PROGRAMME OVERVIEW

Tuesday, June 7	Wednesday, June 8	Thursday, June 9	Friday, June 10
	09:00 **Conference Opening** 09:10 **NMR Development** *Chair: B. Luy*	09:00 **MRI and Diffusion I** *Chair: J.M. Bonny*	09:00 **Application/Foodomics II** *Chair: M. Spraul*
	10:45 Coffee Break, Posters	10:35 Coffee Break, Posters	10:30 Coffee Break, Posters
	11:10 **From Method Development to Application** *Chair: S.B. Engelsen*	11:00 **MRI and Diffusion II** *Chair: J.M. Bonny*	11:00 **Application/Foodomics III** *Chair: D.W. Lachenmeier*
12:00 **Registration**	12:20 Lunch, Posters	12:20 Lunch, Posters	12:15 **Closing Remarks**
	13:30 **Low Field NMR and Other Techniques I** *Chair: J. van Duynhoven*	13:30 **Application/Foodomics I** *Chair: M. Bunzel*	
14:00 **Welcome** 14:10 **Tutorials** *Chair: F. Capozzi*	15:20 Coffee Break, Posters	14:45 Coffee Break, Posters	
	16:00 **Low Field NMR and Other Techniques II** 16:40 **Method and Application** *Chair: A. Fereira*	15:30 **Company Tours** → Bruker → Max Rubner-Institut → Hoepfner Brewery	
17:30 Welcome Mixer	17:40 Finger Food, Posters		
18:30 **Meeting of Scientific Committee** *Chair: J. van Duynhoven*	19:00 **Discussion Session: Quantitative NMR** *Chair: D.W. Lachenmeier*	19:00 Conference Dinner SCHALANDER (HOEPFNER BREWERY)	

Tuesday Afternoon, June 7	
12:00	**Registration**
14:00	**Welcome**
Tutorials, *Chair: F. Capozzi*	
14:10	Introduction to Multivariate Data Analysis for NMR Spectral Data ***W. Kessler***
15:10	Fast Data Acquisition Methods ***W. Bermel, B. Luy***
16:10	Choice of MRI Methods for the Investigation of Various Food Materials ***D. Groß**, V. Lehmann, T. Oerther, K. Zick, S. Schuhmann*
16:40	Technical and Practical Aspects of PFG Diffusion Experiments with respect to Food Applications ***K. Zick***
17:30	Welcome Mixer, EXHIBITION HALL
18:30	**Meeting of Scientific Committee**, *Chair: J. van Duynhoven*, LECTURE HALL

Wednesday Morning, June 8	
NMR Development, *Chair: B. Luy*, LECTURE HALL	
09:00	Conference Opening
09:10	**Plenary:** Microscale NMR Detectors Enable Mass-Limited Spectroscopy ***J.G. Korvink***
09:55	**Invited:** NMR Analysis of Food Extracts through *para*Hydrogen Hyperpolarization ***M. Tessari***
10:25	Structure and Dynamics of D-Fructose and Related Amadori Derivatives ***M. Kaufmann**, C. Mügge, L.W. Kroh*
10:45	Coffee Break, Poster Presentations, EXHIBITION HALL
From Method Development to Application, *Chair: S.B. Engelsen*, LECTURE HALL	
11:10	**Invited:** Diffusion and Multiple-Quantum NMR: Increased Resolution for Enhanced Characterisation of Mixtures ***S. Caldarelli***
11:40	Molecular Mapping of the Amino Acid Perturbated Metabolome of *S. Cerevisiae* by means of a HPLC-NMR Offline Sliced Metabolomics Approach ***R. Hammerl**, O. Frank, T. Hofmann*
12:00	Analysis of the Compositional Changes in Muscular Tissue Thermally Processed by Quantitative Nuclear Magnetic Resonance Spectroscopy (q-NMR) ***D. Pitoux**, M. Bria, V. Achterberg, D. Lioger, H. This*
12:20	Lunch, Poster Presentations, EXHIBITION HALL

Wednesday Afternoon, June 8	
Low field NMR and Other Techniques I, *Chair: J. van Duynhoven*, LECTURE HALL	
13:30	**Invited:** Examples of Low Field NMR in Factory Process and High Pressure Process Environments *M.N. Martin, T.R. Wong, M.J. McCarthy,* ***M.P. Augustine***
14:00	A New 2D T_1-T_2 (IR-FID-CPMG) Method for the Characterization of Food and their Transformation ***C. Rondeau-Mouro****, R. Kovrlija, S. Moussaoui*
14:20	Characterisation of Emulsions by PFG-NMR ***G.H. Sørland***
14:40	Use of Temperature-Controlled Low Field ^{1}H NMR to Study Changes during Simulated Baking of a Flour-Water Model System ***G.M. Bosmans****, J.A. Delcour*
15:00	Low-Field RheoNMR: New Combination of Rheology and TD-NMR to Correlate Mechanical Properties with Molecular Dynamics in Soft Matter *V. Räntzsch, M.B. Özen, K.-F. Ratzsch, G. Guthausen,* ***M. Wilhelm***
15:20	Coffee Break, Poster Presentations, EXHIBITION HALL
Low field NMR and Other Techniques II, *Chair: A. Fereira*, LECTURE HALL	
16:00	TD-NMR as a Method to Determine and Characterize the Water-Binding Capacity of Whey Protein Microparticles *J.P.C.M. Peters, F.J. Vergeldt,* ***H. Van As****, H. Luyten, R.M. Boom, A.J. van der Goot*
16:20	Characterization of Red and White Cocoyam (*Xanthosoma Sagittifolium*) Roots, Flours and Starches during Heating by Low Field NMR ***M. Gudjónsdóttir****, A.A. Boakye, F.D. Wireko-Manu, I. Oduro*
Method and Application, *Chair: A. Fereira*, LECTURE HALL	
16:40	Rapid and Quantitative Assessment of Early Lipid Oxidation in Mayonnaises during Shelf-Life by ^{1}H-NMR ***D. Merkx****, S. Hong, A. Ermacora, J. van Duynhoven*
17:00	Automatized Determination of Ingredients in Non-Alcoholic Beverages with NMR ***S. Ackermann****, K. Dolsophon, T. Thongpanchang, I. Ruge, H. Reusch, D.W. Lachenmeier, M. Bunzel, T. Kuballa*
17:20	Time-Course Evolution of Bioactive Compounds Thermally Treated in Water ***L. Le Falher****, C. Doyen, V. Faugeras, D. Lioger, F.X. Deolarte, H. This*
17:40	Finger Food, Poster Presentations, EXHIBITION HALL
19:00	**Discussion Session: Quantitative NMR**, *Chair: D.W. Lachenmeier* *Experts: T. Schönberger, M. Spraul*, LECTURE HALL

Thursday Morning, June 9	
MRI and Diffusion I, *Chair: J.M. Bonny*, LECTURE HALL	
09:00	**Plenary:** MR Measurements of Phase Transitions Molecular Dynamics in Gels: PGSE MR, MRI and Relaxation Correlations ***J.D. Seymour***
09:45	**Invited:** Physicochemical Characterisation of Multiple W/O/W Emulsions by NMR Diffusometry and Relaxometry ***P. van der Meeren**, L Vermeir*
10:15	NMR Diffusometric Droplet Sizing in Emulsions with Murday-Cotts and Regularization Methods ***J.-H. Sommerling**, A.J. Simon, A. Haber, M. Johns, G. Guthausen, G. Leneweit, H. Nirschl*
10:35	Coffee Break, Poster Presentations, EXHIBITION HALL
MRI and Diffusion II, *Chair: J.M. Bonny*, LECTURE HALL	
11:00	Characterisation of Gel Networks by NMR Nanoprobe Diffusometry *D. de Kort, F. Hoeben, E. Schuster, N. Loren, L.Z. Hohlbein, L. Zuidgeest, M. Emondts, H. Janssen, S. Han, H. Van As, **J. van Duynhoven***
11:20	Use of Multiparametric MRM in Monitoring of the Ham Dry-Curing Process *F. Bajd, M. Škrlep, M. Čandek-Potokar, J. Vidmar, I. **Serša***
11:40	Flow Behaviour of Fat Crystal Dispersions: A Rheo-MRI View ***T. Nikolaeva**, D. de Kort, Voda, H. Van As, J. van Duynhoven*
12:00	Visualisation of Fouling Layer Formation and Flow in Ceramic Hollow Fiber Membranes Using MRI ***F. Arndt**, S. Schuhmann, G. Guthausen, S. Schütz, H. Nirschl*
12:20	Lunch, Poster Presentations, EXHIBITION HALL

Thursday Afternoon, June 9	
Application/Foodomics I, *Chair: M. Bunzel*, LECTURE HALL	
13:30	Kinetic Analysis of the Metabolism of Food Protective Cultures by *In Vitro* NMR and Chemometrics *P. Ebrahimi, F.H. Larsen, H.M. Jensen, F.K. Vogensen,* ***S.B. Engelsen***
13:45	NMR-based Metabolomics to Assess Fruit Quality *P. Schuster, P. Eisenmann, C. Mack, B. Luy, S. Kulling, M. Rist, C. Weinert,* ***C. Muhle-Goll***
14:00	Metabolic Responses of Clams, *Ruditapes Decussatus* and *Ruditapes Philippinarum*, to Short-Term Exposure to Lead and Zinc ***V. Aru****, G. Sarais, F. Savorani, S.B. Engelsen, C. Marincola*
14:15	^{1}H NMR Spectroscopy – A Tool for Authenticity Control of Wine ***R. Godelmann***
14:30	SPE-NMR: Revival of an Old Technique for the Analysis of Wine and Juice ***M. Godejohann****, Y. Jaradat, M. Spraul*
14:45	Coffee Break, Poster Presentations, EXHIBITION HALL
15:30	**Company Tours** → Bruker → Max Rubner-Institut → Hoepfner Brewery
19:00	Conference Dinner, SCHALANDER (HOEPFNER BREWERY)

Friday Morning, June 10	
Application/Foodomics II, *Chair: M. Spraul*, LECTURE HALL	
09:00	**Plenary:** Routine Application of NMR Spectroscopy in Official Food Control **D.W. *Lachenmeier***, *T. Kuballa*
09:45	**Invited:** Metabolomic Investigations of Health Effects of Dairy Products ***M.R. Clausen***, *H. Zheng, B. Amer, C.C. Yde, T. Kastrup Dalsgaard, H.C. Bertram*
10:15	Characterization of Juices from Ancient Danish Apple Cultivars by ^{1}H NMR-Based Metabolomics ***N. Iaccarino***, *C. Varming, M.A. Petersen, F. Savorani, A. Randazzo, S.B. Engelsen*
10:30	Coffee Break, Poster Presentations, EXHIBITION HALL
Application/Foodomics III, *Chair: D.W. Lachenmeier*, LECTURE HALL	
11:00	Metabolomics Analysis of Shucked Mussels' Freshness ***F. Savorani***, *V. Aru, M.B. Pisano, S.B. Engelsen, S. Cosentino, F.C. Marincola*
11:15	Untargeted Analyses of Cowpea Seeds (*Vigna Unguiculata*) Using ^{1}H qNMR Combined with Chemometrics and Solid State NMR ***E.G. Alves Filho***, *L.M.A. Silva, F.H. Larsen, E.S. de Brito*
11:30	^{1}H NMR Metabolite Profiling of Guarana Seeds (*Paullinia Cupana*) from Different Geographic Regions of Brazil ***L.M.A. Silva***, *G.S. Silva, K.M. Canuto, E.S. de Brito, R.M. Jesus*
11:45	Honey-Profiling with NMR ***J. Missler***, *G. Beckh*
12:00	Classification of the Botanical Origin of Honey by ^{1}H NMR in Combination with Chemometric Methods and New Data Fusion Approaches ***N. Gerhardt***, *P. Weller, S. Rohn, M. Ohmenhaeuser, T. Kuballa*
12:15	**Closing Remarks**

LIST OF POSTERS

NMR Development, EXHIBITION HALL, D1-D5	
D1	CLIP-ASAP-HSQC for Fast and Accurate Extraction of One-Bond Couplings from Isotropic and Partially Aligned Molecules *J. Becker,* ***B. Luy***
D2	CLIP-COSY: A Clean In-Phase Experiment for the Rapid Acquisition of COSY-Type Correlations *M.R.M. Koos,* ***J.D. Haller****, B. Luy*
D3	Residual Dipolar Coupling-Accelerated Molecular Dynamics for Structural Elucidation of Small Molecules with Increasing Flexibility ***P. Tzvetkova****, U. Sternberg, T. Gloge, A. Navarro-Vázquez, B. Luy*
D4	Cross-Linked Poly(ethylene Glycol) Diacrylate – A Universal Alignment Medium for the Measurement of Residual Dipolar Couplings ***T. Gloge****, P. Tzvetkova, L. Barner, J. Peters, B. Luy*
D5	Elucidation of Maillard Reaction Pathways by means of the Carbon-Bond Labeling Technique (CABOLA) ***O. Frank****, M. Hegmanns, T. Hofmann*
Low field NMR and Other Techniques, EXHIBITION HALL, L1-L	
L1	Rapid Method to Measure T_1 of Food Products in Single Scans ***L.A. Colnago****, T. Bueno Moraes, T. Monaretto*
L2	Starch Retrogradation Investigated by 1D and 2D NMR *R. Kovrlija, E. Goubin,* ***C. Rondeau-Mouro***
L3	Studies of the Retrogradation Process of Starch in Gels by Using Low Field NMR Method ***H.M. Baranowska****, M. Sikora, M. Krystyjan, A. Dobosz, P. Tomasik, E.M. Kutyła-Kupidura*
L4	Bread Staling: TD-NMR study via T_1-T_2 2D maps *E. Curti, E. Carini, E. Vittadini, M.F. Cobo, T. Bocher, H. Todt*
L5	Pasta Cooking: TD-NMR Study via T_1-T_2 2D maps *E. Curti, E. Carini, E. Vittadini, M.F. Cobo., T. Bocher, H. Todt*
L6	A Combined Rheology and TD NMR Approach for Determining Water Distribution in Protein Blends *B. Dekkers, D.W. de Kort, K.J. Grabowska, B. Tian,* ***H. Van As****, A.J. van der Goot*
L7	The Moisture and Oil Distribution in Tobacco ***T. Li****, Y. Zhang, P. Yang*

L8	Study of the Moisture Equilibrium of Tobacco by Using Spin-Echo Single Point Imaging Sequence ***Y. Zhang**, T. Li, P. Yang*
L9	Correlating Crystallization Kinetics and Rheological Properties of Polyethylene Using a Newly Developed Low-Field RheoNMR Combination ***M.B. Özen**, V. Räntzsch, K.-F. Ratzsch, G. Guthausen, N. Kavak, P.-K. Dannecker, M.A.R. Meier, M. Wilhelm*
Method and Application, EXHIBITION HALL, A1-A	
A1	Quantitative ^{1}H-NMR to Assist the SNIF-NMR Analysis ***R. Popescu**, O.R. Botoran, D. Costinel, R.E. Ionete*
A2	PFG-NMR Analysis of Organic Acids in Oil/Water Emulsions *N. Decourcelle, S. Guégan, F. Courand, J.-F. Le Page, A.G. Mathot, O. Couvert, I. Leguérinel, **C. Rondeau-Mouro***
A3	Improved Methods and Tools for Identification of Mixture Components by NMR ***G. Rheinwald**, S. Golotvin, S. Pol, P. Wheeler, B. Pautler, T. Salbert*
A4	Proton Quantitative Nuclear Magnetic Resonance Analysis (^{1}H q-NMR) of Various Extracts of Raw and Thermally Processed ("Roasted") Coffee (*Coffea arabica* L.) Beans: Influence of the Extraction Process *G. Nord, E. Hamon, D. Aoudé-Werner, H. This*
A5	Determination of Fish Oil Quality by ^{1}H NMR Spectroscopy and Multivariate Statistics ***E. Giese**, O. Winkelmann, S. Rohn, J. Fritsche*
A6	^{1}H NMR Spectroscopy and Chemometrics Evaluation of Non-Thermal Processing of Orange Juice ***E.G. Alves Filho**; L.M.A. Silva; F.H. Larsen; E.S. de Brito*
A7	NMR Metabolomic Investigation of *Calligonum Azel* Maire ***M. Bannour**, A. Khadhri, D.W. Lachenmeier, T. Kuballa, S. Smiti, B. Hanchi*
A8	Quantitative *In-Situ* NMR to Characterize Protein Oxidation and its Dynamics ***G. Pagès**, A. Morisse, P. Gatellier, E. Martineau, P. Giraudeau, J.-M. Bonny*
A9	Quantitative HSQC-NMR Screening of Feruloylated Arabinoxylan Side Chain Profiles in Cereal Grains ***R.R. Schendel**, U. Schmitt, M. Bunzel*
A10	A 2D-NMR-Spectroscopic Profiling Approach to Analyse Structural Elements of Neutral Pectic Side Chains *D. Wefers, **M. Bunzel***
A11	Liquid and Solid-State ^{1}H, ^{13}C and ^{11}B NMR Analysis of Magnesium Fructoborate Complex: Chemical Structure, Identification and Stability Study ***B. Nemzer**, J. Edwards*

A12	Identification and Characterization of Ca and Mg Different Sugar Borate Esters Using Multi Nuclear Liquid and Solid-State NMR ***B. Nemzer**, J. Hunter, J. Edwards*
MRI and Diffusion, EXHIBITION HALL, M1-M	
M1	A Framework for Nucleus Density Quantitative Mapping Corrected for B_1-Errors ***J.-M. Bonny**, S. Clerjon*
M2	Understanding Meat Crust Formation: Validate Mathematical Models from Quantitative Microscopic MRI ***S. Clerjon**, S. Portanguen, A. Kondjoyan, J.-M. Bonny*
M3	Magnetic Resonance Imaging to Monitor the Curing of Century Eggs *C. Hickling, A. Hogg, **R. H. Morris***
M4	Magnetic Resonance as a Tool to Assess Moisture Content in Potatoes for Frying Processes ***E.R. Dye**, M.I. Newton, R.H. Morris*
M5	MRI Study of Staling Process in White Bread: Effect of Bread Improver ***A. Traoré**, L. Linossier, S. Chapron*
M6	Water Diffusion in Biofilms with Different Physical Structures ***M.P. Herrling**, J. Weisbrodt, H. Horn, S. Lackner, G. Guthausen*
Application/Foodomics, EXHIBITION HALL, F1-F	
F1	Food Matrix Description and Stability: A New Perspective from Foodomics ***A. Trimigno**, G. Picone, C. Pineda-Vadillo, D. Dupont, A. Bordoni, F. Capozzi*
F2	NMR Studies of the Quality-Deteriorating Wooden Breast Syndrome in Chicken ***H.C. Bertram**, U.K. Sundekilde, M.K. Rasmussen, P. Brandt, J.F. Young*
F3	Characterization and Identification of Biomarkers from Deterioration in Freshwater Fish by NMR and Chemometrics ***L.M. Lião**, V.S. Pinto. I.S. Flores*
F4	Extensive Regulation of Diurnal Transcription and Metabolism by Glucocorticoids *B.D. Weger, M. Weger, **B. Görling**, C. Gobet, M. Yildiz, C. Keime, G. Poschet, B. Jost, N. Krone, R. Hell, T. Akcay, T. Güran, F. Gachon, B. Luy, T. Dickmeis*
F5	Rapid Identification of Imitation Cheese and Imitation Ice Cream Based on Vegetable Fat Using NMR Spectroscopy and Chemometrics ***R. Brendel**, T. Kuballa, D.W. Lachenmeier, R. Godelmann, C. Andlauer, Y.B. Monakhova*
F6	Classification of the Botanical Origin of Honey by ^{1}H NMR in combination with Chemometric Methods and New Data Fusion Approaches ***N. Gerhardt**, P. Weller, S. Rohn, M. Ohmenhaeuser, T. Kuballa*

F7	Definition of Monofloral and Polyfloral Honeys Based on NMR Metabolomic Profiling ***E. Schievano**, C. Finotello, J. Uddin, S. Mammi, L. Piana*
F8	Characterization of Lignin Structures of Plant Based Foods by 2D-NMR Spectroscopy ***J. Schäfer**, M. Bunzel*
F9	Longitudinal Metabolic Profiling during Growth and Storage of Apples from Different Production Systems Studied by ^{1}H HR-MAS NMR ***M. Vermathen**, M. Marzorati, G. Diserens, D. Baumgartner, C. Good, F. Gasser, P. Vermathen*
F10	Untargeted NMR Apectroscopic Analysis of the Metabolic Variety of Apple Cultivars ***P. Eisenmann**, M. Ehlers, C. Weinert, M. Rist, B. Luy, C. Muhle-Goll*
F11	Variation of Blueberry's Metabolic Profile: The Influence of Ambient and Genetic Factors ***A.P. Sobolev**, D. Capitani, N. Proietti, M. Delfini, S. Carradori, F.R. De Salvador, L. Mannina*
F12	Fingerprint Profile by ^{1}H NMR and Chemometric Analysis of Freeze-Dried Açaí Berry Pulp ***T. da Conceição Alves**, A.G. Ferreira, M. do Socorro Padilha de Oliveira, R. de Andrade Mattietto*[2]
F13	Study of Lipoxigenase Enzyme Activity in Common Beans by NMR and UV Spectroscopies ***L.M. Lião**, A.K. Silva, P.Z. Bassinello, A.C. Lanna*
F14	Authentication of Saffron (*Crocus sativus* L.) Using ^{1}H NMR Spectroscopy ***S. Schumacher**, S. Mayer, C. Sproll, T.Kuballa, D.W. Lachenmeier*
F15	HR-MAS NMR Spectroscopy on the Quality Control of Green Tea ***A. Barison**, M. de Fátima Costa Santos*
F16	Investigation of the Impact of UV-C Treatment on Grape Must Using Untargeted NMR Spectroscopy ***L.A. Kromm**, K.Briviba, M.R. Stahl, T.Kuballa, D.W. Lachenmeier*
F17	Whisky Analysis through the Application of NMR Metabolomic Techniques ***N. MacKinnon**, C. Trautwein, J.G. Korvink*
F18	Nontargeted NMR Analysis to Detect Hazardous Substances Including Methanol in Unrecorded Alcohol from Russia ***T. Hausler**, M. Neufeld, J. Rehm, T. Kuballa, D.W. Lachenmeier*
F19	Classification of Italian Vinegar by Foodomics Approach ***G. Picone**, M. Sacco, A. Trimigno, F. Capozzi*
F20	HR-MAS NMR as Technique to Monitor *In-Vivo* Growth and Real-Time Fermentation Patterns of *Saccharomyces Cerevisae* ***C. Trautwein**, M.V. Meissner, J. Höfflin, J.G. Korvink*