nutritional sciences open journal (1)6, 135-140.

Keywords: triolein, secondary oxidation products, 2,4-DNPH, α-tocopherol, β-carotene

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THE UNIQUE CHEMISTRY OF MANUKA HONEY
(LEPTOSPERMUM SCOPARIUM)

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Manuka honey is well known for its unique antibacterial effect, which is due to high amounts of the 1,2-dicarbonyl compound methylglyoxal (MGO). MGO and its precursor dihydroxyacetone (DHA) are found in Manuka honeys in amounts of up to 700 and 1600 mg/kg, respectively, whereas conventional honeys contain only 5–10 mg/kg of DHA and MGO (1). MGO and DHA are highly reactive substances, leading to a variety of unique chemical reactions during Manuka honey maturation and storage. 2-Acetyl-1-pyrroline (2-AP), which is formed during Strecker degradation of proline and MGO, was identified and quantified in Manuka honey for the first time. The 2-AP concentration in Manuka honey ranges from 0.1 to 0.5 mg/kg and correlates with the MGO content. 2-AP in conventional honeys usually was below 0.1 mg/kg. Glycation of proteins can lead to the formation of advanced glycation end products (AGEs). After isolation of honey proteins via dialysis or acid precipitation and subsequent enzymatic hydrolysis, carboxyethyllysine (CEL) and a methylglyoxal-derived hydroimidazolone (MG-H1), specific MGO-derived glycation compounds, were identified in Manuka honey using HPLC-MS/MS. Amounts ranging between n.d. –103.0 μmol/mmol leucine for CEL and n.d. –24.1 μmol/mmol leucine for MG-H1 were quantified for Manuka honey. Corresponding concentrations in non Manuka honeys were between n.d.-tr. and n.d.-0.7 μmol/mmol leucine for CEL and MG-H1, respectively. CEL and MG-H1 concentrations correlated strongly with the MGO content of the honeys. To obtain further information about the structure of Manuka honey proteins, the fluorescence properties of honey proteins (excitation at 350 nm, emission at 450 nm) were analyzed. Protein isolated from Manuka honey showed significantly higher fluorescence intensities when compared to non-Manuka honey protein. The fluorescence intensities correlated with the corresponding MGO contents. To characterize the reactions responsible for the increase of fluorescence in Manuka honey, protein fractions were analyzed by gel permeation chromatography. The studies showed that the molecular weight fraction above 500 kDa is significantly increased in Manuka honey protein, whereas non-Manuka honey proteins are mainly distributed between 100 to 500 kDa. This leads to the conclusion, that MGO is responsible for protein polymerization in Manuka honey. The unique MGO-derived reactions distinguish Manuka honey from other honey varieties. These modifications directly depend on the MGO content of the honey and could therefore be a suitable parameter to characterize Manuka honey and assess the quality of commercial samples.


Keywords: manuka honey, methylglyoxal, glycation, fluorescence
Poster session
EFFECT OF VARIOUS COOKING TECHNOLOGIES ON QUALITY AND STARCH NUTRITIONAL PROPERTIES OF PULSES

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Pulses are important part of a healthy-balanced diet as being low in fat and a good source of protein, slowly digestible starch, dietary fiber and bioactive components. This nutrient composition makes pulses promising food ingredients for processing healthy foods. The present study investigated the effect of different cooking technologies and solutions on quality and starch nutritional properties of three pulses (lentils, faba beans and peas). Starch nutritional fractions were based on controlled conditions of enzymatic digestion in vitro. Resistant starch was measured based on the AOAC (Method 2002.02). Four cooking methods including traditional boiling, pressure, microwave heating and slow cooking were investigated with the use of water, salt, sugar or citric acid as a cooking medium. Firmness of cooked pulses was significantly influenced by type of cooking technology and cooking solution. In addition, time of cooking significantly varied among cooking methods which could indicate different amounts of energy consumed by each cooking method. Concentration of cooking solutions also affected firmness and cooking time of pulses. Nutritional properties of starch varied among pulses and cooking technologies. In general, the results demonstrated that processing technology could have significant effects on the quality and nutritional properties of cooked pulses.

Keywords: pulses, processing, starch, quality, nutrition

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VOLATILE COMPOUNDS PROFILE OF MICROWAVE TREATED TART CHERRY PUREES WITH ADDITION OF SUGARS DURING STORAGE

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Tart cherry puree as a semi-product can be used for preparation of different products like pies, cakes, bakery products and dairy based products. Different additives, such as sugars, are usually used to achieve high quality of the puree required for further processing. In this study, tart cherry purees were prepared with the addition of 10% sucrose or trehalose. The profile of volatile compounds determines the aroma properties of product and depends on additives used, as well as the processing method. Tart cherry puree samples were prepared by pasteurisation and microwave treatment. In the untreated sour cherry puree, 22 volatile compounds were identified which have been divided into four groups: terpenoids, carbonyl compounds, alcohols and esters. Results of volatile compounds analyses of prepared samples (with addition of sugars, prepared by pasteurisation and using microwave treatment) were compared to untreated tart cherry puree with no additives. Comparison of microwave treated versus pasteurised purees indicated a higher retention of alcohols and esters in the microwaved puree. Carbonyl compounds were determined in higher amounts in both samples compared to the untreated puree but at a much higher level in the pasteurised puree. Comparing the microwaved versus pasteurised samples, both with and without the addition of sugars, microwaved samples had higher retention of all compounds except carbonyl compounds. Within the microwaved puree samples, higher retention of carbonyl compounds and alcohols was determined in puree with added sucrose, while samples with trehalose had a higher retention of terpenoids and esters. In pasteurised purees, trehalose addition resulted in higher retention of terpenoids, esters and carbonyl compounds. After one month of storage at room temperature, carbonyl compounds have been lost in all samples. In untreated puree, only alcohols were retained during storage while the addition of sugars enabled the retention of esters and terpenoids as well as alcohols. Microwaved puree with added trehalose had the highest retention of esters and terpenoids. Based on our results, it can be concluded that both matrix composition (in this case the type of added sugar used) and processing method (microwave treatment versus pasteurisation) greatly influenced the retention of volatile compounds of tart cherry purees after the preparation of puree samples as well as during processing.

Keywords: tart cherry purees, microwaves, pasteurisation, sugars, volatile compounds

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TEXTURE AND AROMA PROFILE OF SOUR CHERRY FILLINGS

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Sour cherry fillings can be used as the semi-product for preparation of different products like pie, cakes, bakery products, milk products. It is necessary to obtain high quality of the semi-product that could be used in further processing and usually different additives are used, such as hydrocolloids and sugars. In this study, the sour cherry fillings were prepared with the addition of hydrocolloids (guar gum or xanthan; 0.6%) and sugars (sucrose or trehalose; 50%). Textural parameters that were selected for comparison of samples were firmness, consistency, cohesiveness and index of viscosity. Samples prepared with the xanthan had higher firmness than guar gum samples, and in both case samples with addition of trehalose had lower values of the firmness. Values of consistency were the same in samples guar gum/sucrose and xanthan/sucrose, also the same values were determined in guar gum/trehalose and xanthan/trehalose. Samples with trehalose addition had lower values of consistency than sucrose samples. Cohesiveness and index of viscosity were higher in samples that were prepared with guar gum, and samples with sucrose addition had higher values of these parameters. In sour cherry puree, 22 aroma compounds were identified which were divided into four groups: terpenoids, carbonyl compounds, alcohols and esters. Aroma compounds of sour cherry fillings were compared to aroma compounds of sour cherry puree. In all filling samples, carbonyl compounds were determined in higher amount than in puree. Terpenoids and esters were retained in higher amount in samples when trehalose was added, while alcohols were determined in higher amount in samples with sucrose. Matrix composition and interactions during processing greatly affected texture and aroma compound retention in sour cherry fillings.

Keywords: sour cherry fillings, hydrocolloids, sugars, texture, aroma

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AROMATIC PROFILE OF RASPBERRY CREAM FILLINGS WITH SUGARS, MODIFIED STARCHES AND HYDROCOLLOIDS

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Knowledge of the aroma properties has great significance for fruit product processing as well as fruit product acceptability. Fruit products based on raspberry are usually obtained from puree. Due to evaluation of organoleptic properties of final product it is necessary to understand the properties of aroma puree as well as influence of different additives and processing methods. The objective of this study was to investigate the retention of aroma compounds in raspberry cream fillings with addition of sugars (sucrose, sucrose/fructose or sucrose/trehalose), modified starches (tapioca or corn starch) and hydrocolloids (karaya or guar gum). For this purpose, raspberry cream fillings were prepared with different combinations of sugars, sugars/modified starches and sugars/hydrocolloids. The aroma profile of raspberries was determined in fresh, pasteurized raspberry puree and in prepared raspberry cream fillings. Determination of aroma profile of raspberry samples was carried out by gas chromatography with mass spectrometry. In raspberry puree, eighteen aroma compounds were identified which were divided into three groups: terpenoids, carbonyl compounds and acids. After pasteurisation, retention of terpenoids was 45%, carbonyl compounds 60% and acids 81%. In the case of samples prepared by different sugar combinations, the highest retention of terpenoids was observed in sugar/trehalose samples, 70%, but there was no significant difference for acids and carbonyl compounds between samples with sugar addition. Terpenoids and carbonyl compounds had the highest retention in samples with sucrose/trehalose and modified starches additions (83%) while acids were retained in the highest amount in sucrose/starches samples (45%). In the case of hydrocolloids addition, samples with addition of sucrose/trehalose and karaya had the highest retention of terpenoids (87%) and carbonyl compounds, while samples with addition of sucrose and hydrocolloids had the highest addition of acids. Matrix composition and interactions during processing greatly affected aroma compound retention in raspberry cream fillings.

Keywords: raspberry fillings, sugars, modified starches, hydrocolloids, aroma compounds

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TEXTURAL PROPERTIES OF MODEL SYSTEMS OF HYDROCOLLOIDS AND SUGARS

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Texture is one of very important food quality properties. Different additives have influence on aroma and colour of fruit products, but their influence on texture should not be neglected. Hydrocolloids and sugars are additives that are very often used in preparation and formulation of fruit products. The aim of this study was to prepare model systems of hydrocolloids (guar gum or xantan; in amount of 0.6 %) and sugars (sucrose or trehalose; in amount of 30, 40 or 50%) in order to investigate influence of different sugars and their amount on textural properties of selected hydrocolloids. Textural parameters that were selected for comparison of model systems were firmness, consistency, cohesiveness and index of viscosity. Xantan systems without sugar addition had higher values of firmness (13.324 g) and consistency (115.68 g) than guar gum systems. Both systems had the same value of cohesiveness and index of viscosity. Addition of both sugars in different amount caused change of textural parameters. With increase of sugars amount increase of all textural parameters occurred. With addition of sugars, firmness of both hydrocolloid systems increased. In the case of guar gum there was no difference between addition of 30% of sucrose or trehalose, while with addition of 40 and 50% of sugar significant difference between sugars were obtained. Addition of trehalose had higher impact on guar gum firmness, and the higher values of those systems were observed. In the case of xantan, addition of sucrose (all amounts) caused higher increase of firmness than addition of trehalose. The same tendency of sugars influence was observed in the case of consistency. There was no difference in cohesiveness and index of viscosity when 30% of sugars were added to guar gum systems. When 40 and 50% of trehalose were added, guar gum systems had significantly higher values of cohesiveness and index of viscosity. In the case of xantan, sugar amount did not cause difference in cohesiveness and index of viscosity. Specific molecular interactions between sugars and hydrocolloids appear to have a significant contribution to textural parameters. Even though, sucrose and trehalose are chemical isomers, it is obvious that interactions between those sugars and hydrocolloids, as well as sugar amount had high impact on textural parameters of model systems hydrocolloids and sugars.

Keywords: model systems, hydrocolloids, sugars, textural properties

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FREE MCPDS, THEIR ESTERS AND GLYCIDYL-ESTERS IN FOOD: PRECISION AND ACCURACY FOR MONITORING FOOD PRODUCTS AND MITIGATION PROCESSES

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2- and 3-monochloropropene-1,2-diol (2- and 3-MCPD) are important food processing contaminants. 3-MCPD is classified as a possible human carcinogen (according to IARC), and European Commission (EC) has already set limitations in food1. The toxicity of 2-MCPD is still under investigation and long term studies are required to properly assess its harmfulness. Esters of 3-MCPD, 2-MCPD and glycidyl esters form during high temperature oil refining and are contaminants of processed vegetable oils.

A recent EFSA scientific opinion showed that those esterified forms undergo extensive hydrolysis upon ingestion, thus generating high quantity of toxic MCPDs. This is a problem primarily linked to vegetable oils and fats, but also to derived foods such as bakery products. In particular, it was recently found that the vegetable oils contain not negligible concentration of these contaminants as well as margarines, creams, chocolate creams and many other foods made with vegetable oils and animal fats. That has raised much concern, considering that those oils are very much used as ingredient for foods and baby food as well.

In long-term toxicological studies, administration of 3-MCPD to laboratory animals led to an increase in cell count (hyperplasia) in renal tubules as the most sensitive endpoint. Higher doses triggered benign tumours in treated animals. A tolerable daily intake (TDI) of 0.8 μg/kg bodyweight per day was established and the mean exposure to 3-MCPD was above the TDI for ‘Infants’, ‘Toddlers’ and ‘Other children’.

Due to the carcinogenic and genotoxic potential of glycidol, it is not possible to derive any safe intake quantities for glycidyl fatty acid esters [studies on bioavailability have shown that glycidyl fatty acid esters are hydrolyzed (de-esterified) during digestion, and the free glycidol is almost completely released]. There is therefore a need to minimize esters’ concentrations in accordance with the ALARA principle (as low as reasonably achievable).

Given the importance of monitoring the presence of free as well as esterified MCPDs and glycidyl esters in compliance with EC Recommendation2, MérieuxNutriSciences developed and improved analytical methods based on official JRC-standards to fully validate a precise, accurate and complete panel of analyses for:

- 2-MCPD (2-Monochloropropene-1,2-diol)
- 3-MCPD (3-Monochloropropene-1,2-diol)
- 2-MCPD esters (2-Monochloropropene-1,2-diol fatty acid esters)
- 3-MCPD esters (3-Monochloropropene-1,2-diol fatty acid esters)
- Glycidol esters (Glycidyl fatty acid esters)

To ensure accurate results, the method allows a proper and extensive hydrolysis of fatty acid esters in the sample. Moreover, the use of isotopically labeled internal standards implies to minimize uncertainty.

More than 90% of 1000 samples analyzed in 2016 were consistent with EFSA data and results3.

(1) Commission Reg (EC) 1881/2006
(2) Commission Recommendation 2014/661/EU
(3) EFSA Scientific Opinion (3 march 2016) - doi: 10.2903/j.efsa.2016.4426

Keywords: MCPD, MCPD esters, glycidyl esters, food processing contaminants
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PROMOTION OF MAILLARD REACTIONS BY CHITOSAN-GENIPIN FILMS IN MODEL WINE SOLUTIONS

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Chitosan-genipin (Ch-Ge) films have been proposed as wine preservative due to their antimicrobial and antioxidant properties. However, wines treated with Ch-Ge films showed a significant higher content of furfural and benzaldehyde in relation to untreated wine. The formation mechanism of these compounds, described as volatile products of Maillard reactions (VPMR) [1], was never proposed. Therefore, the main purpose of this work was to understand the role of Ch-Ge films on the formation mechanism of VPMR. The wine model solution was prepared containing Ch-Ge film and arabinose (Ara) allowed to detect the presence of furfural, confirming its formation by reaction between the amino group of chitosan and the aldehyde group of Ara, giving rise to an imine and later leading to its dehydration. Using a wine model solution containing Ch-Ge film and phenylalanine (Phe), it was observed the formation of benzaldehyde. In order to explain the reaction of formation of benzaldehyde, wine model solutions were prepared separately using glycerol (plasticizer) and genipin (cross-linker) used to prepare Ch-Ge films, together with Phe. These experiments allowed to observe benzaldehyde in wine model solutions with genipin, but not with glycerol. In fact, the secoiridoid as genipin can be in equilibrium between hemiacetal group of close form and the carbonyl groups of dialdehydic open–ring form that, if not involved in the cross-linking, can react with the amino group of Phe and promoting the formation of benzaldehyde through a Strecker reaction. In conclusion, Ch-Ge films are able to promote the formation of volatile compounds by reaction with sugars and amino acids present in foods.


Keywords: chitosan-genipin film, volatile compounds, maillard reaction, strecker reaction

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PESTICIDES HOUSEHOLD PROCESSING FACTORS OF NATURALLY CONTAMINATED FRESH TOMATOES AND APPLES

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Pesticides use is increasing as a modern technological tool for extensive crops and horticulture in Argentina and globally. The latest food chain concerns greatly with the risk of human dietary exposure for many residues of authorized and non-authorized active ingredients in fruits and vegetables. Fresh apple and tomato, usually with skin, are products of high consuming rates in Argentina, even including the infant diet cluster. Providing safe products to consumers is a constant concern for producers, legislators and also for housewives who demand procedures to safely treat the food they provide to their own families. This work aims to study the chemical behavior of pesticide residues found in samples of fresh tomato and apples, naturally contaminated during the production in commercial productive greenhouses, submitted to household processing such as washing and peeling. The analytical methodology developed and validated for this study, comprised a previous step of extracting analytes from samples as they were collected with acetonitrile and buffering salts, followed by a multi-residue method searching for 64 pesticides, using liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS). Raw tomatoes harvested from two farms from Santa Fe Province (in the central region of the country) and fresh apples from Rio Negro Province (in the Andinean region) stored using SmartFreshSM technology, were submitted to experimental assays. Both types of samples were found to contain pesticide residues as follows: azoxystrobin, carbendazim, difenoconazole, flubendiamide, imidacloprid and pyraclostrobin in tomatoes, and carbaryl, carbendazim, chlorantraniliprole, chlorpyrifos, imazalil and thiabendazole in apples. All concentrations found were below the National MRIs (Res 934/10, SENASA). In both types of contaminated samples, peeling and washing treatments with tap water, acidic solutions (acetic acid 2% and 5% v/v) and alkaline solutions (sodium bicarbonate 2% and 5% v/v) were applied. Peeling was the most effective with a reduction of residue concentrations ranging from 65% (imidacloprid) to 98% (difenoconazole) for tomatoes and above 90% for all compounds in apples. Washing with tap water also achieved a reduction of the six residue compounds found in the samples. Finally, the results obtained by washing with acid and alkaline solutions were highly variable depending on the pesticide and the concentrations of solutions used. Results of calculated processing factors for household treatments were compared with other values, scarcely existent in bibliography under the same experimental conditions, being a good contribution to the available data for refinement of acute and chronic dietary risk assessment of an interesting group of pesticides and popular food such as tomatoes and apples.

Keywords: household processing factors, pesticides, apples, tomatoes

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REDUCTION AND TRANSFORMATION OF DEOXYNIVALENOL DURING THERMAL PROCESSING

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Mycotoxins, toxic secondary metabolites produced by fungi, contaminate a wide range of food commodities. Thermal treatment during food processing remains one of the most important factors to reduce the mycotoxin contamination in a finished food product [1]. The degradation of the parent compound can result in the formation of products with altered chemical structures (modified mycotoxins). Little information on modified mycotoxins is available except for those originating from deoxynivalenol (DON). When heated in aqueous NaOH solution, DON was found to degrade to norDONs and DONlactones, which have also been found in food samples from the market [2]. However, studies on the fate of DON during thermal food processing left contradictory conclusions. While extrusion cooking was found to effectively reduce DON levels in a study by Cazzaniga et al. [3], other authors reported only moderate effects or no reduction at all [4,5]. Therefore, the panel on Contaminants in the Food Chain (CONTAM) emphasized the need for further work to identify modified mycotoxins not yet characterized and for more information on their chemical structures [6]. Within a recently granted EU project, “MyToolBox”, thermal processing factors which are relevant for the reduction of mycotoxins and their transformation into modified forms are explored. The ultimate goal of this contribution is to understand the degradation process of DON during food production. NorDONs and DONlactones were produced after thermal treatment of 90 mg DON in 0.1M NaOH for 1 hour. The formed compounds were isolated by reversed phase preparative chromatography and their structures were confirmed by MS and NMR. The obtained substances will be used as reference standards to develop a LC–MS/MS based method for the determination of DON degradation products in finished food.

(6) CONTAM Scientific Opinion on the risks for human and animal health related to the presence of modified forms of certain mycotoxins in food and feed EFSA Journal 2014;12(12):3916.

Keywords: food processing, deoxynivalenol, mycotoxins, LC-MS
AUTHENTICATION OF MEAT AND MEAT PRODUCTS USING LC-MS/MS - TARGET PROTEOMIC ANALYSIS APPROACH

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Food adulteration is a growing problem worldwide, meat and meat products are no exception. Serious problem is accidental or fraudulent blending of meat from different species or complete substitution, for example the horse meat scandal in Europe in 2013. A new method based on mass spectrometric identification of animal species in both raw and processed meat and meat products was established for the purposes of the official control. This method, with a target proteomic analysis approach, is based on MRM detection of unique peptides in tryptic digest of protein extracts via LC–MS/MS (QqQ). Unique peptides were selected by means of Skyline software and come from different muscle proteins. The method was optimized for identifying of different meat samples of eight animal species (beef, pork, horse, sheep, chicken, turkey, duck and rabbit) in one run with detection limits between 1 and 5 % of added/non-declared meat species.

Keywords: authentication, meat species, peptides, mass spectrometry
ANALYSIS OF CHEMICAL COMPOSITIONS AND CORDYCEPIN IN TOCHUKASO MUSHROOM

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The Cordyceps species fungi, belonging to Ascomycetes are parasites feeding on insects generally called Tochukaso (summer grass, winter worm). The host insects are various and Tochukaso is composed of a fruit body of Cordyceps sinensis and its parasitic host larva. It has been used as a traditional herbal medicine in Korea, Japan, and China. In this study, chemical compositions and Cordycepin, the index compound in Tochukaso, were investigated. Nutritional compositions of three Tochukaso species (P. tenuipes hosted by Larva and pupa, C. militaris, C. sinensis) were compared. Fruiting body and host fractions were separately analyzed. The portion of fruiting body part of P. tenuipes (36.6%) was higher than the host part (10.2%) by pupa. Carbohydrate content of C. sinensis (39.6%) was higher by 2.5~7 times than those of the others, suggesting due to the polysaccharides. Protein content of C. sinensis and C. militaris was 25.8% and 75.1%, respectively. Crude lipid content of C. sinensis was 10.3%, while that of C. militaris was 3.9%. From the mineral analysis, C. sinensis was shown to have the lowest in Ca content, but extremely higher in Fe content by 30~75 times than the others. Vitamin A content of C. militaris was 308.9 IU/100g. This is higher by 2 times than those of the other species. Saturated fatty acid composition was highest in P. tenuipes (pupa, 27.7%), while unsaturated fatty acid was highest in P. tenuipes (larva, 83.3%). Aspartic acid, glutamic acid, and glycine were abundant in all species. Cordycepin content of C. militaris analyzed by HPLC was higher by 20~50 times than those of the other two species.

Keywords: tochukaso, chemical composition, cordycepin, Cordycpes militaris

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Caseins represent about 80% of the proteins in bovine milk. Due to their flexible and open molecule structure, the caseins show very good emulsifying, gelling and foaming properties [1] and are, therefore, widely used in food production. A common procedure in industry to alter those techno-functional properties involves the application of microbial transglutaminase to induce protein cross-linking [2]. The reaction of milk proteins with reducing sugars via Maillard reaction (glycation) can also lead to a formation of protein cross-links, but includes an additional derivatization of the protein side chains, resulting in various other structures like Amadori products and advanced glycation end products (AGEs). The aim of our study was to investigate the relationship between new structural features evolving during different stages of Maillard reaction and the gelling properties of casein in comparison to enzymatic cross-linking with microbial transglutaminase on a molecular level. Sodium caseinate was heated in the dry state at 60 °C with reducing sugars or treated with microbial transglutaminase at 40 °C. The formation of Amadori products and protein cross-linking was examined by amino acid analysis and gel permeation chromatography, respectively. For techno-functional characterization, acid casein gels were prepared by addition of glucono-δ-lactone and gel strength was measured with a Texture Analyzer. Our results showed an increase in gel strength up to 164 and 387% after glycation and enzymatic treatment of caseins, respectively. For both types of modification, cross-linked casein dimers and trimers contribute considerably to the formation of stronger gels. The increase in gel strength of the glycate casein gels was furthermore independent from the amount of sugars covalently bound to the proteins during early Maillard reaction but strongly limited when an oligomerisation degree of about 50% was exceeded. The increase in gel strength of enzymatically treated casein gels remained unaffected by that critical threshold of protein cross-linking, which was for both types of modification associated with an exponential rise of the polymer fraction. We postulate, that the size and shape of casein polymers differ significantly between glycated and enzymatically treated caseins and have a strong influence on the formation and stability of the gel network built up of intensively modified caseins.

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(2) M. Kieliszek & A. Misiewicz, Folia Microbiol. 2014, 59, 241

**Keywords:** casein, techno-functionality, Maillard reaction, microbial transglutaminase, protein cross-linking
P13
INFLUENCE OF CYCLODEXTRINS ON ACE-INHIBITORY DIPEPTIDES PRESENT IN PROTEIN HYDROLYSATES

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Bioactive peptides can be released from food proteins by fermentation, enzymatic hydrolysis or during gastrointestinal digestion. We focused on peptides acting as inhibitors of the angiotensin-converting enzyme (ACE) in vitro, which plays an important role in blood pressure regulation in vivo [1]. Potent ACE-inhibitory dipeptides contain an amino acid with a bulky and hydrophobic side chain in the C-terminal position, such as tryptophan, tyrosine or phenylalanine [2]. A limiting factor for a possible activity in vivo is their low bioavailability (below 0.1 %), which is due to proteolytic degradation [3]. Cyclodextrins (CD), cyclic starch degradation products of 6 (α-CD), 7 (β-CD) or 8 (γ-CD) glucose units, can form complexes with hydrophobic compounds. Complexation of aromatic amino acids could lead to an increased bioavailability of the corresponding dipeptides. Furthermore, the sensory quality of bitter-tasting hydrolysates can be improved by the addition of cyclodextrins [4]. The aim of this work was to determine the influence of the addition of α-, β- and γ-CD on the stability of selected dipeptides in protein hydrolysates towards simulated gastrointestinal digestion. Therefore, it was first clarified whether the aromatic amino acids tryptophan, tyrosine and phenylalanine form complexes with these cyclodextrins. Two-dimensional NMR measurements (e.g. ROESY-NMR) provided information about molecular interactions. It was shown that the hydrophobic side chain of the respective amino acids can penetrate into the cavity of the cyclodextrins. 1H-NMR spectroscopy was used to characterize the formation of corresponding complexes. For all amino acids analysed, the calculated association constants were less than 600 M⁻¹, indicating only weak interactions, whereby tryptophan and β-CD formed the most stable complexes. The effect of α-, β- and γ-CD on selected potent ACE-inhibitory tryptophan- and tyrosine-containing dipeptides in whey and rice protein hydrolysate was investigated by simulated gastrointestinal digestion. Only the addition of β-CD resulted in a significantly higher residual amount of as well as tryptophan- and tyrosine-containing dipeptides up to 50 %. Moreover, initial investigations on the taste of rice protein hydrolysate have shown that the addition of β-CD can significantly reduce their bitterness.

(2) J. Wu, QSAR Comb Sci. 2006, 27, 873-880.

Keywords: plant protein hydrolysates, bioactive dipeptides, cyclodextrin, digestion, sensory analysis
FREE MAILLARD REACTION PRODUCTS IN MILK FROM “ORGANIC” AND “CONVENTIONAL” FARMING

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The organic production of food plays a dual societal role. On the one hand it supplies a specific market as a response to a consumer’s demand for organic products, on the other hand delivers foods which contribute to the protection of the environment and animal welfare. Furthermore, the idea of organic farming is increasingly gaining popularity in the context of the Council Regulation (EC) No 834/2007 on organic production and labelling of organic products. From intervention studies it is known that some Maillard Reaction Products (MRP) (e.g. pyrraline) could be detected after ingestion in urine [1]. Therefore, a transition of protein-bound MRPs from the diet into free MRPs in the milk seems probable. As MRPs do not belong to the constituents of natural food resources of ruminants, they potentially could be indicators of the use of heat-treated fodder (e.g. feed pellets), which is common in conventional farming. Using LC-MS/MS and isotopically labeled standard substances, quantitation of free Maillard reaction products (MRPs), namely, Nε-(carboxymethyl)lysine (CML), 5-(hydroxymethyl)-1H-pyrrole-2-carbaldehyde (pyrraline, PYR), Nδ-(5-hydro-5-methyl-4-imidazolon-2-yl)-ornithine (MG-H), in bovine milk was achieved. When comparing commercial milk samples labeled as originating from “organic” or “conventional” farming, respectively, significant differences in the content of free PYR (organic milk, 20–300 pmol/mL; conventional milk, 400–1000 pmol/mL) were observed. An analysis of feed samples indicated that rapeseed and sugar beet are the main sources for MRPs in conventional farming. As the components of concentrated feed do not belong to the natural food sources of ruminants, free MRPs in milk might serve as indicators for an adequate animal feeding in near-natural farming and can be suitable parameters to distinguish between an “organic” and “conventional” production method of milk. [2] Further studies indicate, that the distinction between “organic” and “conventional” production with other milk products, namely, quark, buttermilk, yogurt and cheese, is also possible.


Keywords: Maillard reaction, organic and conventional farming, milk, food authenticity

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CANCELED
Decompressed heat pump drying technique is a new drying method for food system. Drying is carried out by a heat pump in low air pressure, which is better than the vacuum freeze drying and the hot air drying method in terms of reducing the drying time and improving efficiency. In this study, we investigated the change of the properties on the dried aronia by the decompressed heat pump dryer (DHPD) which is capable of the retention of flavor, nutrition, appearance and color. To confirm the structural safety and drying mechanism of the decompressed heat pump dryer, the structure was analyzed using MSC’s Marc and the air flow was measured using ANSYS. For the vacuum drying, DHPD works in the range of 0 ~ -4,500 mmAqg vacuum and 20 ~ 65°C temperature. In this study, we carried out aronia drying in 0 ~ -3,000 mmAqg vacuum and 45°C temperature. The eco-friendly air extraction device was used for 0~-3,000 mmAqg of low air pressure and two stage condenser for obtaining 20~65°C of heat pump extraction temperature. To compare with the conventional vacuum freeze dryer, various quality properties of dried aronia were investigated; moisture content, polyphenol content, flavonoid content and anthocyanin content. Antioxidant activity of dried aronia was determined by the free radical scavenging activity using DPPH method. The drying yield of aronia was 82.5% in vacuum freeze drying and 92% in DHPD. Flavonoid contents were 109.4 mg/g and 271.8 mg/g by vacuum freeze drying and DHPD, respectively. Polyphenol contents were shown as 109.4 mg/g for vacuum freeze drying and 271.8 mg/g for decompressed heat pump drying. The content of anthocyanin was 3 times higher in heat pump drying (69.2 mg/100 g) than that of the vacuum freeze drying (17.9 mg/100 g). EDA (Electron Donating Activity) calculated from DPPH method was 29.8% in vacuum freeze drying and 69.8% in DHPD. From these results, Decompressed Heat Pump Dryer (DHPD) is thought to be more effective tool than the conventional freeze drying method to get the better quality of foods.

**Keywords:** decompressed dryer, heat pump, aronia, antioxidant activity

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P17
IDENTIFICATION OF BIPHENYLS - CONTAMINANTS RESPONSIBLE FOR OFF-FLAVOUR IN SOFT DRINKS

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Contamination of soft drinks is one of the manufacturer’s main risks and can result in expensive recalls and discredit the brand. Off-flavour can occur for a variety of reasons and chemical contamination of raw material is one of the least likely and is difficult to be detected as a source of off-flavour. Presented real case study proved a link between the identification of biphenyl and biphenyl derivatives in used preservatives (benzoates) and off-flavoured drinks. The project had the following four phases: 1) assessment of the probable cause of off-flavour based on sensory evaluation and GC–MS–Olfactometry profiling of volatiles; 2) quantification of biphenyls, characterisation of their sensory and chemical properties; 3) screening of commercially available benzoates for the presence of biphenyl and its derivatives; 4) the proposal of corrective measures to eliminate the incidence of off-flavour in soft drinks.

Keywords: off-flavour, beverages, biphenyl, gas chromatography - olfactometry
EVALUATION OF COCOA PRODUCTS QUALITY AND AUTHENTICITY BY DART/TOF-MS

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The work focuses on the optimization and validation of direct analysis in real time (DART) coupled with time of flight detector (TOF) for the evaluation of the quality and authenticity of selected cocoa products (cocoa powders and cocoa drinks). The ionization mode, the optimal ionization temperature and solvent for sample extraction were optimized. The characteristic compounds of the analysed cocoa products (theobromine, caffeine, phenolic and flavonoid substances) were detected. A set of samples of cocoa powders (17) and cocoa drinks (12) were analysed. The possibility of using DART for analysis of caffeine and theobromine was confirmed. HPLC/DAD and DART/TOF-MS methods for determination of theobromine and caffeine were compared. The correlation equation between these methods were: theobromine: cocoa powders: DART = 1.6294 × HPLC - 1.4147; cocoa drinks: DART = 1.0398 × HPLC - 0.0211 and caffeine: cocoa powders: DART = 1.0098×HPLC - 0.0169; cocoa drinks: DART = 0.7705 × HPLC + 0.0064. The results show that the DART/TOF-MS technique has a great potential for the evaluation of the quality and authenticity of cocoa products, especially for fast screening.

Keywords: Theobroma cacao, beverages, mass spectrometry, alkaloids
P19
CANCELLED
UNRAVELLING COMPLEX REACTION PATHWAYS - FATE OF 14C-LABELLED AGROCHEMICALS IN FOOD PROCESSING - FIRST RESULTS

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Analysing the fate and metabolism of ingredients or environmental and technical contaminations in complex matrices, such as food, is a major challenge in food technology. Modern food processing aims to combine more and novel ingredients and to apply combinations of physical processing factors. By using radioactively labelled precursors their remains, metabolites, and fragments can easily be identified and monitored along food processing chains. As pesticide residues are of major public concern, our long-term project focuses on the fate of selected pesticides. We aim to reveal possible hazardous compounds that have not yet been identified with common techniques and to optimize food processing strategies to yield safer food. First results of this project indicate that current guidelines to elucidate the fate of pesticides (e.g. OECD 507) do by far not represent all chemical reactions in food processing. Additional degradation products were observed e.g. of the imidazole fungicide Prochloraz when traditionally processed in the presence of rapeseed oil. One of the technical metabolites cannot have been formed by simple bond breakage. On the basis of MS/MS-data, it is assumed that this product containing the trichlorophenol moiety results from a chemical reaction with any matrix component from rapeseed oil. This observation demonstrates the limitations of the OECD guideline in which such matrix effects cannot be discovered. These first results show that further investigations on the fate of chemicals in food processing have to be conducted and that real food processing steps need to be considered regulating pesticides. Thereby it is possible to fully elucidate and assess hazards caused by unknown technical metabolites.

Keywords: fate of pesticides, radioactive tracing, food processing
P21
CANCELLED
FORMATION OF MAILLARD REACTION PRODUCTS DURING ROASTING OF HAZELNUTS

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Hazelnut (Corylus avellana) belongs to the Betulaceae family and is native in Europe, western Asia and some areas of the United States [1]. Turkey is the world’s largest producer of hazelnuts (up to 650,000 tons in 2012) while Germany is the main importer (2012 up to 56,000 tons) [2]. Within a Turkish-German Food Research Network between Hacettepe University Ankara, Turkey, and the Technische Universität Dresden, Germany, chemical reactions occurring during hazelnut roasting with regard to food quality and safety are studied. In this study, N-ε-fructosyllysine (FruLys), as an indicator for the early stage Maillard reaction, and pyrraline (PYR), N-ε-carboxymethyllysine (CML), formyline (FOR) and maltosine (MAL), as products of the advanced stage Maillard reaction were quantitated in Turkish Tombul hazelnuts after laboratory roasting at temperatures between 150 and 170°C for 15 up to 60 min. The protein-bound Maillard reaction products FruLys, PYR, FOR and MAL were quantitated after a three steps enzymatic hydrolysis. CML was analyzed after reduction with sodium borohydrid and acid hydrolysis. The quantitation of the Maillard products, except PYR, was carried out via HPLC–ESI–MS/MS in MRM mode and standard addition. PYR analysis, a HPLC-UV method using a phenyl column was applied. Lysine modification was determined after acid hydrolysis with cation exchange chromatography and ninhydrin postcolumn derivatization. The amount of the Amadori-Product FruLys, main product of the early stage Maillard reaction, was 1.7 mmol/kg protein in raw hazelnuts and decreased rapidly during temperature treatment. The advanced glycation endproducts (AGEs) PYR (0.4 mmol/kg protein), CML (0.2 mmol/kg protein) and FOR (10 μmol/kg protein) were present in very low amounts in raw hazelnuts. MAL was not detectable in raw hazelnuts. During roasting, the values for the AGEs increased continuously with rising temperature and heating time until certain maximum values. Under severe heating conditions, a decrease was observed. For PYR, the main Maillard reaction product, a maximum value of 4.1 mmol/kg protein after roasting for 45 min at 160°C was measured. Degradation of Pyrraline started after 45 min at 160°C and 30 min at 170°C, indicating that both roasting temperature and heating time are important factors influencing formation and degradation of Maillard reaction products.


Keywords: Maillard reaction, hazelnuts, roasting
ENZYMATIC CROSSLINKING OF CASEIN MICELLES UNDER ALKALINE CONDITIONS

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In the present study, we analyzed the potential of enzymatic crosslinking of casein micelles under alkaline conditions in order to prepare defined structured aggregates which have the potential to be used as nanocarriers. For this, microbial transglutaminase (mTG) [EC 2.3.2.13] which catalyzes an acyl transfer reaction between protein-bound glutamine and lysine, resulting in a stable, tridimensional network, was used [1]. Casein micelles, crosslinked by mTG (8 U/g protein, 40 °C, 5 60 min) at a pH value of 7.9 were compared to samples incubated at the physiological pH value of milk (pH 6.8). The extramicellar protein fraction (analyzed via Bradford assay and gel permeation chromatography, following ultracentrifugation), particle size distribution (Dynamic Light Scattering) and reactivity of each casein (HPLC) were investigated for sample characterization. During alkalisation, a swelling of the casein micelles was observed, which initially results in a higher hydrodynamic diameter, followed by a loss of casein due to dissociation from the micelles and final disintegration of the micelles. Enzymatic crosslinking in alkaline milieu compensates the destabilizing effect of the increased pH value: the original size distribution as well as the natural percentage of extramicellar casein are readjusted. In addition, the reaction behavior of individual caseins is affected. Beside κ- and β-caseins also the α-caseins, which are located in the inner of the casein micelles, could be crosslinked by microbial transglutaminase. Our results present the possibility to modify the structure of nanocarriers like casein micelles under alkaline conditions by enzymatic crosslinking.


Keywords: casein micelles, microbial transglutaminase, milk proteins, nanocarrier

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INFLUENCE OF THE CASEIN MICELLE STRUCTURE ON THE MAILLARD REACTION

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The caseins from bovine milk represent approximately 80% of the total milk proteins. They mainly consist of the \( \alpha \)S1-, \( \alpha \)S2-, \( \beta \)- and \( \kappa \)-caseins and associate in colloidal aggregates, the casein micelles, ranging from 50 to 500 nm [1]. During the heating of milk, several reactions, including the Maillard reaction, occur [2]. Glycation reactions between carbonyl groups of reducing sugars and amino acid side chains have been investigated in a number of studies for nonmicellar caseinate. These studies mainly have shown the formation of the Amadori compound N\( \varepsilon \)-fructosyllysine, representing a marker for the “early” stage of the Maillard reaction, but also, in significant smaller amounts, the formation of the advanced glycation endproducts (AGE) N\( \varepsilon \)-carboxymethyllysine (CML) and pyrraline in caseinate and \( \beta \)-casein model solutions [3,4]. It is conceivable that defined hydrophobic and hydrophilic regions within the micelles may influence the course of the Maillard reaction at individual casein molecules. In the present study, the casein micelles were isolated by ultracentrifugation at 100,000 \( \times \) g (1 h, 20°C) and resuspended in synthetic milk ultrafiltrate. After heating the suspensions of micellar casein and, for comparison, also of nonmicellar sodium caseinate in the presence and absence of glucose for 0 - 4 h at 100°C, the resulting Maillard reaction products N\( \varepsilon \)-fructosyllysine, CML and pyrraline were quantitated by LC-ESI-MS/MS and HPLC-UV/DAD. The formation of Amadori products were in the same range for both micellar and nonmicellar caseins, indicating that reactive amino acid side chains within the micelles are accessible for glucose in a comparable way as in nonmicellar casein. However, significant differences were observed concerning the formation of the AGEs CML and pyrraline. CML could be quantitated in significantly higher amounts in nonmicellar casein, whereas in the micelles the pyrraline formation was significantly increased. As it is known that pyrraline is formed predominantly in food with lower water content, the higher formation of pyrraline within the casein micelles could be the consequence of the proposed irregular water distribution [5]. It is conceivable that partial “dry” areas exist within the micelles, in which pyrraline was formed preferentially. From the behavior of the casein micelles during glycation, more details can be learned about the casein micelle structure and could be incorporated in the discussions about the micelle models.


Keywords: casein, micelle, Maillard reaction
P25

BIODEGRADABILITY OF TOXIC COMPOUNDS OF SEEDS FROM BRAZILIAN FRUITS AFTER NATURAL SOLID-STATE FERMENTATION

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Brazil produces a great variety of tasty endemic fruits, very popular among both local population and tourists. Those fruits are commonly consumed fresh but in the last few years, several industrial derivatives such as ice-creams, jellies, liqueurs and desserts began to appear in the markets, increasing opportunities for expansion of food industries and exportation to other countries. Previous researches revealed the presence of toxic compounds inside the seeds of some of those fruits, similarly as it happens in other common fruits, such as peaches, cherries, plums and almonds. The risk of intoxication is minimal when those fruits are consumed fresh, but it significantly increases during industrial derivatives manufacturing, since seeds might be broken during automatic pulp removal. Toxins of seeds from fruits known as Araticum (Annona crassiflora), Cagaita (Eugenia dysenterica) and Mangaba (Hancornia speciosa), have been recently studied in order to characterize their toxic potential, chemical structure, thermal sensitivity and action mechanisms. This work aims to study biodegradability of seed toxins after natural fermentation with both mixed cultures and isolated endophytic micro-organisms: two bacteria, two molds and one yeast, preliminarily identified as Coccus, Lactobacillus, Penicillium, Aspergillus and Saccharomyces, respectively. Solid-state fermentation was performed adding 5 ml of mixed cultures or isolated micro-organisms onto 5 g of each toxic seeds previously crushed. Seed toxicity after fermentation was evaluated by bioassay with Artemia salina. Mixed culture fermentation reduced toxicity values 80% (Araticum), 78.3% (Cagaita) and 81.7% (Mangaba). Fermentation with both isolated bacteria caused a significant toxicity decrease in Mangaba seeds only, but did not show any effect on Araticum and Cagaita seeds. Mold-1 induced degradation of Cagaita and Mangaba toxins, while Mold-2 enabled detoxification of all three studied seeds. Saccharomyces fermentation did not significantly reduced seeds toxicity, but the presence of toxic compounds apparently did not affect yeast growth and neither ethanol production. These results evidence de presence of toxins with different structure and action mechanisms, and consequently, with different sensitivities to biodegradation, being the Mangaba seed toxins the most sensitive and Araticum toxins the most resistant. From the safety point of view, these findings could be useful during manufacturing of industrial derivatives of those fruits, suggesting that in the event of seed breaking during pulp removal, fermented products could contain reduced amounts of toxic compounds.

Keywords: food toxins, biodegradation, bioassay, kernels, endophytics

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Support of Small farmers and New Agricultural Cooperatives that are created in Georgia after 2013 by adoption of new Law on Agricultural Cooperatives in Georgia by the Parliament of Georgia was a major step to forward of the Agrarian Reforms in Georgia. All food providers in Georgia are contributing only 20 % of local production and import amount is 80%, nevertheless the role of small/family farming does not appear to be central in the debate on the future of agriculture and food and nutrition security and it seems actually minor compared to large farm structures and relative benefits of economies of scale, which largely dominate on the local markets. Small farmers Ag Cooperatives have provide additional environmental and social sustainability services. These include their ability to maintain more diverse mixed production systems and consequently preserve biodiversity, their role of labor-inclusive family farms but also potential generators of new jobs, their contribution in maintaining an adequate rural/urban balance and enabling territorial development their role in soil and natural resource protection/preservation

Nevertheless, it is a fact that the environmental, social, cultural and organizational fragmentation of small Ag Cooperative’s limits their ability to cope with economic (market dynamics) and environmental (climate change) jeopardies, which overall makes the small Farmers exist systems week and un-resilient, if not adequately supported. The reasons for this current scenario can be searched in political, social, economic and environmental determinants. Among these, the inability to connect the small/family farm to an organic and structural developmental process that looks at the system rather than single part(s) of it has been one major constraint. This shortcoming has confined small farms to remote/scattered entities that, at the very best, need to be helped in producing their own food, because they do not have much chance to exit from that status and to be integrated in a global equitable development. How improve Rural Advisory and Extension Systems for better outcomes to make Ag Cooperatives more stable and structurally developed are central role of RAS Systems for ensuring job creation, societal growth and overall, Food and Nutrition Security. Many State Supported programs and projects has been attempted to improve and develop in Georgia Ag Cooperatives systems through a Technology Transfer programs and targeted projects. For this working group we will put in place a bottom-up system in which Ag Coops will design their industry development by analyzing challenges and opportunities ahead of them. For this to be accomplished, the foresight component will have a pivotal role in the structure and implementation of Climate Smart Agriculture, Innovative Technologies and Strong Advisory and Policy Analyses Supports.

Keywords: small farmers, sustainability, agricultural cooperatives, food security, Georgia, green economy
Polysaccharides are the major components of green coffee beans. The most abundant ones are galactomannans, followed by arabinogalactans. Although it is known that galactomannans and arabinogalactans are modified during the roasting process, namely by reaction with proteins, chlorogenic acids, and sucrose, leading to the formation of melanoidins, the exact structures of the roasting-induced compounds derived from coffee polysaccharides are far to be completely elucidated. This is due to their diversity and the higher structural complexity of the new structures formed [1].

The use of simple model systems, comprising few populations of molecules able to provide information concerning the specific reactions occurring inside the coffee beans, together with mass spectrometry analysis, allow to obtain an overall view of the structural modifications in coffee polysaccharides promoted by roasting. Based on this thesis, oligosaccharides structurally related to the backbone of galactomannans, (β1→4)-D-mannotriose, and the side chains of arabinogalactans, (α1→5)-L-arabinotriose (Ara3), alone or in mixtures with 5-O-caffeoylquinic acid, the most abundant chlorogenic acid in green coffee beans, and dipeptides used as models of proteins, were submitted to dry thermal treatments, mimicking the coffee roasting process [2-5]. The oxidation of Ara3 induced by hydroxyl radicals was also studied, since these radicals seem to be involved in the modification of the polysaccharides during roasting [6]. New structural modifications induced by thermal and oxidative treatment of the model compounds were identified by mass spectrometry-based analytical strategies, either by direct analysis or coupling with high-performance liquid chromatography. Roasted coffee polysaccharide-rich samples were also analysed, validating the conclusions achieved with the model systems.


Keywords: polysaccharides, roasting, structural changes, melanoidins, mass spectrometry

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P28 FORMATION OF 3,4-DIDEOXYGLUCOSONE-3-ENE IN BEER THROUGH 3-DEOXYHEXOSONE INTERCONVERSION

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Heating and storage of food leads to sugar degradation with the formation of 1,2-dicarbonyl compounds, among which the hexose degradation products 3-deoxyglucosone (3-DG) and 3-deoxygalactosone (3-DGal) predominate [2]. The highest concentrations of 3-DGal can be found in beer and malt beer, and its formation through 3-deoxyhexosone interconversion from 3-DG has been proposed [1,2,3]. This study was undertaken in order to get further insight into the mechanism of formation of 3-DGal and the relevance of intermediate 3,4-dideoxyglucosone-3-ene (3,4-DGE). 3,4-DGE is a cytotoxic compound that has already been quantitated in heat-sterilized peritoneal dialysis solutions [4,5]. First, wort boiling was simulated by incubating 3-DG and 3-DGal in a mash buffer for up to 2 h at 70-100 °C in the presence and the absence of amino acids. Quantitation of 1,2-dicarbonyl compounds was performed after derivatization to the stable quinoxalines by RP-HPLC-UV on a phenyl column or RP-HPLC-MS/MS, respectively [2,3]. A survey of commercial beer and malt beer samples was performed thereafter. Heating of 3-DG and 3-DGal under the conditions of wort boiling leads to the accumulation of intermediate 3,4-DGE. The latter compound is rehydrated to 3-DG and 3-DGal on prolonged heating, what can explain the unexpectedly high concentrations of the galactose derivative 3-DGal in beer. 32 beer samples of different types (Pilsner, dark, wheat, and malt beer) showed strongly diverging concentrations of 3-DG (18–120 mg/L) and 3-DGal (4–40 mg/L). Only the (Z) derivative of 3,4-DGE was found to be of importance both in model systems and in commercial beers. Its concentration was ca. 10% that of 3-DGal (0.3-4.8 mg/L). All products were most abundant in malt beer. However, the ratio of 3-DG to 3-DGal was different in model systems (ca. 12) and commercial samples (2.5–4). 3-Deoxyhexosone interconversion is an important chemical reaction in foods such as beer and malt beer leading to the formation of relatively high concentrations of 3-DGal and 3,4-DGE. Differences in the extent of 3-deoxyhexosone interconversion can be a key to the understanding of aroma alterations during storage of beer.


Keywords: Maillard reaction, beer, caramelization, 3,4-dideoxyglucosone-3-ene, 3-deoxyglucosone
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EXAMINATION OF ACRYLAMIDE IN MILK WITH DIFFERENT TYPES OF COFFEE

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Acrylamide in foods is produced by Maillard reaction of asparagine and carbonyl (created by reducing sugars) at temperatures above 120°C, although asparagine heat may itself be converted to asparagine acrylamide with decarboxylation and deamination, which in practice can’t happen without the presence of sugar. Redox reaction of acrylamide with potassium permanganate, resulting with changes in colour is used as a base method, supported by spectrophotometry measurements of sample absorbance at 355 nm. Acrylamide (AA) migration from different types of coffee (1- ground coffee, 2- instant coffee and 3- cocoa) to milk drinks. Acrylamide was determined in 10 samples content of 100 ml long-life milk (pasteurized) with 0.5 g of three types of coffee, obtained results of concentration, C are: C1AA = 63.53 mg/l, RSD = 9.82%; C2AA = 136.30 mg/l, RSD = 5.77% and C3AA = 24.93 mg/l, RSD = 5.93% respectively, quantities much lower than those found in pure coffee extracts, which means that milk, used as a dilution factor in everyday habits, leads to reduced acrylamide daily intake. Food that contributes most to acrylamide intake are treated potatoes, bakery products and other cereal products, but this research shows that are also coffee, cocoa powder, and instant coffee. It is a concern for many institutions, aware about carcinogenicity and toxicity that acrylamide can provoke to human health.

Keywords: acrylamide, milk, coffee, cocoa, instant coffee
BIOGENIC AMINES IN DIFFERENT CHEESE VARIETIES RETAILED IN AUSTRIA

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High concentrations of biogenic amines (BA) can be found due to microbial activity intrinsic to typical fermented foods such as wine, fermented meat and especially cheese. During cheese ripening, accumulated free amino acids may act as precursors for the conversion into BA mostly affected by bacterial decarboxylases of a contaminating microflora. Thus, BA in food are of main concern in relation to food spoilage and food safety aspects. The objective of this study was to analyse BA concentrations in various commercial cheese samples (n = 151) representing most common cheese varieties using UHPLC. In general, cumulative BA levels varied to a great extent with exceptional samples having amounts up to 150-300 mg/100 g cheese (e.g., Tiroler Graukäse with 313 mg/100 g or Tiroler Almkäse with 185 g/100 g), whereas only 5% of the analyzed cheeses showed total concentrations higher than 90 mg/100 g (median 5.7 mg/100 g). Regarding the most relevant biogenic amines, histamine was found in 79% of all samples, with maximum concentrations for Tiroler Almkäse (116 and 82 mg/100 g), but only 5% of the cheeses had a histamine level above 17 mg/100 g (median 0.9 mg/100 g). For tyramine (72% occurrence), highest values were found for Algunder Graukäse (160 mg/100 g), Tiroler Almkäse, French raw milk cheese, Olmützer Quargel or Harzer cheese (each ~50 mg/100 g; median 1.0 mg/100 g). Putrescine was detected in 70% of the cheeses (up to 80 mg/100 g for some acid-curd cheeses; median 0.6 mg/100 g). Cadaverine was found in 47% of the samples, with highest concentrations for Harzer cheese and Olmützer Quargel (127 and 75 mg/100 g, median 0.2 mg/100 g). Tryptamine had the lowest occurrence (15%) and a median concentration of 0.3 mg/100 g. In conclusion, high (and toxicologically critical) levels of BA are definitely not associated with a certain type of cheese, but may vary depending on a large number of different incalculable factors (e.g., hygiene during cheese manufacturing, number and class of contaminants, degree of proteolysis in cheese).

Keywords: biogenic amines, cheese varieties, UHPLC, histamine, tyramine
TRANSFER OF CAROTENOIDS FROM SUPPLEMENTED FEED INTO EGGS

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Carotenoids are mostly yellow and orange pigments found in plants, some fungi, algae and microorganisms, they are significant for human health because of their important biological properties. Humans and animals cannot synthetize carotenoids so it is crucial to include them into the diet. Some of carotenoids are provitamins A, effective antioxidants or important for eye health. For example, lutein and zeaxanthin, present in macula lutea, are known for reducing macular degeneration. These two xanthophylls are the most abundant carotenoids in egg yolk. This makes eggs a valuable source of bioavailable lutein and zeaxanthin. Eggs are also an excellent source of complete protein, omega-3 and omega-6 fatty acids, bioavailable iron and vitamins. It is known that carotenoids can be transferred from feed into animal tissue and products such as salmon, poultry meat or eggs. The influence of feed supplementation on carotenoid content in egg yolk was investigated. Natural carotenoids sources which can be added into chicken feed are especially petals of marigold flowers and some algae, for example Chlorella and Scenedesmus.

The aim of this research was to determine the content of carotenoids in egg yolks from laying hens which were fed for one month by feed fortified with marigold petals, algae (Chlorella, Scenedesmus, Japonochytrium, Schyzochytrium, Trachydiscus, Ulkenia) or feed fortified by yellow pigments Xamacol. An increased content of carotenoids and a positive change in color was expected in egg yolk samples when fortified feed was used.

For the determination of carotenoid content high performance liquid chromatography coupled with a diode array detector (HPLC/DAD) was used.

Acquired data showed that the feed with marigold petals and algae Chlorella caused a significant increase of carotenoids (mainly lutein) in yolk samples. Unlike the shiny yellow color of these samples, the color of the yolks from hen fed by special feed with Xamacol is intense orange but without corresponding carotenoids content. In these samples, canthaxantin, a pigment originally absent in eggs, was found.

Keywords: carotenoids, feed, egg yolk, HPLC/DAD

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THE INFLUENCE THERMAL STABILIZATION ON POPPY SEEDS

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Poppy seeds obtained from Papaver somniferum L. plants are widely used in the Central and Eastern Europe as fillings of cakes and in desserts, on a top of various dishes, and/or to produce edible oil. With regards to a possible presence of narcotic opium alkaloids, public concern regarding health risks associated with a dietary exposure to these hazardous secondary metabolites exits. Overall, more than 50 different opium alkaloids occur in poppy plants, they are concentrated mainly in poppy capsules. Improper harvesting and/or processing practices may cause contamination by these alkaloids on the surface of poppy seeds. In the recent years, Czech Agriculture and Food Inspection Authority has notified of a numerous cases of mixing high quality food poppy seeds with those originated from ‘technical’ plants with high content of opium alkaloids grown primarily for pharmaceutical purposes. To reduce elevated levels of opium alkaloid, markers of such illegal practices, washing or soaking in acidified water, sometimes in combination with grinding or ‘thermal stabilization’ can be used. However, such treatments typically result in reduction of sensorial quality and/or shelf life of the poppy seeds. The purpose of the presented study was to document the dynamics of changes induced in opium alkaloids profiles and metabolome fingerprints in poppy seeds by holding them for a various time periods at 100°C. The possibly identified markers of this process are assumed to help in recognition of adulteration practice. Ultra high performance liquid chromatography coupled with tandem high resolution mass spectrometry (UHPLC-HRMS/MS) was used for this purpose.

Keywords: opium alkaloids, poppy seeds, fingerprint, UHPLC-HRMS/MS

Acknowledgement: This work was supported by the “National Program of Sustainability I” - NPU I (LO1601 - No.: MSMT-43760/2015) and the specific university research (MSMT No 20-SVV/2016).
Galactolipids are biologically active polar lipids, basically a diacylglycerols with one or two bound galactose units. According to the number of bound molecules of galactose, they can be divided into two main groups: monogalactosyldiacylglycerols (MGDG) and digalactosyldiacylglycerols (DGDG). A large number of individual galactolipids exist, they differ in fatty acids bound in their molecule.

It has been suggested, that galactolipids are a group of compounds responsible for beneficial effect of rose hips and food supplements based on rose hips on human health. Clinical studies, indeed, have shown that galactolipids may help patients suffering from inflammatory diseases like osteoarthritis in a way of pain reduction, symptom alleviation and prevention.

The presented study was focused on a search for new, other than rosehips, sources of galactolipids. Using the ultra performance liquid chromatography coupled with high-resolution tandem mass spectrometry (U-HPLC-MS/MS, Synapt G2, Waters) various plant matrices like cannabis were analyzed. Several samples of food supplements already available at the market were also tested. In total, 43 different galactolipids, 24 MGDGs and 19 DGDGs, were identified in examined samples. The generated data confirmed that green parts of plants like ginkgo biloba or cannabis are comparably good sources of galactolipids as rose hips. High content of galactolipids was also confirmed in food supplements made from microalgae like chlorella or spirulina, which have never been reported to contain galactolipids. The follow up study will be focused on a more in-depth investigation of these ‘novel’ sources of galactolipids, including their isolation and bioactivity characterization.

Keywords: galactolipids, biological activity, plant matrices, microalgae, U-HPLC-MS/MS

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BIOLOGICALLY ACTIVE CONSTITUENTS IN HEMP OIL AT THE CZECH MARKET

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Cannabinoids represent a group of biologically active chemicals naturally occurring in Cannabis plants. These compounds pass into the cannabis derived products (hemp oil, hemp seeds) and are also present in products containing hemp or hemp extracts (CBD-oil, cookies, lollipops, etc.). Given the increasing demand for cannabis and cannabis products, it is necessary to monitor the cannabinoid content in these products (especially the level of psychotropic Δ9-tetrahydrocannabinol (because of the legislative limit). In the case of CBD-oils, it is also necessary to control the content of CBD content declared by the manufacturer. For the analysis of cannabinoids, we used the method of ultra-high performance liquid chromatography coupled with a high resolution mass spectrometric detector (UHPLC-HRMS). Furthermore, we focused on the analysis of fatty acids in hemp oils. Hemp oil is a relatively expensive commodity, and due to its optimum ratio of ω6 / ω3 (3:1) fatty acids is becoming an increasingly popular foodstuff. The aim of this/our study was to determine whether the composition of fatty acids in hemp oils matches the expected values and to reveal if there is any adulteration by less valuable plant oils. The oxidation stability in relation to CBD content was assessed, too.

Keywords: cannabinoids, hemp oil, fatty acid, UHPLC-HRMS

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AMBIDENT MASS SPECTROMETRY EMPLOYING DIRECT ANALYSIS IN REAL TIME (DART) IONIZATION SOURCE FOR MONITORING OF LARD AUTOXIDATION

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There is a considerable interest in the characterisation of thermos-oxidative properties of the unsaturated fatty acids, their esters and kinetics of their autoxidation. Unsaturated fatty acids (free and especially bounded in triacylglycerols) are the major components of vegetable fats. Their peroxidation does not only deteriorate flavour and taste of oil containing foods, but also causes e.g. mutagenesis, heart diseases and carcinogenesis. Addition of antioxidants is the most common practice used to delay fat oxidation. Although synthetic antioxidants are widely used in the food industry, researchers have recognized the need to identify new natural antioxidants for use as safe additives in the food industry. From many antioxidants that have been isolated from vegetables so far, the extracts from rosemary leaves have shown the highest activities and are regarded as natural alternatives to synthetic antioxidants.

In this study, the Shaal test as a standard test for assessment of oxidative stability and new approach represented by direct analysis in real time ionization coupled with high resolution mass spectrometry (DART-HRMS) were used. The assessment of oxidative changes in lard samples influenced by addition of various antioxidants (tocopherol, commercially available rosemary extract and in-laboratory prepared extract of dried rosemary leaves) was performed. In oxidized pork lard samples, both primary and secondary low molecular weight oxidation products of triacylglycerols were observed and tentatively identified based on accurate mass measurement.

Addition of antioxidants in samples of fat extended significantly the induction period of lard increasing the oxidative stability of fat. For samples which were incubated in an oven, induction period of lard with added tocopherol was prolonged by 18 days, commercial rosemary extract by 57 days, extract prepared from dried rosemary plants at a concentration of 6.25 g/kg by 112 days, 12.5 g/kg by 153 days compared to pure lard without the addition of antioxidants.

Keywords: Direct analysis in real time (DART), mass spectrometry, lard, autoxidation, natural antioxidant

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CHANGES IN LIPID FRACTION OF CZECH CARP (CYPRINUS CARPIO L.) DURING A LONG-TERM STORAGE

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The growing living standards of modern society in recent years are, unfortunately, linked to increased incidence of cardiovascular disease, especially atherosclerosis. A part of other factors, diet is affecting the quality and condition of cardiovascular system. In this context, a sufficient intake of omega-3 fatty acids is considered as beneficial. While marine fish and products thereof are the major sources of these compounds, their amount in fresh water fish is fairly lower. In the Czech Republic, carp (Cyprinus carpio L.) is the most commonly farmed fish. To increase its nutritional value, feeding stuffs enriched by plant oils with high content alfa-linoleic acid have been used to produce ´omega carps´. The objective of the current study was to assess a large set of carps available at the Czech market and those from feeding experiments (provided by Faculty of Fisheries and Protection of Waters University of South Bohemia in České Budějovice) in terms of fatty acids composition and to monitor the oxidative changes of lipid fraction of fillets differing in unsaturated fatty acids content during their storage (-18°C). The products originated from oxidized lipids which may have an adverse impact on sensorial properties and, possibly, on consumers´ health were evaluated.

Keywords: Cyprinus carpio L., lipid fraction, oxidation, frozen storage, DART-HRMS

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PRODUCTION OF CHICKEN MEAT AND EGGS WITH ADDED VALUE - OMEGA-3 PUFA AND ORGANIC SELENIUM ORIGINATING FROM MICROALGAE

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Polyunsaturated fatty acids (PUFAs) with long chain (C > 18), which cannot be synthetized by higher plants, are essential especially for the development of brain and eyes correctors in children and for cardiovascular health in adults. If these PUFAs would be incorporated into the food chain (livestock are fed with additives containing PUFAs), production of foods e.g. meat, eggs or milk enriched with these health beneficial substances is feasible. The consumption of such functional foods may then replace the currently commonly used dietary supplements. Besides flaxseed, which contains mainly PUFAs with shorter chain (α-linolenic acid), is the only commercially available source of long-chain PUFAs fish oil. However, this commodity is not very convenient for the production of OMEGA foods. Nevertheless, it is known that some microalgae are capable of synthesizing PUFAs. Eustigmatophyte microalgae with nutritionally balanced composition of PUFAs and other compounds with antioxidant effects seem to be perspective. In addition, microalgae, which are exposed to selenium in the form of selenite, are able incorporate that element to its cells and organoselenium compounds with higher biological availability are formed. The aim of this study was to develop new feed supplements for poultry, based on microalgae and flaxseed, with high content of PUFAs and organic selenium compounds and other bioactive substances. It will improve health and quality of breeds and new functional foods with higher content of PUFA and selenium could be produced. As a promising source of EPA eustigmatophyte microalgae Trachydiscus minutus with a high growth rate and productivity, excellent biotechnological parameters, resistance in large-scale cultivation and resistance against contamination, was identified. Microalgae Chlorella sp. cultivated in a medium containing inorganic form of selenium was selected as a good source of organic selenium. Total selenium content was 650 μg/g (59% bonded in selenomethionine and 3% in selenocystine). In our experiment, various ratios of flax seed and algae (Trachydiscus, Chlorella) added in to the feed were tested and parameters of lipid metabolism in poultry, conversion rate and biotransformation of PUFAs and biotransformation of selenium in chicken meat and eggs were monitored. As regards eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA), eggs containing higher amount of DHA can be labelled as “increased omega-3 fatty acids” (Commission Regulation EC 1924/2006 and 432/2012). Regarding the increased content of alpha-linolenic acid (ALA), which was presented in meat due to the supplementation with flax seed (1%), can be also labelled as “increased omega-3 fatty acids”. The content of EPA and DHA in a chicken muscle was very low and corresponded to the content of EPA + DHA in the meat supplemented only with flax seed. Addition of Trachydiscus algae therefore had no effect on a content of polyunsaturated fatty acids with long chain.

Keywords: PUFA, microalgae, organic selenium, functional food

Acknowledgement: This study was supported by the Technology Agency of the Czech Republic, project No TE01020080, Centre of competence for bio-refining research, and project No TA03011027 Innovative functional food and feed additives and with content of Omega-3 poly-unsaturated fatty acids produced by Trachydiscus minutus microalgae.
HERBAL TEAS: POTENTIAL CONTAMINATION BY PLANT ALKALOIDS

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Plant alkaloids are secondary metabolites produced by a wide variety of plant species. The present study is focused on pyrrolizidine, tropane, quinolizidine, and ergot alkaloids which can contaminate food crops when alkaloids producing weeds are co-harvested. The main alkaloid producers are plants of Brassicaceae, Convolvulaceae, Solanaceae, Senecio, Fabaceae, and Claviceps family. As concerns tropane alkaloids, besides (-)-hyoscyamine and (-)-scopolamine as the main representatives, over 200 further species are known. Similarly, besides of heliotrine, motocrotaline, lycopsamine, retosine, senecionine, seneciphylline, senkirkine or their N-oxides, as the most wellknown representatives of pyrrolizidine alkaloids, approximately 600 different species have been identified. Recently, the occurrence of alkaloids in herbal teas has gained increasing attention of European Food Safety Authority (EFSA). The aim of the present study was to determine the concentrations of alkaloids levels in pre-packed teabags of herbal teas sold in supermarkets and pharmacies at the European market. Moreover, the transfer of alkaloids from dry matter to tea infusion has been assessed, which illustrates the real risk for consumers resulting from tea consumption. A simple aqueous-methanolic extraction, followed by separation on C-18 based ultra-high performance liquid chromatography and tandem mass spectrometric detection represented by triple quadrupol mass was employed.

Keywords: plant alkaloids, tea, tea infusions, risk assessment

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PRE- AND POST-HARVEST CHANGES OF S-ALK(EN)YL-L-CYSTEINSULPHOXIDES AND OTHER BIOLOGICALLY ACTIVE COMPOUNDS IN GARLIC

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The use of garlic (Allium sativum) as a spice and/or a natural remedy has a long history. Both flavor and biological activity are determined by organo-sulphur compounds, mainly S-alk(en)yl-L-cysteinsulphoxides (ACSO). A wide range of factors may have an impact on concentrations of these compounds, such as the genetic background of the respective cultivars, environmental factors during growth, and storage conditions. This extensive study aimed to characterize the differences between immature, freshly harvested and stored garlic representing various cultivars, in order to find the best one in terms of biologically active compounds content and their dynamics over the time. This knowledge is specifically important for the producers of garlic-based supplements. Within four years of study (2013–2016), more than 200 samples of Czech garlic involving 24 cultivars grown at several locations were examined. Analyses included, in addition to determination of ACSO (alliin, methiin, isoalliin and propiin) and total phenolics, also an untargeted approach, metabolomic fingerprinting. The results showed a high natural variability between harvest years and growing localities, on this account identification of the 'best' cultivar was rather difficult. During storage, an enormous increase in isoalliin content in all samples occurred. This compound is a precursor for the development of blue-green discoloration; therefore, stored garlic is not suitable for technological processing. Fingerprinting approach showed additional changes mostly in amino acids content.

Keywords: garlic, Allium sativum, S-alk(en)yl-L-cysteinsulphoxides, total phenolics, metabolomic fingerprinting

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PCR-BASED FISH MEAT AUTHENTICATION

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The most common determination of fish species is based on morphological traits. This approach faces more and more complications as the level of processing of fish flesh into products of food industry and/or complex dishes produced in gastronomy makes morphological markers less available. Another factor preventing morphological determination is the character of marine fish trade and import of this fish into landlocked countries like the Czech Republic. These are often transported in the form of frozen blocks, also devoid of morphological characteristics. It is therefore critical to have a method for species determination independent on size, intactness or level of processing of the sample, available as a versatile tool. Towards this end, methods of molecular biology based on Polymerase Chain Reaction (PCR) appear as the best tool due to their high level of sensitivity and specificity in raw as well as technologically processed fish meat, even in the form of complex food products. The presented analysis is performed as an amplification of nuclear gene encoding important protein of fish muscles parvalbumin, also known as a major allergen connected with fish consumption. Here, within the scope of Real-Time PCR (qPCR) set of primers together with fluorescent dye-conjugated probe, both specific to second intron of protein coding region of Black seabream (Spondyliosoma cantharus) were designed and tested. Specificity of this set was validated on panel of 19 different fish species representing the most common and important fraction of the spectrum of the locally traded species, i.e. for instance Carp (Cyprinus carpio), Tench (Tinca tinca), Nile tilapia (Oreochromis niloticus) and others. Efficiency of the method was determined from calibration curve based on points of five levels of DNA concentration. Quantitative PCR presented here was proven as highly efficient and specific method for Black seabream (S. cantharus) species identification.

Keywords: PCR, fish meat, authentication
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SHORT STUDY TO VERIFY OF FORMATION OF PHTHALIMIDE FROM PHTHALIC ACID AND AMMONIUM IN PEPPERMINT PLANT

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The definition of the residue of the fungicide folpet changed to the sum of folpet and phthalimide [PI] expressed as folpet [1]. The consideration of the metabolite PI is new. Besides folpet, PI is also a metabolite of other pesticides like phosmet, ditalimfos und thioclorfenphim. Especially in dried matrices like tea, herbs and tea infusion commodities, PI is often detectable without any findings of folpet. This is equally true for both organic and conventional sectors. So it is implausible to deduce these findings from the use of folpet or other pesticides. Besides that, in all samples containing PI, Relana® member labs also detected also phthalic acid anhydride [PSA] [2] with the constant proportion. Both can be formed from phthalic acid, which is a common contaminant [3] and is known as a precursor of PSA and PI. We tested the formation of PI from phthalic acid and a nitrogen source, ammonia. Nitrogen is generally very important for the growth of every plant, but in the agriculture it is absolutely necessary for fast growing leafy commodities like teas, herbs etc. [4]. To avoid the influence of possible contaminations, we worked with deuterated phthalic acid. As a source of ammonia we used urea. The application was done through the soil. Five days later after the application, we harvested the peppermint leaves and analyzed a part of them for PI D4. We could only find a small traces of the PI D4 (< 0.01 mg/kg) in fresh leaves. Another part of the leaves was dried by 60 °C for ca. 1 hour. We found 0.18 mg/kg PI D4 in dried peppermint leaves. One possible source of PI in dried leafy commodities is phthalic acid. With intensive nitrogen fertilizing and additional drying (dehydration), the phthalimide formation is possible.

(1) Regulation (EU) 2016/156 of 18 Jan. 16
(2) Relana®, position papers 16-03, “phthalimid: metabolite or unavoidable artefact”

Keywords: phthalimide, phthalic acid

Acknowledgement: colleagues from Thermo Fisher Scientific GmbH Im Steingrund 4 - 6/63303 Dreieich/Germany For the HR-GC-MS (Orbitrap) for structure confirmation
WHEY PROTEIN INTERACTIONS WITH BERRY TANNIN

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Dairy whey proteins are one of the highly nutritious food ingredients available for commercial use not only because they contain high concentration of all the essential amino acids compared to any other natural food protein source, but also due to the high content of branched chain amino acids that contribute to the structure of food. Beta-lactoglobulin (\(\beta\)-Lg) (50-62\% of WP) and \(\alpha\)-lactalbumin (ALA) (20-25\% of WP) are the most important protein in whey proteins. On the other hand, polyphenols such as procyanidins and ellagitannins are known to possess significant binding affinity to proteins. The binding process leads to the formation of soluble and insoluble protein-polyphenol interactions, that may affect the quality of protein containing food. This research aims to elucidate antioxidant and other protein-tannin interactions in dairy foods by using up-to-date analytical approaches to investigate oxidation, adduct formation, and binding reactions both in model solutions and in food matrices containing dairy whey proteins and plant tannins. \(\beta\)-Lg and ALA was digested by modified trypsin and the subsequent peptides were fractionated with preparative-HPLC. Three peptides, LIVTQTMK, ALPMHIR, and IPAVFK were isolated from enzymatic digestion of \(\beta\)-Lg.

Oxidation of the peptides with and without sanguiin H-6 was monitored by LC–ESI–MS for up to 7 days. Sanguiin H-6 showed radical scavenging activities toward oxidation of the selected peptides. An interaction product was found with sanguiin H-6 and peptide LIVTQTMK by using MS and supported by sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS–PAGE). An observable (haze) but unstable interaction product of sanguiin H-6 with peptide ALPMHIR, but no detectable interaction products were seen with peptide IPAVFK. The selected Peptide LDQWLCEK from ALA containing specific amino aids prone to oxidation was seen with peptide ALPMHIR, but no detectable interaction products were seen with peptide IPAVFK. The selected Peptide LDQWLCEK from ALA containing specific amino aids prone to oxidation was selected for interaction with procyanidin B2 or PF during oxidation in the ratio of peptide to tannin 10:1 and 1:1. Both procyanidin B2 and PF showed radical scavenging activities toward oxidation of the selected peptide. Several interaction products were identified between procyanidin B2 and peptide LDQWLCEK by using size-exclusion chromatography (SEC) and supported by MS. Tryptophan, cysteine, and lysine are the most likely groups of peptide LDQWLCEK to be oxidized. The higher the ratio of the procyanidin, the less and slower were the oxidized forms of LDQWLCEK generated. Moreover, procyanidin B2 protected peptide LDQWLCEK from oxidation and degradation of during the oxidation procedures, whereas peptide LDQWLCEK also prevented procyanidin B2 from degradation. Tryptophan (W) and Lysine (K) might be the amino acid prone to interact with procyanidin B2. Larger molecular size interaction products were generated during the oxidation most likely due to crosslinking. Thus, protein-tannin interaction does take place during oxidation leading to both degradation and interaction products.

Keywords: peptides, tannins, protein-phenolic interaction, protein oxidation, LC-ESI-MS
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PLASMA LIPIDOME PROVIDES A CLEAR MESSAGE ON PARENTERAL NUTRITION

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Full parenteral nutrition is a way of keeping alive patients with severe conditions such as short bowel. However, the process poses not only inconvenience but also a health risk as the patients are constantly in a septic state. To this day no information exists if the process of metabolizing nutrients acquired directly from plasma differs from that in normal state (healthy patients). For this purpose, non-targeted approach based on supercritical fluid chromatography-high-resolution mass spectrometry (SFC-HRMS) was employed. The data obtained were evaluated both by supervised (PCA) and supervised (OPLS-DA) multivariate methods. The differences observed between patients and control group were mainly caused by compounds rich on polyunsaturated fatty acids originating from fish oils used for production of nutritional emulsions. After eliminating this influence, the differences between patients and control groups were still observable. However, the identification of such compounds (biomarkers) is rather hard except for their probable elemental composition. With regards to a possibility to get a more in-depth insight into metabolic processes in respective patients, this challenge (biomarkers structure identification) will be addressed in follow-up studies.

Keywords: high resolution mass spectrometry, supercritical fluid chromatography, parenteral nutrition

Acknowledgement: This work was supported by the Operational Programme Prague - Competitiveness (CZ.2.16/3.1.00/21537 and CZ.2.16/3.1.00/24503) and by the “National Program of Sustainability I” - NPU I (LO1601 - No.: MSMT-43760/2015.
In food industry, the demand for liquid syrups at the expense of sucrose has increased in last decades. Irrespective of numerous technological and economical benefits, the massive use of fructose-containing sugar sweeteners is connected with some negative nutritional implications. One of the potential drawbacks is higher formation rate of reactive carbonyl species (RCS), which arise mainly from reducing carbohydrates. Among the most reactive RCS rank carbaldehyde derivatives and alpha-dicarbonyl compounds in particular. Their presence in foods is associated with certain risks such as damage of macromolecules with glycation mechanisms or mutagenic activity. However, the extent of metabolic transfer of these reactive substances into the body, which results in direct risk of in vivo carbonyl stress, is often overestimated. In this work, RCS levels were evaluated in carbonated beverages with various sugar sweeteners, in the syrups themselves, in syrups used as sweeteners in kitchen or as nutraceuticals, in honey, and other products. The alpha-dicarbonyl compounds were determined by derivatisation with o-phenylenediamine and analysed with high-performance liquid chromatography on C18 or phenyl RP stationary phases and diode array detection. We investigated the relationships between the content of alpha-dicarbonyl compounds, carbaldehydes and active-methylene reducing compounds on the one hand and the decrease of saccharides and redox potential on the other. Within the complex reaction pathways of sugar caramelization, an assessment of relative importance of parent sugar, pH of beverages, storage time and other conditions on RCS levels and the relative (trans)formation rates was performed. The data revealed that the kind of sugar sweetener may not be the deciding factor determining the levels of alpha-dicarbonyl compounds in carbonated soft drinks. Their concentration and profile is significantly affected also by pH of beverages, storage conditions, access of oxygen and storage time. Levels of alpha-dicarbonyl compounds found in soft drinks were comparable to those in the corresponding syrups. Since the concentration of sugars in soft drinks amounts to around 10 %, it is evident that the concentration of alpha-dicarbonyl compounds increases several times during manufacture and storage of soft drinks. Moreover, relatively more fragmentary alpha-dicarbonyl compounds were present in carbonated drinks compared to syrups. The results confirmed that the kinetics of sucrose inversion and 3-deoxyhexos-2-ulose (3-DG) formation/transformation in carbonated soft drinks are differently pH-dependent. The formation rate of 5-(hydroxymethyl)furan-2-carbaldehyde (HMF) was higher in soft drinks with fructose syrups than with the glucose ones, which indicates probable easier pathway via fructofuranose dehydration than via 3-DG from glucose.

**Keywords:** fructose syrups, soft drinks, caramelization, alpha-dicarbonyl compounds, HMF
METHYLGLYOXAL AND DIHYDROXYACETONE PRESENT IN MANUKA HONEY (LEPTOSPERMUM SCOPARIUM) ARE INHIBITORS OF JACK BEAN UREASE

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Manuka honey contains methylglyoxal (MGO) and dihydroxyacetone (DHA) in amounts of up to 700 and 1600 mg/kg, respectively. Both compounds are found in significantly lower amounts in non-Manuka honeys (1). MGO is responsible for the exceptional antibacterial activity of Manuka honey against pathogenic organisms. The gram-negative bacterium *Helicobacter pylori* colonizes the human stomach and causes chronic inflammation or gastric ulcers. The enzyme urease is an important virulence factor of *Helicobacter pylori*. It catalyzes the reaction of urea to carbon dioxide and ammonia, which neutralizes the acidic environment of the stomach. Manuka honey inhibits *Helicobacter pylori* growth in-vitro (2). Until now, little is known about the honey compounds and the mechanism responsible for the inhibition. The aim of the study was to characterize the effect of the compounds MGO and DHA and commercial honeys, including Manuka and non-Manuka varieties, on urease. Urease from jack bean (*Canavalia ensiformis*) was used for the studies. A new enzymatic assay based on photometric detection of ammonia after the reaction with ninhydrin at 440 nm was developed to study urease activity and inhibition. MGO and DHA were identified as urease inhibitors with IC₅₀ values of 2.8 and 5.0 mM, respectively. Manuka honey with naturally present MGO and DHA, inhibited urease dose-dependently. Inhibition of 50% of enzyme activity was achieved with 5.5% solution (w/v) of commercial Manuka honey containing MGO 595 mg/kg and DHA 1549 mg/kg. Comparable inhibition of urease was found for aqueous solutions of MGO and DHA. Non-Manuka honeys and artificial honey, which lack MGO and DHA, showed significantly less urease inhibition with IC₅₀ values of 15 to 30% (w/v). Moreover, the inhibitory effect of Manuka honey was significantly reduced after the addition of glyoxalase and glutathione, which react with methylglyoxal and thus make it unavailable for urease inhibition. Therefore, the pronounced inhibition of urease by Manuka honey compared to non-Manuka honeys is mainly due to the presence of MGO and DHA. The inhibition of urease with MGO and DHA may contribute to the inhibitory effect of Manuka honey on *Helicobacter pylori*.


**Keywords:** manuka honey, methylglyoxal, dihydroxyacetone, urease, ninhydrin
BIOCONTROL OF OCHRATOXIN A DURING COCOA POST-HARVEST TREATMENTS

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Ochratoxin A (OTA) is a carcinogenic and nephrotoxic mycotoxin produced by fungal species such as Aspergillus and Penicillium. Previous studies showed that during post-harvest treatments, it is possible for cocoa beans to be contaminated by OTA which is resistant to chemical and physical treatments. This work studied the biocontrol of OTA in cocoa fermentation by using A. carbonarius, it’s a high OTA producing mold and Rhizopus a non-producing one mold. After purification on PDA medium, the conidia of A. carbonarius and Rhizopus of the same age were harvested by scratching in a solution of physiological liquid. After counting the spores at the hematometer, suspensions calibrated at 106 and 104 conidies.ml-1 were obtained by dilutions of suspensions for preparations of inoculas. Some healthy cocoa pods were inoculated only with suspensions of A. carbonarius or Rhizopus while others were co-inoculated with the suspensions of both molds. The pods thus inoculated were incubated in a climatic room with 60% relative humidity at 30°C for 4 and 8 days. After incubation, beans were extracted and OTA dosed. When the concentration in conidia of A. carbonarius was lower or similar to Rhizopus, there was no production of OTA during the first four days of incubation. However, when the conidia concentration of A. carbonarius was greater than that of Rhizopus, 36.2 μg.kg-1 of OTA was obtained after four days. But after 8 days, this content decreased to 6.2 μg.kg-1.

Keywords: Bio-control, ochratoxin A, cocoa, post-harvest, treatments

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3-MCPD (3-chloropropane-1,2-diol) and its fatty acid esters are contaminants that are formed during processing and manufacture of certain foods and food ingredients. Velíšek et al. (1978) were the first to report the discovery of MCPD esters as reaction products of hydrochloric acid with TAG and in acid-hydrolyzed vegetable protein (HVP). 3-MCPD might also be formed in the food as a result of a reaction between a chlorine source and a lipid source. This reaction is accelerated during the heat processing of foods. The project focuses on the study of reaction mechanisms leading to the formation of esters of 3-MCPD and glycidol esters of fatty acids in model systems, because the knowledge of its main roads, products and reaction kinetics (influenced by temperature, time, concentration of reactants, etc.) can help predict the concentration of esters 3-MCPD and glycidol in real matrices (food) and help find appropriate detoxification processes. In this work, we observed dependence of monopalmitine, dipalmitine and tripalmitine decomposition on temperature and water content. The model mixtures were then analyzed by gas chromatography with mass spectrometric detection.

**Keywords:** 3-MCPD esters, Glycidyl esters, Kinetics
P48 INTERFACIAL CONCENTRATIONS OF PHENOLIC ANTIOXIDANTS IN MODEL FOOD EMULSIONS: EFFECTS OF ACIDITY AND SURFACTANT CONCENTRATION

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In bulk solution, the empirical rate laws for interfacial kinetics are usually expressed in terms of the reactant concentrations at the reaction site and the treatment of chemical reactions begins with the rate law for bimolecular reactions between a substrate A and a reactant B. However, in multiphasic systems such as oil-in-water emulsions, molecules and ions are exchanged between the different regions and, after bulk mixing, the distributions of the reactants within the system are determined by their relative solubilities in the oil, interfacial and aqueous regions. Partitioning of antioxidants, AOs, in food emulsions is of particular importance because the efficiency of antioxidants to inhibit the oxidation of lipid-based emulsions depends on several factors including their nature and their concentration at the reaction site, which can be very different from the bulk concentration, making them to be more or less efficient. Determining the distribution of AOs in emulsified systems is a difficult task for two main reasons. 1) Partitioning of AOs depends on both the solvating properties of the oil, aqueous and interfacial regions of the emulsion and on their ability of solutes to form intra- and intermolecular hydrogen bonds with the solvent. Their relative contributions cannot be determined solely on the basis of the molecular structure of the AOs and thus partitioning needs to be determined experimentally for each antioxidant. 2) The physical impossibility of separating the interfacial region from the oil and aqueous regions (classical methods employed to determine the distribution of reactants in binary systems cannot be employed without disrupting the existing equilibria). As a consequence, the distribution of AOs in emulsions needs to be assessed in the intact emulsions. Here we have analyzed the effects of acidity and of surfactant concentration on the distribution and efficiency of phenolic acids in stripped olive oil-in-water emulsions stabilized with Tween 20. Most phenolic acids distribute exclusively between the water (w) and interfacial (I) regions. The partition constant values PWI values are independent of emulsifier concentration, but change substantially with acidity following sigmoidal curves with upper limits of PWI = 280 (gallic acid) and PWI = 590 (caffeic acid) at high acidity. Increasing either the acidity or the surfactant volume fraction produces substantial changes in the concentrations of AOs in the interfacial region. [1,2]


Keywords: antioxidant interfacial concentration, antioxidant efficiency, food emulsions, pseudophase kinetic model, kinetics
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