



abiosus e.V.

Non-Profit Association for the Advancement of Research on Renewable Raw Materials

10th Workshop on Fats and Oils as Renewable Feedstock for the Chemical Industry

**March 17-19, 2019
Karlsruhe, Germany**

in Cooperation with

Agency of Renewable Resources (FNR)



Scientific and Organizing Committee

Ursula Biermann, University of Oldenburg, Oldenburg, Germany

Norbert Holst, Agency of Renewable Resources (FNR), Gülzow, Germany

Michael A. R. Meier, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Jürgen O. Metzger, *abiosus* e.V. and University of Oldenburg, Oldenburg, Germany

Acknowledgement

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Program

Lectures and Posters

Sunday, March 17, 2019

Registration

Registration will be open from 15:00 - 19:00

15.45 **Welcome and Opening**

Jürgen O. Metzger, *abiosus* e.V.

Michael A. R. Meier, KIT

16.00 – 17.30 *First Session*

Chair: Michael A. R. Meier

16.00 – 16.30 **At Long Last: Olefin Metathesis Production of Macrocyclic Musk from a Biomass at High Concentration (M)**

L1 Karol Grela, Biological and Chemical Research Centre, Faculty of Chemistry University of Warsaw and Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland

16.30 – 17.00 **Future of Surfactants: Sustainability fuels Innovation (M)**

L2 Dirk Kuppert, Clariant, Frankfurt, Germany

17.00 – 17.30 **Bio-Derived Molecular Materials: Ability to Adapt, Clean and for Energy Storage (M)**

L3 George John, The City College of New York, Center for Discovery and Innovation, New York, USA

17.30 – 20.30 **Poster Session and Opening Mixer**

Posters will be displayed until the end of the workshop

(M) Main Lecture 30 min. including discussion

(D) Discussion Lecture 20 min. including discussion

Monday, March 18, 2019

9.00 – 10.30 *First morning session*

Chair: Johannes Kabisch

9.00 – 9.30 **Alteration of Lipase Selectivity for Fatty Acid Enrichment by Protein Engineering (M)**

L4 Katja Zorn¹, Isabel-Oroz-Guinea¹, Henrike Brundiek², Uwe T. Bornscheuer¹, ¹ Institute of Biochemistry, Greifswald University, Greifswald, Germany, ² Enzymicals AG, Greifswald, Germany

9.30 – 9.50 **Synthesis of 100% renewable glycolipids from lignocellulose (D)**

L5 Katrin Ochsenreither, S. Siebenhaller, C. Syldatk, Karlsruhe Institute of Technology (KIT), Institute of Process Engineering in Life Sciences, Section II: Technical Biology, Karlsruhe, Germany

9.50 – 10.10 **Cyanide-free Chemoenzymatic Approach towards Fatty Nitriles and Aliphatic Dinitriles Based on Renewable Feedstocks (D)**

L6 Harald Gröger, Chair of Organic Chemistry I, Faculty of Chemistry, Bielefeld University

10.10 – 10.30 **Enzymatic synthesis of peracids with lipase/acyltransferase for tailored *in situ* epoxidation in mild conditions (D)**

L7 Rebecca Re,¹ Johanna Proessdorf,¹ James J. La Clair¹, Michael D. Burkart¹, Maeva Subileau,^{1,2} ¹ Department of Chemistry and Biochemistry, UC San Diego, La Jolla, United States, ² Montpellier SupAgro, UMR 1208 IATE, 2 Place Viala, 34060 Montpellier Cedex 2, France

10.30 – 11.00 **Coffee break**

11.00 – 12.30 *Second morning session*

Chair: Uwe Bornscheuer

11.00 – 11.30 **Oleaginous Yeasts as Microbial Cell Factories for the Renewable Production of Lipids and Lipid Derived Products (M)**

L8 Stefan Bruder, Silke Hackenschmidt, Eva Moldenhauer, Felix Bracharz, Johannes Kabisch, Computer-aided Synthetic Biology, TU Darmstadt, Darmstadt, Germany

11.30 – 11.50 **Biobased materials and foams from algae or jojoba oils (D)**

L9 Claire Negrell^a, Adrien Cornille^a, Sylvain Caillol^a, Chakib Mokhtari^b, Fouad Malek^b, ^a Institut Charles Gerhardt UMR 5253 – CNRS, UM, ENSCM, Montpellier, France. ^b Laboratoire de Chimie Organique, Macromoléculaire et Produits Naturels – Université Mohamed 1^{er} – Faculté des Sciences, Oujda, Maroc

- 11.50 – 12.10 **Sustainable synthesis of bio-based surfactants from cashew nutshell liquid (CNSL) (D)**
L10 Valentina Bragoni, J. Pollini, R. K. Rit, R. Kirchmann, A. S. Trita, Lukas J. Gooßen, Ruhr Universität Bochum, Bochum (Germany)
- 12.10 – 12.30 **Innovative Concepts for Homogeneous Catalyst Recycling: Novel Solutions in the Functionalization of Unsaturated Oleo Chemicals (D)**
L11 T. Seidensticker, J. Vondran, N. Herrmann, D. Vogt, TU Dortmund University, Laboratory of Industrial Chemistry, Dortmund/Germany
- 12.30 – 14.00 **Lunch break**
- 14.00 – 15.30 *First afternoon session*
Chair: Karol Grela
- 14.00 – 14.30 **From Pheromones to Functional Polymers: Ring-Opening Polymerization of Macrolactones from Long-Chain Hydroxyacids (M)**
L12 Andreas Heise, Department of Chemistry, Royal College of Surgeons in Ireland (RCSI), Dublin , Ireland
- 14.30 – 14.50 **Sustainable epoxidation of Cynara cardunculus seed oil with hydrogen peroxide (D)**
L13 Rosa Turco, Riccardo Tesser, Rosa Vitiello, Vincenzo Russo, Martino Di Serio, Università di Naples Federico II, Department of Chemical Sciences, Napoli, Italy
- 14.50 – 15.10 **Organocatalytic cleavage of fatty acid derivatives to aldehydes and esters (D)**
L14 Nam Duc Vu, Souleymane Bah, Elsa Deruer, Boris Guicheret, Estelle Métay, Nicolas Dugué, Marc Lemaire, University Lyon 1, Villeurbanne, France
- 15.10 – 15.30 **Selective Oxidations of Unsaturated Fatty Acids and Bio-sourced Feedstocks (D)**
L15 Mukund P. Sibi, Department of Chemistry and Biochemistry, North Dakota State University, Fargo, ND, USA
- 15.30 – 16.00 **Coffee break**

- 16.00 – 17.30 *Second afternoon session*
- Chair: *Eric Monflier*
- 16.00 – 16.30 **Bioeconomy in figures - with a focus on the use of oils and fats in the chemical industry (M)**
L16 Michael Carus, Nova-Institut, Germany
- 16.30 – 17.00 **Enhancing the physical-mechanical properties of vegetable oil-based waxes using simple, safe and sustainable chemical modifications (M)**
L17 Eliane Goossens¹, Peter Tollington², ¹ Cargill R&D Centre Europe, Vilvoorde, Belgium, ² Cargill Bio-Industrials Europe, Schiphol, The Netherlands
- 17.00 – 17.20 **Current Development in biobased polyester : PRIC range (D)**
L18 Marie Reulier, ITERG, Canejan, France
- 17.20 – 17.40 ***N,N*-Dimethylglucamine – A Sustainable Solution for Paints & Coatings (D)**
L19 Adriana Grossmann, Clariant Produkte (Deutschland) GmbH, Burgkirchen, Germany
- 19.30 *Conference Dinner*
- Achat Plaza Karlsruhe**

Tuesday, March 19, 2019

9.00 – 10.30 *First morning session*

Chair: Dean Webster

9.00 – 9.30 **Chemical Synthesis of High-Melting Bacterial Polyesters and Chemically Recyclable Polymers (M)**

L20 Eugene Y.-X. Chen, Department of Chemistry, Colorado State University, Fort Collins, United States

9.30 – 9.50 **Plant oil-based Poly(Alkyl Methacrylate) as Viscosity Control Additive for Mineral and Vegetable Oils (D)**

L21 Juliette Lomege, Vincent Lapinte, Claire Negrell, Jean-Jacques Robin, Sylvain Caillol, Institut Charles Gerhardt, CNRS UMR-5253, Ingénierie et Architectures Macromoléculaires, Montpellier, France

9.50 – 10.10 **Development of New Bio-based Innovative and Responsive Materials Based on Fatty Acid Derivatives (D)**

L22 Khantutta-Kim Tremblay-Parrado, Luc Avérous, BioTeam/ICPEES-ECPM, Université de Strasbourg, Strasbourg, France

10.10 – 10.30 **Roots towards innovation in sustainable poly(2,5-furandicarboxylate)s polymeric materials (M)**

L23 Andreia F. Sousa, CICECO - Aveiro Institute of Materials, Departamento de Química, Universidade de Aveiro, Aveiro, Portugal

10.30 – 11.00 **Coffee Break**

11.00 – 12.30 *Second morning session*

Chair: Eva E. Malmström

11.00 – 11.30 **Sustainable Terpene-Based Biopolymers and Novel Functional Biomaterials (M)**

L24 Malte Winnacker, Jacob Sag, Andreas Beringer, Bernhard Rieger, WACKER-Lehrstuhl für Makromolekulare Chemie and Catalysis Research Center, TU München, Garching bei München, Germany

11.30 – 11.50 **Renewable polyamides via thiol-ene click' chemistry and long-chain aliphatic segments (D)**

L25 Phan Huy Nguyen, Steven Spoljaric, Jukka Seppälä, Polymer Technology, Department of Chemical and Metallurgical Engineering, Aalto University School of Chemical Engineering, Aalto, Finland

- 11.50 – 12.10 **Sustainable Cellulose modification via transesterification using high oleic sunflower in a DBU-CO₂ switchable solvent system (D)**
L26 Kelechukwu (Kenny) N. Onwukamike,^{1,2} S. Grelier,² E. Grau,² H. Cramail,² M.A.R. Meier¹, ¹ Institute of Organic Chemistry (IOC), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany. ² Laboratoire de Chimie des Polymères Organiques, Université de Bordeaux, UMR5629, CNRS - Bordeaux INP - ENSCBP, Pessac Cedex France.
- 12.10 – 12.30 **Non-isocyanate bio-based polyurethanes through reactive extrusion (D)**
L27 Fiona Magliozzi,^{1,2} Etienne Grau^{1,2}, Guillaume Chollet³, Henri Cramail^{1,2}, ¹Univ. Bordeaux, LCPO, UMR 5629, Pessac, France ²Bordeaux INP, LCPO, UMR 5629, Talence, France, ³ITERG, F-Canéjan, France
- 12.30 – 14.00 **Lunch break**
- 14.00 – 15.30 *Afternoon session*
Chair: Eugene X.-Y. Chen
- 14.00 – 14.30 **Epoxidized Sucrose Esters as a Platform Technology for High Performance Thermosets (M)**
L28 Dean C. Webster, North Dakota State University, Fargo, North Dakota, USA
- 14.30 – 15.00 **Recent Advances in Hydroformylation, Hydrohydroxy-methylation and Hydroaminomethylation of Oleochemicals (M)**
L29 Eric Monflier, University of Artois, Unité de Catalyse et Chimie du Solide, UMR CNRS 8181, Faculté des Sciences Jean Perrin, Lens, France
- 15.00 – 15.30 **Renewable building blocks for potential use in coatings (M)**
L30 Eva E. Malmström, KTH Royal Institute of Technology, Stockholm, Sweden
- 15.30 **Poster Award and Closing Remarks**
Best Poster Award
Award committee: Eliane Goossens, Andreas Heise, George John, Malte Winnacker
- 15.45 **End of Workshop**

Poster

- P1 **Sustainable Preparation of Catalytically Active Ag/AgBr Janus Nanoparticles Under Sun light using Renewable Surface Active Ionic Liquid**
Gurbir Singh, Komal, Tejwant Singh Kang*, Department of Chemistry, UGC Sponsored Centre for Advanced Studies (CAS-II), Guru Nanak Dev University, Amritsar, India
- P2 **Inherently Green and Thermally stable Microemulsions**
Manvir Kaur, Gurbir Singh, Tejwant Singh Kang*, Department of Chemistry, UGC-Centre for Advance Studies – II, Guru Nanak Dev University, Amritsar, India
- P3 **Nicotine-based Renewable Surface Active Ionic Liquids: Self-assembly and Their Application as Greener Oil Herding Agents**
Gurbir Singh,[†] Raman Kamboj, Venus Singh Mithu,[†] Vinay Chauhan, Taranjeet Kaur,[#] Gurcharan Kaur,[#] Sukhprit Singh,^{†,*} Tejwant Singh Kang^{†,*}
[†]Department of Chemistry, UGC-centre for Advance Studies – II, [#]Department of Biotechnology, Guru Nanak Dev University, Amritsar, India.
- P4 **Green Initiative to Prepare Glass Fibre Reinforced Composite based on Vegetable Oil Polyester Thermoset Matrices**
Abhishek Chowdhury, Prashant Anthony, Sam Higginbottom University of Agriculture, Technology and Sciences, Allahabad, Uttar Pradesh, India
- P5 **Oxidative processes towards 12-OPDA as a precursor of jasmonic acid**
Jana Löwe, Karl-Josef Dietz and Harald Gröger, Chair of Organic Chemistry I, Faculty of Chemistry, Bielefeld University, Bielefeld, Germany
- P6 **Ruthenium-catalyzed hydroaminomethylation of vegetable oils**
Kévin Cousin, Frédéric Hapiot, Eric Monflier, Univ. Artois, CNRS, Lens, France
- P7 **Retardation of lipid oxidation in (o/w) and (w/o) emulsion systems with addition of natural terpene molecules**
Olivia Dhara*, Mahua Ghosh, Department of Chemical Technology, University College of Science and Technology, University of Calcutta, Kolkata, India
- P8 **Functionalized polyurethanes for surface coatings**
Philipp Schmidt, Steven Eschig, Fraunhofer Institute for Wood Research Wilhelm-Klauditz-Institut WKI, Braunschweig, Germany
- P9 **Stereo selective synthesis of cyclic carbonates based on renewables**
Vivian Stefanow, Thomas Werner, Leibniz Institute for Catalysis at University of Rostock, Rostock, Germany
- P10 **Synthesis of bio-sourced Non-Isocyanate Polyurethanes and their incorporation into water-borne NIPU-Acrylic hybrid systems**
Boris Bizet^{1,2}, Étienne Grau¹, José M. Asua², Henri Cramail¹
¹LCPO – UMR 5629, Université de Bordeaux, CNRS, ENSCBP / Bordeaux INP – 16, PESSAC, France ; ²POLYMAT, University of the Basque Country UPV/EHU, Centro Joxe Mari Korta –San Sebastián, Spain

- P11 **Agglomerated stone materials based on acrylated vegetable oils as thermosetting binder**
Stefano Zeggio, Fabio Bassetto, Breton SpA, Castello di Godego, Italy
- P12 **Sustainable synthesis of bio-based surfactants from cashew nutshell liquid (CNSL) (D)**
Valentina Bragoni, J. Pollini, R. K. Rit, R. Kirchmann, A. S. Trita, Lukas J. Gooßen, Ruhr Universität Bochum, Bochum (Germany)
- P13 **Selective product crystallization as a recycling strategy in the methoxycarbonylation of renewable resources**
N. Herrmann, D. Vogt, T. Seidensticker, TU Dortmund University, Dortmund, Germany
- P14 **Castor Oil Based Polyurethane Perlite Composites with Low Thermal Conductivity**
Gokhan CAYLI, Milkah Wairimu MURUMI, Istanbul University Cerrahpasa, Istanbul, Turkey
- P15 **New Series of Epoxidized Sunflower Oil Based Flame Retardant Monomers: Synthesis and Characterization**
Gokhan CAYLI, Necla BEKTAS, Demet GURBUZ, Adem CINARLI, Istanbul University-Cerrahpasa, Istanbul, Turkey
- P16 **Synthesis and Characterization of Epoxy Acrylate Derivative of Methyl Ricinoleate**
Gokhan CAYLI¹, Pinar CAKIR HATIR², ¹ Istanbul University Cerrahpasa, Istanbul, Turkey, ² Istanbul Arel University, Istanbul, Turkey
- P17 **Polymerization of PEP Resole with Different Types of Oils**
Gokhan CAYLI¹, Pinar CAKIR HATIR², Selim KUSEFOGLU³, ¹ Istanbul University-Cerrahpasa, Istanbul, Turkey, ² Istanbul Arel University, Istanbul, Turkey, ³ Bogazici University, Istanbul, Turkey
- P18 **Epoxy Derivative of Maleate Ester of Castor Oil: A New Alternative to Unsaturated Polyesters**
Gokhan CAYLI¹, Pinar CAKIR HATIR², ¹ Istanbul University-Cerrahpasa, Istanbul, Turkey, ² Istanbul Arel University, Istanbul, Turkey
- P19 **Properties of Epoxidized Maleinated Castor Oil / Hydroxyapatite Composites**
Gokhan CAYLI¹, Yesim Muge SAHIN², Erdi BULUS², Demet Sezgin MANSUROGLU², ¹ Istanbul University-Cerrahpasa, Istanbul, Turkey, ² Istanbul Arel University, Istanbul, Turkey
- P20 **The Effect of Plant Oil-Based Monomer Unsaturation on Properties of Latexes and Latex Materials with High Biobased Content**
Zoriana Demchuk¹, Oleh Shevchuk², Vasylyna Kirianchuk², Ananiy Kohut², Stanislav Voronov², Andriy Voronov¹, ¹Coatings and Polymeric Materials Department, North Dakota State University, Fargo, ND, USA, ²Organic Chemistry Department, Lviv Polytechnic National University, Lviv, Ukraine

- P21 **Synthesis of novel acrylated cardanol diphenyl phosphate based reactive diluent for UV curable flame retardant coating application**
Ganesh Phalak, Shashank Mhaske, Institute of Chemical Technology, Mumbai, India
- P22 **Modified Fatty raw materials as PHBV PLASTICIZERS**
Hanna Nosal¹, Marek Warzala¹, Kevin Moser², Andrei Holzer², Dorota Stańczyk¹,
¹Institute of Heavy Organic Synthesis "Blachownia", Kedzierzyn-Kozle, Poland,
²Fraunhofer Institute for Chemical Technology, Pfinztal, Germany
- P23 **Autoxidation of oils according to their composition: Applications to the drying of alkyd paints**
Raphael Lebeuf, Laura Dubrulle, Pr. Véronique Rataj, Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, Lille, France
- P24 **Oxo-functionalization of unsaturated lipids by a photooxidation / molybdate catalysis sequence**
Raphael Lebeuf, Pr. Véronique Rataj, Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, Lille, France
- P25 **A specific kinetic study to understand better the ring-opening of epoxydes from unsaturated fatty acid systems**
Julien Peyrton, Luc Avérous, BioTeam/ICPEES-ECPM, UMR CNRS 7515, Strasbourg, France
- P26 **Sustainable synthesis of ureas and amines via CO₂-based Lossen rearrangement**
Luca Filippi, Michael a. R. Meier*, Karlsruhe Institute of Technology (KIT), Institute of Organic Chemistry (IOC), Karlsruhe, Germany
- P27 **Immobilized Molecular Catalysts for Lipid Isomerization**
Felix Einsiedler, Stefan Mecking, Chair of Chemical Material Science University of Konstanz, Konstanz, Germany
- P28 **Immobilized Olefin Metathesis Catalysts for the Conversion of Renewable Raw Materials**
Stefanie Kulpa, Natalie Schunck, Stefan Mecking, Chair of Chemical Material Science University of Konstanz, Konstanz, Germany
- P29 **Modification of starch via the Biginelli multicomponent reaction**
Eren Esen, Michael A. R. Meier, Institute of Organic Chemistry (IOC), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
- P30 **Enzymatic conversions of renewables to tailor-made glycolipid biotensides in uncommon media**
André Delavault, Jens Grüninger, Christoph Syldatk; Karlsruhe Institute of Technology (KIT); Institute of Process Engineering in Life Science; Section II: Technical Biology, Karlsruhe, Germany

- P31 **Synthesis and Copolymerization of Biginelli-Polycondensates**
J. T. Windbiel, M. A. R. Meier, Karlsruhe Institute of Technology, Karlsruhe, Germany
- P32 **Microbial synthesis of long chain sophorolipids and their potential as emulsifiers**
Christian Zerhusen, Timo Bollmann, Birgit Glösen, Ulrich Schörken, TH Köln, Cologne University of Applied Sciences, Leverkusen, Germany
- P33 **Pheno- and genotypic characterization of three *Yarrowia lipolytica* strains**
Silke Hackenschmidt, Stefan Bruder, Felix Bracharz, Johannes Kabisch
 Computer-aided Synthetic Biology, TU Darmstadt, Darmstadt, Germany
- P34 **Sustainable synthesis of biobased recyclable thermosets**
P. S. Löser¹, M. A. R. Meier¹, A. Llevot², ¹ Karlsruhe Institute of Technology, Karlsruhe, Germany; ² University of Bordeaux, Bordeaux, France
- P35 **Single cell oil production by *Y. lipolytica* for the chemical conversion to hydrocarbons**
Eva J. Moldenhauer¹, Stefan Bruder¹, Martin Peters², Andreas Menne², Stefan Junne³, Johannes Kabisch¹, ¹ Computer-aided synthetic biology, Technical University of Darmstadt, Germany, ² Fraunhofer UMSICHT, Oberhausen, Germany, ³ Department of Bioprocess Engineering, Technical University of Berlin, Germany
- P36 **A novel approach on isomerization of long chain carboxylic acids based on inspiration from isomerization of hydrocarbons**
Maghrebi Ramin¹, Bondioli Paolo³, Chiaramonti David^{1,2}, ¹ Department of Industrial Engineering, University of Florence, Italy, ² RE-CORD, Research and Demonstration for R&D, Florence, Italy, ³ Innovhub Stazioni Sperimentali per l'Industria S.r.l., Milan, Italy
- P37 **Structural investigation of natural deuterated phospholipid multilayers**
Krishna Batchu, Yuri Gerelli, Michael Haertlein, Giovanna Fragneto
 Institute Laue-Langevin, Grenoble, France
- P38 **Optimization of the extraction of glucose monodecanoate synthesized in deep eutectic solvents by response surface modeling**
Rebecca Hollenbach, Christoph Syldatk, Karlsruhe Institute of Technology, Karlsruhe, Germany
- P39 **Plant Oil-Based Monomers for Reversible Deactivation Radical Polymerisation**
P.B.V. Scholten,^{1,2} C. Detrembleur,² M.A.R. Meier¹, ¹ Karlsruhe Institute of Technology, IOC, Materialwissenschaftliches Zentrum MZE, Karlsruhe, Germany; ² Université de Liège, Center for Education and Research on Macromolecules, CESAM Research Unit, Liège, Belgium
- P40 **Progress in homogeneously catalyzed oxidation reactions of fatty acids – sustainability through catalyst recycling**
Johanna Vondran, Dieter Vogt, Thomas Seidensticker, Technical University, Dortmund, Germany

Abstracts

Part 1: Lectures

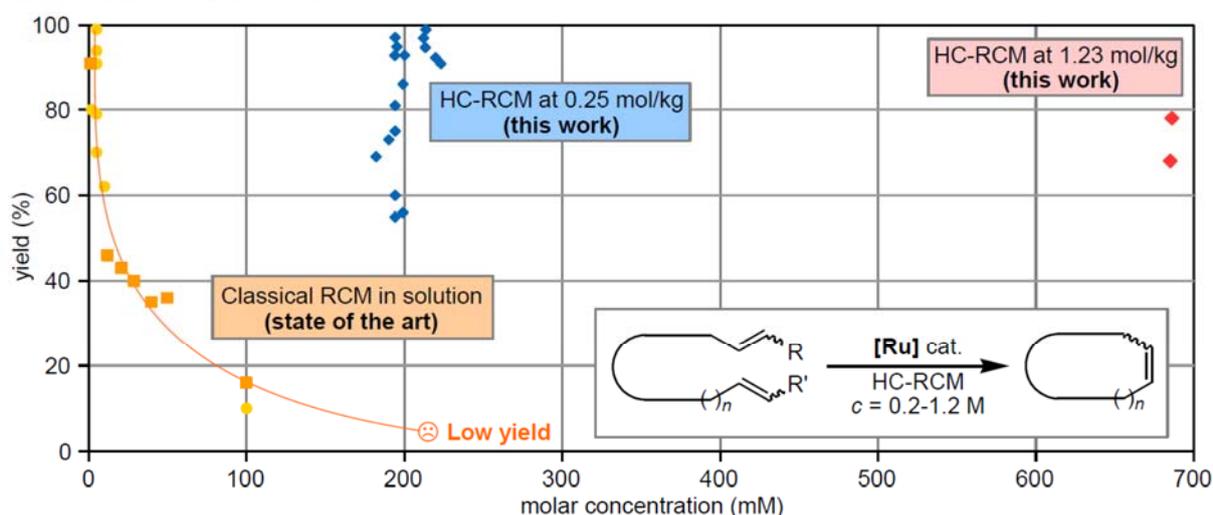
At Long Last: Olefin Metathesis Production of Macrocyclic Musk from a Biomass at High Concentration

Karol Grela^{1,2}

¹ Organometallic Synthesis Laboratory, Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Warsaw, Poland

² Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland
prof.grela@gmail.com

Macrocyclic lactones, ketones, and ethers can be obtained in the High-Concentration Ring-Closing Metathesis (HC-RCM) reaction in high yield and selectivity at concentrations 40 to 380 times higher than those typically used by organic chemists for similar macrocyclizations.



The new method consists of using tailored ruthenium catalysts together with applying vacuum to distill off the macrocyclic product as it is formed by the metathetical backbiting of oligomers. Unlike classical RCM, no large quantities of organic solvents are used, but rather inexpensive nonvolatile diluents, such as natural or synthetic paraffin oils. Moreover, use of a protecting atmosphere or a glovebox is not needed, as the new catalysts are perfectly moisture and air stable. In addition, some other cyclic compounds previously reported as unobtainable by RCM in neat conditions, or in high dilutions even, can be formed with the help of the HC-RCM method [1].

[1] Sytniczuk, A.; Dąbrowski, M.; Banach, Ł.; Urban, M.; Czarnocka-Śniadała, S.; Milewski, M.; Kajetanowicz, A.; Grela, K. "At Long Last: Olefin Metathesis Macrocyclization at High Concentration" *J. Am. Chem. Soc.* **2018**, *140*, 8895-8901.

Future of Surfactants: Sustainability fuels Innovation

Dirk Kuppert, Clariant, Frankfurt, Germany
dirkroland.kuppert@clariant.com

Steadily rising demand and simultaneous decline of resources are creating global challenges in areas such as energy supply, resource efficiency, waste prevention, nutrition, consumer care and mobility. While discussing the future of surfactants these challenges are highly ranked on corporate agendas. New and innovative products are the result of a well-structured innovation process that incorporates sustainability aspects at an early stage, combined with state-of-the-art technology. Moreover, developing customized and holistic solutions requires close collaboration with external partners creating new innovation ecosystems.

A new platform of sugar-based surfactants with a broad range of application fields and the conversion of agricultural residues into bio-based products are just two examples presented to demonstrate next generations of sustainable product solutions.

Bio-Derived Molecular Materials: Ability to Adapt, Clean and for Energy Storage

George John, Department of Chemistry and Biochemistry, The City College of New York, NY 10031 & Ph.D. Program in Chemistry and Biochemistry, The Graduate Center of the City University of New York, New York, NY 10016.
gjohn@ccny.cuny.edu

Developing functional materials from renewable resources would be fascinating yet demanding practice, which will have a direct impact on industrial applications, and economically viable choices. This talk discusses an emerging model of generating new chemicals, intermediates and materials in a 'biorefinery'. Our continued efforts in this area have led us to develop new molecular materials through non-covalent synthesis of amphiphilic molecules derived from industrial by-products and co-products. The family of new materials generated include emulsions, molecular gels, solid bilayers, scintillating gels, battery components and liquid crystals. More recently, harnessing the availability of 'chiral pool' of carbohydrates and selectivity of enzymes catalysis, our laboratory produced an array of amphiphilic molecules from simple sugars and sugar alcohols conjugating with appropriate fatty acids. Intriguingly, following the principles of green and supramolecular chemistry, we have developed building blocks-to-assembled materials *viz* vegetable oil structuring agents and green battery components. Redox-active organic compounds are re-emerging in the energy storage community bringing with them interesting opportunities such as design flexibility, lightweight, low cost and/or restrained environmental burden. These results will lead to efficient molecular design of supramolecular architectures and next generation multifunctional materials from underutilized plant/crop-based renewable feedstock.

Selected References

1. Silverman, J. R.; Samateh, M.; John, G. Functional Self-Assembled Lipidic Systems Derived from Renewable Resources, *Eur. J. Lipid Sci. Technol.* 2016, 118, 47–55.
2. Gupta, D.; Sarker, B.; Thadikaran, K.; John, V.; Maldarelli, C.; John, G. Sacrificial Amphiphiles: Eco-friendly Chemical Herders as Oil Spill Mitigation Chemicals, *Science Advances*, 2015, 1, e1400265.
3. Faure, L.; Nagarajan, S.; Hwang, H.; Montgomery, C. L.; Khan, B. R.; John, G.; Koulen, P.; Blancaflor, E. B.; Chapman, K. D. Synthesis of Phenoxyacyl-Ethanolamides and Their Effects on Fatty Acid Amide Hydrolase Activity, *J. Biol. Chem.* 2014, 289, 9340-51.
4. Jadhav, S. R.; Hwang, H.; Huang, Q.; John, G. Medium-Chain Sugar Amphiphiles: A New Family of Healthy Vegetable Oil Structuring Agents, *J. Agric. Food Chem.* 2013, 61,12005-11.
5. Jadhav, S. R.; Vemula, P. K.; Kumar, R.; Raghavan, S.; John, G. Sugar-derived phase-selective molecular gelators as model solidifiers for oil spills, *Angew. Chem. Int. Ed.*, 2010, 49, 7695-7698.

Alteration of lipase selectivity for fatty acid enrichment by protein engineering

Katja Zorn¹, Isabel-Oroz-Guinea¹, Henrike Brundiek², Uwe T. Bornscheuer¹

¹ Institute of Biochemistry, Greifswald University, Greifswald, Germany

² Enzymicals AG, Greifswald, Germany

uwe.bornscheuer@uni-greifswald.de

Lipases belong to the α/β -hydrolase fold family and they widely applied in industrial processes [1]. Each industrial application needs particular reaction conditions (e.g. substrate selectivity or stability towards temperature, pH and/or organic solvents) that must be tolerated by the biocatalyst and to achieve this, protein engineering can be applied [2].

The present study focuses on the enhancement of lipase selectivity by protein engineering and its application for the enrichment of long chain fatty acids such as erucic acid and gondoic acid from natural oils, which are interesting building blocks for the chemical industry. From a range of commercial lipases, lipase CAL-A was chosen and subjected to rational design. Three different amino acids present in the binding pocket of CAL-A were identified, allowing the design and creation of three combinatorial mutant libraries. The performance of more than 4500 clones was verified using our fully automatized robotic platform LARA [3]. The most selective variants were chosen and used for confirmation of their activity and selectivity towards fatty acid ethyl esters and oil fractions containing the desired fatty acids [4] including scale up [5].

[1] Bornscheuer, U. T., *Eur. J. Lipid Sci. Tech.*, 2014, 116, 1322-1331.

[2] Zorn, K. et al., *Prog. Lipid. Res.*, 2016, 63, 153-164.

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Synthesis of 100% renewable glycolipids from lignocellulose

Katrin Ochsenreither, S. Siebenhaller, C. Syldatk
Karlsruhe Institute of Technology (KIT), Institute of Process Engineering in Life Sciences,
Section II: Technical Biology, Karlsruhe, Germany
Katrin.ochsenreither@kit.edu

Glycolipids are non-ionic surfactants occurring in numerous products of daily life. Due to their surface-activity, emulsifying properties and foaming abilities they can be applied in food, cosmetics and pharmaceuticals. Enzymatic synthesis of glycolipids based on sugar and fatty acids or their respective esters is often catalyzed by using esterases or lipases in reaction media of low water activity, e.g. organic solvents or deep eutectic solvents (DES). DES offer several advantages, as being cheap, biological degradable and easy to produce. In general, DES consists of a mixture of a quaternary ammonium- or phosphonium salt and a hydrogen-bond donor. By interaction of both components the melting point of the mixture is strongly decreased resulting in a liquid solution at room temperature. When using a sugar as hydrogen-bond donor, the sugar can act simultaneously as substrate for glycolipid production.

The aim of the presented study was to produce glycolipids from completely renewable resources using eco-friendly enzymatic catalysis. To achieve this goal, beech wood cellulose fiber hydrolysate was used as the sugar component and part of the DES solvent system as well as the carbon source for the biotechnological production of the fatty acid component of the glycolipid. Fatty acids were gained from single cell oil produced by the oleaginous yeast *Cryptococcus curvatus* cultivated with cellulose fiber hydrolysate as carbon source. Immobilized *Candida antarctica* lipase B (former Novozyme 435) was used as the biocatalyst in DES to achieve the esterification between sugar and fatty acid. Synthesis products were detected and characterized using TLC, MS and NMR. Using this approach, glycolipids were successfully synthesized which are 100 % of renewable origin. This study shows that cellulose hydrolysates from wood are promising substrates for establishing biorefineries.

Cyanide-free Chemoenzymatic Approach towards Fatty Nitriles and Aliphatic Dinitriles Based on Renewable Feedstocks

Harald Gröger

Chair of Organic Chemistry I, Faculty of Chemistry, Bielefeld University,
harald.groeger@uni-bielefeld.de

Aliphatic linear nitriles and dinitriles are widely used in industry as solvents, intermediates for the production of surfactants and life sciences products as well as precursors for polymers, respectively. In this contribution we report a chemoenzymatic approach towards such linear aliphatic nitriles as well as dinitriles, which avoids the utilization of cyanide as a reagent being used in many chemical syntheses of nitriles.

As for the production of aliphatic nitriles (fatty nitriles) the developed process is based on an initial transformation of fatty aldehydes into the corresponding aldoximes and subsequent enzymatic dehydration using an aldoxime dehydratase from *Bacillus* sp.. It is noteworthy that these processes run at high substrate loadings of up to 1.4 kg/L as shown for the synthesis of *n*-octanenitrile. This substrate loading is one of the highest ever reported in biocatalysis. The aliphatic aldoximes are readily available starting materials being easily prepared from fatty aldehydes via spontaneous condensation with the bulk chemical hydroxylamine. Simple work up by only separation of the solvent-free organic product phase without need for further purification is another advantage.

Furthermore, this chemoenzymatic concept was utilized for an alternative route towards adiponitrile and related linear α,ω -dinitriles.¹ Albeit being produced on ca. 1 million tons scale, a drawback of today's dominating process for adiponitrile is the need for large amounts of highly toxic hydrogen cyanide. In this contribution, a cyanide-free approach towards such dinitriles is presented based again on dehydration of α,ω -dialdoximes using aldoxime dehydratases at ambient conditions. A selective synthesis of adiponitrile with substrate loadings of up to 100 g/L and yields of up to 80% was achieved.¹

¹ T. Betke, M. Maier, H. Gruber-Wölfler, H. Gröger, *Nature Commun.* **2018**, *9*, 5112.

Enzymatic synthesis of peracids with lipase/acyltransferase for tailored *in situ* epoxidation in mild conditions

Rebecca Re,¹ Johanna Proessdorf,¹ James J. La Clair¹,
Michael D. Burkart¹ and Maeva Subileau,^{1,2}

¹ Department of Chemistry and Biochemistry, UC San Diego, 9500 Gilman Dr., La Jolla CA 92093-0358, United States

² Montpellier SupAgro, UMR 1208 IATE, 2 Place Viala, 34060 Montpellier Cedex 2, France
maeva.subileau@supagro.fr

Nowadays, epoxides are appearing in a wide array of commodity chemicals, materials and pharmaceuticals, and renewed attention has turned to explore chemo-enzymatic routes to circumvent the harsh and complex conditions usually required in chemistry. In this context, lipases/acyltransferases, known to preferentially catalyze acyltransfer to other nucleophiles but water, appear as enzymes of choice to allow peracids synthesis in the presence of low hydrogen peroxide concentration. Here we present a two-phase enzymatic system using an improved mutant of the lipase/acyltransferase CpLIP2 from *Candida parapsilosis*, that allows to effectively generate peracids which in turn allow *in situ* epoxidation of olefins. We demonstrate the approach by application to a wide range of lipid and olefin epoxidation with low amount of hydrogen peroxide and enzyme, in simple aqueous medium. The system opens valuable perspectives of applications, toward the sustainable synthesis of epoxidized oil for bio-based materials but also of fine chemicals.

Oleaginous Yeasts as Microbial Cell Factories for the Renewable Production of Lipids and Lipid Derived Products

Stefan Bruder, Silke Hackenschmidt, Eva Moldenhauer, Felix Bracharz,
Johannes Kabisch
Computer-aided Synthetic Biology, TU Darmstadt, Darmstadt, Germany
johannes@kabisch-lab.de

Oleaginous yeasts are potent hosts for the renewable production of lipids, fatty acids and derived products, such as biofuels. For Example several promising processes have been described that produce hydrocarbon drop-in biofuels based on fatty acid decarboxylation and fatty aldehyde decarbonylation. Unfortunately, besides fatty aldehyde toxicity and high reactivity, the most investigated enzyme, aldehyde-deformylating oxygenase, shows unfavorable catalytic properties which hindered high yields in previous metabolic engineering approaches. To demonstrate an alternative alkane production pathway for oleaginous yeasts, we describe the production of biodiesel-like odd-chain alkanes and alkenes, by heterologously expressing a recently discovered light-driven oxidase from *Chlorella variabilis* (CvFAP) in *Yarrowia lipolytica*.

In order to optimize this process we developed and 3D printed custom LED systems for microwell plates and our bioreactors. Besides this enzyme based process we will as well present our experiences with the pilot scale production, extraction and chemical hydrocracking of lipids produced by *Y. lipolytica*.

Biobased materials and foams from algae or jojoba oils

Claire Negrell^{a*}, Adrien Cornille^a, Sylvain Caillol^a, Chakib Mokhtari^b, Fouad Malek^b

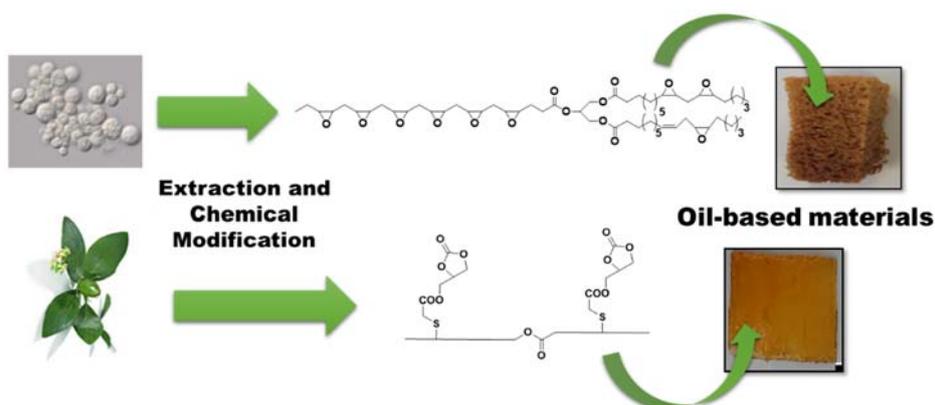
^aInstitut Charles Gerhardt UMR 5253 – CNRS, UM, ENSCM – 240 avenue Jeanbrau, 34296 Montpellier, France.

^bLaboratoire de Chimie Organique, Macromoléculaire et Produits Naturels – Université Mohamed 1^{er} – Faculté des Sciences, Bd Mohamed VI, 60 000 Oujda, Maroc

* claire.negrell@enscm.fr

All vegetable oils are not equivalent in terms of double bonds functionality or chemical structure. For example, linseed, soybean and canola oils contain respectively 6.6, 4.6 and 3.9 double bonds per triglyceride, while palm oil contains 1.7 double bonds per triglyceride. Hence, jojoba is the only plant species known to use liquid wax esters as a seed storage. It is a vegetable oil obtained from the crushed bean of the jojoba shrub (*Simmondsia chinensis*) and is almost entirely (~97%) composed of two mono-unsaturated hydrocarbon chains linked by an ester moiety [1]. In the other side, microalgae are, first, a potential source of renewable energy but could also interesting lead to a platform for oleochemicals. The oil obtained from *Schizochytrium* microalgae, is a triglyceride with a high content in saturations (around 10) [2], could be dedicated to the synthesis of polymer materials.

Chemical modifications were made on algal and jojoba oils to obtain new functional buildings blocks. Fully biobased materials were synthesized, characterized and compared with classic vegetable oils. This work highlighted the originality of jojoba oil to obtain linear as well as cross-linking polymers [3,4] and the interesting thermos-mechanical superiority of algal oil material with their high content in reactive functions. Finally, the addition of a blowing agent led to the synthesis of algal oils derived foams with interesting properties. Finally, algal oil and jojoba oil demonstrated interesting potential as a viable starting material for fully biobased materials and foams [5].



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Sustainable synthesis of bio-based surfactants from cashew nutshell liquid (CNSL)

Valentina Bragoni, J. Pollini, R. K. Rit, R. Kirchmann, A. S. Trita and Lukas J. Gooßen
Ruhr Universität Bochum, Universitätsstr 150, 44801, Bochum (Germany)
Valentina.bragoni@rub.de

Cashew nutshell liquid (CNSL) is an inedible waste by-product of the cashew nut processing. It is an excellent candidate for the synthesis of bio-based synthetically valuable compounds, as its production does not compete with the land use for food production.^[1,2] CNSL is a mixture of phenols bearing a 15-carbon side chain with different degrees of unsaturations.^[3,4]

We have developed an eco-friendly and waste minimised concept for the synthesis of amine-based surfactants from CNSL (Fig. 1).^[5] The key step of the procedure is a reductive amination of CNSL in water. The resulting cyclohexyl amine derivatives were further converted into *N*-oxide, betaine and quaternary ammonium tensides. The *N*-oxide was produced in one-pot with water as the solvent in a process with an E-factor of 2.

During the refining of the CNSL, the anacardic acid fraction was separated off. The synthetic value of this byproduct was demonstrated in a three-steps synthesis of a tyrosinase inhibitor.^[6] The process occurred *via* ethenolysis and subsequent cross-metathesis using a first generation Hoveyda–Grubbs catalyst, which was reused as precatalyst in a subsequent hydrogenation step.

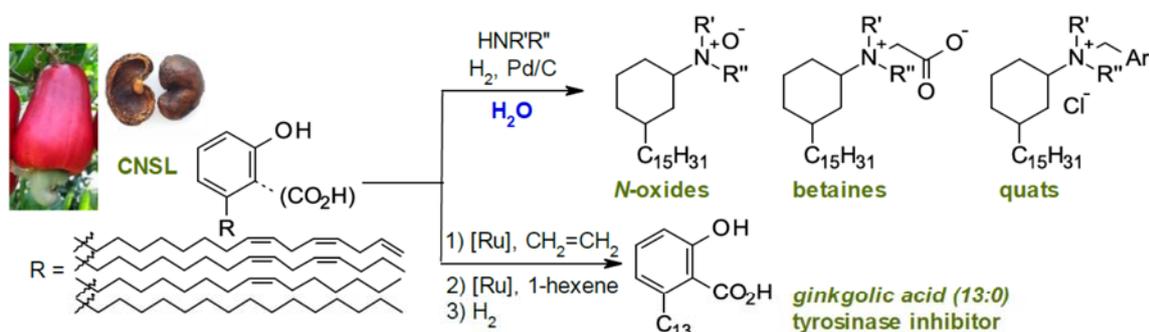


Figure 1. Synthesis of surfactants and biological active compounds from CNSL

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Innovative Concepts for Homogeneous Catalyst Recycling: Novel Solutions in the Functionalization of Unsaturated Oleo Chemicals

T. Seidensticker, J. Vondran, N. Herrmann, D. Vogt
TU Dortmund University, Laboratory of Industrial Chemistry, Dortmund/Germany
thomas.seidensticker@tu-dortmund.de

Renewable Resources, such as oleo compounds, have shown to be promising feedstocks in the synthesis of linear, bifunctional monomers for e.g. polycondensates by selectively attaching various functional groups to C=C double bonds. In these transformations, homogeneous transition metal catalysis certainly possesses greatest potential, regarding selectivity, atom economy and mild reaction conditions.

In a nutshell: Converting oleo chemicals into polymer precursors *via* homogeneous transition metal catalysis can play a great role in the future chemical industry from both, sustainability and economic aspects.

However, for such transformations to become competitive to existing synthesis routes and attractive to be run on a continuous and larger scale, different major challenges remain in the downstream process beyond chemistry: efficient product separation considering sufficient purity, recovery of the precious homogeneous catalyst including recycling, etc., only to name a few. Established concepts already operated in industry addressing these points are not applicable one-to-one to the conversion of oleo chemicals, due to their generally higher boiling points, their polarity and the usually very sensitive nature of the applied transition metal catalytic system.

Hence, for all the numerous homogeneously catalysed transformations of oleo chemicals towards the synthesis of polymer precursors, novel solutions for sustainable processes have to be developed in order to allow a successful and economically viable transfer into larger-scale.

In the present contribution, some of these concepts developed at TU Dortmund will be highlighted. Among these are thermomorphic solvents (TMS) systems and the innovative approach of selective product crystallization. Additionally, these concepts will be discussed with regard to potential implementation into continuous processes.

From Pheromones to Functional Polymers: Ring-Opening Polymerization of Macrolactones from Long-Chain Hydroxyacids

Andreas Heise

Department of Chemistry, Royal College of Surgeons in Ireland (RCSI), 123 St. Stephen's Green, Dublin 2, Ireland.
andreasheise@rcsi.ie

Recent advances in the ring-opening polymerisation (ROP) of macrolactones (MLs) have afforded access to novel, potentially degradable polymeric materials featuring long aliphatic chains. These developments extend the synthetic robustness and versatility of ROP to a greater range of interesting monomers, many of which can be derived from sustainable or renewable feedstocks, to access polymeric materials boasting a diversity of properties and potential applications. This paper will discuss current strategies to catalyse the ROP of MLs, and highlights recent developments in the preparation, functionalisation, and application of materials featuring poly(macrolactone)s (PMLs).

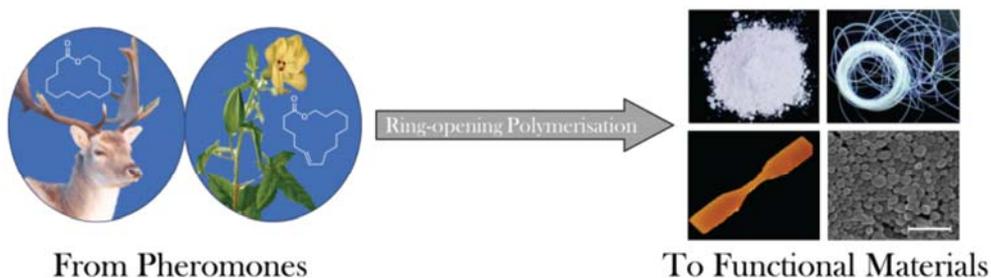


Figure 1: Saturated and unsaturated macrolactones can be polymerised into functional polymers and materials.

L13

Sustainable epoxidation of *Cynara cardunculus* seed oil with hydrogen peroxide

Rosa Turco, Riccardo Tesser, Rosa Vitiello, Vincenzo Russo, Martino Di Serio
Università di Naples Federico II, Department of Chemical Sciences, Napoli, Italy
diserio@unina.it

Cynara Cardunculus (Cardoon) is a Mediterranean region-native plant, which grows on arid and contaminant lands, in harsh habitat conditions, characterized by high temperature, salinity and drought. Therefore, it does not compete with edible resources. The Cardoon is botanically related to the sunflower. It can be considered as an oil crop; the seed yield has been estimated at 1.36 t/(ha year), the content of oil is about 25-33% with a composition based mainly on mono-, di- and triglyceride, similar to that of the sunflower. This work aimed to study of the epoxidation of Cardoon oil, as cheap, waste and non-edible oil, in order to obtain sustainable chemical products, addressed to be used in alternative to petro-based one in PVC or bioplastic. Cardoon seed oil was successfully epoxidized by hydrogen peroxide in presence of a commercial γ -alumina as heterogeneous solid catalyst. A strong influence of the impurities content on activity of alumina in epoxidation was observed. The presence alkali metals, such as sodium, were found to deactivate the medium-strength Lewis acid sites, leading a decrease of double bonds conversion. While an increase in SiO₂ content was found to ruin the selectivity to epoxide, through epoxy ring opening reactions.

Organocatalytic cleavage of fatty acid derivatives to aldehydes and esters

Nam Duc Vu, Souleymane Bah, Elsa Deruer, Boris Guicheret, Estelle Métay,
Nicolas Duguet and Marc Lemaire
University Lyon 1, Villeurbanne, France
nicolas.duguet@univ-lyon1.fr

The C=C bond(s) of unsaturated vegetable oil derivatives offers an excellent site for functionalization but also for cleavage reactions to give to valuable building blocks for a wide range of applications.

In this context, we have recently developed two complementary methods for the valorization of oleochemical 1,2-diols. First, the fatty diols were converted to the corresponding α -hydroxyketones through dehydrogenation^[1] and these derivatives were organocatalytically cleaved to aldehydes through a retro-benzoin process.^[2] Advantageously, both reaction proceed under solvent-free conditions. Moreover, the fatty α -hydroxyketones were further converted to the corresponding fatty 1,2-diketones that were cleaved to esters using organocatalysis.

The aldehydes and esters obtained through these methods are excellent building-blocks for the preparation of bio-based surfactants and polymers.

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Selective Oxidations of Unsaturated Fatty Acids and Bio-sourced Feedstocks

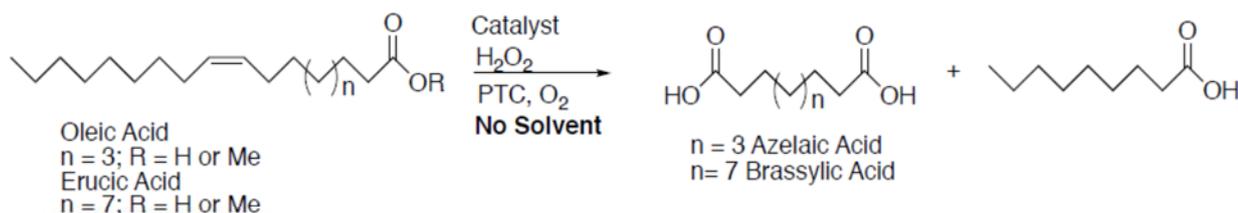
Mukund P. Sibi

Department of Chemistry and Biochemistry, North Dakota State University, Fargo, ND, USA

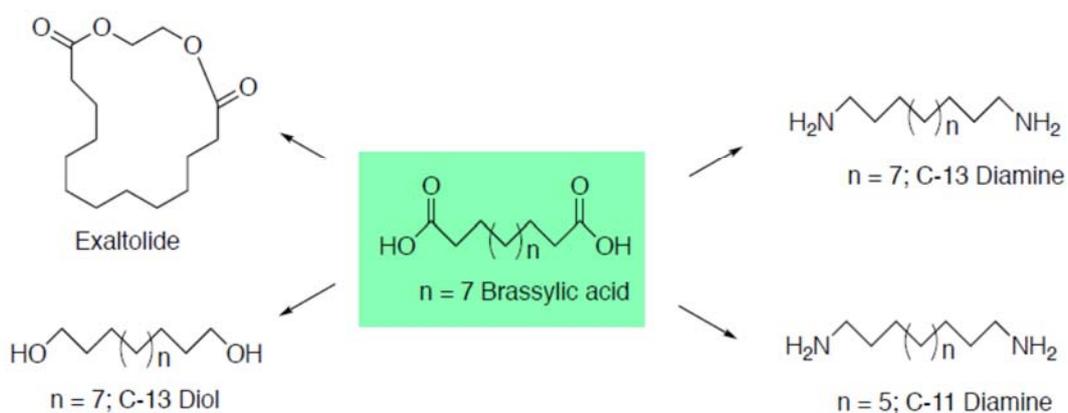
Mukund.Sibi@ndsu.edu

Oxidation plays an important role in the preparation of carboxylic acids which are valuable precursors for polyesters and polyamides. Our group has developed a green method for the synthesis of diacids from unsaturated fatty acids readily available from oil seeds. The preparation of azelaic and brassylic acids (Scheme 1) and their conversion to other monomers will be presented (Scheme 2). Additionally, a chemoselective oxidation of bio-sourced feedstocks to important furanics will also be presented.

Scheme 1. Green Oxidation of Unsaturated Fatty Acids Using Molecular Oxygen



Scheme 2. Conversion of Brassylic Acid to Useful Compounds



L16

Bioeconomy in figures - with a focus on the use of oils and fats in the chemical industry

Michael Carus
nova-Institut GmbH, Huerth, Germany
michael.carus@nova-institut.de

The presentation will show the latest market data on Bioeconomy in the European Union, nova-Institut is yearly providing the Bio-Based Industry Consortium (BIC) in Brussels. The data will include data on turnover, employment and bio-based shares for the European Union and the member states. In addition market data on bio-based building blocks and polymers (for the year 2018) will be presented.

After this general overview on status and outlook of the European Bioeconomy, the presentation will focus on the use of oils and fats in the (oleo)chemical industry in the world and especially in Europe. This will include castor oil, palm oil, rape seed oil any many others (including animal fats, used cooking oil, Glycerol) in a wide range of applications such as lubricants, polymers (PA, Epoxy, NOP, Bio-Naphtha). Here again a status and outlook will be presented.

Enhancing the physical-mechanical properties of vegetable oil-based waxes using simple, safe and sustainable chemical modifications

Eliane Goossens¹, Peter Tollington²

¹ Cargill R&D Centre Europe, Vilvoorde, Belgium

² Cargill Bio-Industrials Europe, Schiphol, The Netherlands

eliane_goossens@cargill.com

peter_tollington@cargill.com

Hydrogenated vegetable oils (HVOs) are increasingly finding application as a substitute for (semi)refined paraffin waxes; they offer good price economy, a wide range of melting points and a sustainable, renewable feedstock with consumer appeal.

Despite their positive credentials, HVOs display functional shortcomings that limit their use in applications originally developed around paraffin feedstocks. Specifically, paraffin exhibits excellent plasticity and cohesiveness, physical properties which are essential in e.g. paper coating and some candle-making processes, but are largely absent in HVOs.

In order to overcome these significant limitations, Cargill has investigated the modification of HVOs using simple and affordable chemical processes transferable to existing food refinery infrastructure. The goal of this work is to achieve “paraffin-like” properties in the modified HVOs (including smooth and predictable crystallization behavior), while retaining the attractive features of HVOs described earlier.

Partial (trans)esterification of the HVOs with other lipid-derived species was the synthetic route selected as a basis for the chemical modifications investigated. Formation of the resulting complex lipid mixtures was monitored using gel permeation chromatography, and detailed chemical characterization was carried out using high temperature gas chromatography coupled with mass spectrometry.

Crystal morphology was studied using microscopy and XRD, while thermal properties such as melting profiles were assessed using conventional solid fat content measurement (NMR) and DSC. Mechanical properties such as flexural and compressive strength, hardness and brittleness were quantified using a TA.XT plus texture analyser. The melting temperatures of the modified HVOs ranged between 40 and 60 °C. The hardness values ranged from 4 times softer to 2 times harder than beeswax. Brittleness values could be reduced below that of beeswax. The products showed a high cohesiveness and several did not break under compression.

The application of these advanced scientific tools has revealed new understanding of the structure-performance relationships in complex lipid mixtures. Our study confirms that HVOs can be modified to substantially match the textural characteristics of paraffin and beeswax. The versatile nature of the modification and blending techniques used allow for a wide range of thermal and mechanical properties, which can thus be tailored to the application of interest. Finally, the scalability of the synthesis was successfully demonstrated on a refinery pilot plant unit.

Current Development in biobased polyester : PRIC range

Marie REULIER

ITERG, Rue Gaspard Monge – ZA PESSAC – CANEJAN, 33610 CANEJAN, FRANCE
m.reulier@iterg.com

ITERG, in collaboration with the Laboratoire de Chimie des Polymères Organiques in Bordeaux, has developed, few years ago, a range of polyesters from vegetable oil. These estolides have been tested in different applications and their potential seem to be huge and still underestimated.

Their uses in packaging, cosmetics, lubricant are actually evaluated and performance improvements have been achieved. Due to constant innovation, new fields of application are targeted such as coatings, surfactants, or paraffin substitution.

About twenty polymers have been approved internally and ITERG is able to produce them at the ton scale. The interest of PRIC range is based on the ability to tune polyester structure according to customer needs.

Technico-economic and environmental assessments have helped to better position our products in relation to markets.



New Biobased Polyesters

A new range of biobased polyesters, with hydroxyl or carboxylic functionalities, is now available from ITERG.

This range consists of more than 95% renewable carbon and is compatible with REACH regulation.

GAMME PRIC

Markets
This range of polyesters offers number of potential applications as additives and platform biomolecules in fields of coating, paint, adhesive, lubricant, fuel, construction (insulation...), plastics and materials, cosmetics, automotive, packaging...

Performances
Hydrophobicity, plasticizer, texturizer, lubrication, reinforcement to shock, binder, water repellent....etc.

ITERG
Expert in Fats and Oils

> Polyesters Polyols

Functionality	Acid Value mg KOH/g	Hydroxyl Value mg KOH/g	Iodine value g Iode/100 g	Dynamic Viscosity 20°C mPa.s	Density 20°C	Molar Mass g/mol PS		% of Renewable Carbon Atoms	
						Mn	Mw		
PRIC 100	~1	≤ 1	25 – 35	85 – 95	900 – 1400	0.9 – 1	2200 – 3000	3800 – 5300	>95%
PRIC 100H	~1	≤ 1	15 – 30	< 5	2100 – 2600	0.9 – 1	2800 – 3100	5800 – 6500	>95%
PRIC 212	~2	≤ 1	70 – 80	85 – 95	600 – 800	0.9 – 1	2000 – 2300	2800 – 3200	>95%
PRIC 215	~2	≤ 1	170 – 180	80 – 90	300 – 400	0.9 – 1	1100 – 1300	1500 – 1700	>95%
PRIC 2205H	~2	≤ 1	16 – 20	< 10	2800 – 3500	0.9 – 1	2600 – 3300	5500 – 6800	>95%
PRIC 222	~2	≤ 1	55 – 61	70 – 80	900 – 1300	0.9 – 1	1800 – 2400	2500 – 3100	>95%
PRIC 222H	~2	≤ 1	55 – 61	< 10	1750 – 2150	n.d.	2400 – 3000	3300 – 4100	>95%
PRIC 225	~2	≤ 1	95 – 105	60 – 70	1200 – 1400	0.9 – 1	1600 – 2000	1900 – 2300	>95%
PRIC 225H	~2	≤ 1	95 – 105	< 10	1400 – 2000	0.9 – 1	1500 – 2300	1800 – 2700	>95%

> Polyesters Acid

Functionality	Acid Value mg KOH/g	Hydroxyl Value mg KOH/g	Iodine value g Iode/100 g	Dynamic Viscosity 20°C mPa.s	Density 20°C	Molar Mass g/mol PS		% of Renewable Carbon Atoms	
						Mn	Mw		
PRICA 100	~1	20 – 30	< 20	85 – 95	2000 – 2500	0.9 – 1	2500 – 3000	5000 – 5600	>95%
PRICA 100H	~1	20 – 30	< 20	< 10	4600 – 4800	0.9 – 1	3000 – 3600	6200 – 8600	>95%
PRICA 232	~2	75 – 85	< 20	85 – 95	2800 – 3200	0.9 – 1	1500 – 2000	2600 – 3000	>95%
PRICA 232H	~2	75 – 85	< 20	< 10	2800 – 3200	0.9 – 1	1500 – 2000	2600 – 3000	>95%

Description of the biobased polyesters range

***N,N*-Dimethylglucamine – A Sustainable Solution for Paints & Coatings**

Adriana Grossmann
Clariant Produkte (Deutschland) GmbH, Burgkirchen, Germany
adriana.grossmann@clariant.com

Sustainability is one of the five important pillars in Clariant's corporate strategy.[1] As a globally leading company in the field of speciality chemicals, Clariant puts strong emphasis on environmental protection and safety in all its activities.

A successful example for a sustainable product is Clariant's neutralizing agent Genamin® Gluco 50, which is a 50 wt% aqueous solution of *N,N*-dimethylglucamine in water. The structure of this speciality amine is derived from the renewable feedstock glucose and comprises a renewable carbon index of 75%. Only the two methyl groups of the amine functionality, arising from methylamine and formaldehyde, have a synthetic origin.[2] Additionally, *N,N*-dimethylglucamine is not only free of volatile organic compounds and semi volatile organic compounds but also completely hazard label-free for which reason it is suitable for ecolabeled paints. Other neutralizing compounds, such as aminomethyl propanol or ammonia are hazardous towards health and the environment and have furthermore no bio-based origin. The *N,N*-dimethylglucamine is therefore an ideal eco-friendly alternative. Moreover, it is multifunctional since it combines the neutralizing effect with its feature as compatibilizer and stabilizer. Therefore, less formulation work and less raw material handling are required than with the common single-purpose neutralizing agents.

In this presentation the advantages of Clariant's bio-based neutralizing agent *N,N*-dimethylglucamine are described in comparison to current products on the market.

[1] Integrated report 2017, Clariant. [2] Genamin® Gluco 50 has 8 carbon atoms, of which the sugar carbons (6) are renewable, i.e. the product has a RCI (renewable carbon index) of 75%. The other two carbons at the aminogroup are synthetic in origin.

Chemical Synthesis of High-Melting Bacterial Polyesters and Chemically Recyclable Polymers

Eugene Y.-X. Chen

Department of Chemistry, Colorado State University
Fort Collins, CO 80523-1872, United States
eugene.chen@colostate.edu

Poly(hydroxyalkanoate)s, naturally produced by bacteria and other living microorganisms from biorenewable resources such as carbohydrates and fats, are an important class of commercially implemented aliphatic polyesters as biodegradable and/or biocompatible materials. Typically, they are perfectly isotactic, crystalline materials possessing physical and mechanical properties suitable for substituting petroleum plastics, but their high production costs and low production volumes render them impractical in many applications as biorenewable and biodegradable "green" commodity thermoplastics. Hence, there has been increasing interest in synthetic equivalents of such polyesters via catalytic polymerization of renewable building blocks toward the cost-effective, large-scale production for commodity applications.

Current practices in the generation and disposal of synthetic polymers are largely unsustainable and also causing severe worldwide polymer pollution and an enormous materials value loss. Several solutions have been intensively pursued to address this global challenge but the current solutions suffer from either significant materials value and quality losses or unintended environmental consequences. The development of chemically recyclable polymers that can be completely and repeatedly depolymerized back to their building-block monomers for virgin-quality polymer reproduction provides a practical approach to achieving a circular economy and addressing polymer pollution. However, realizing such sustainable polymers must meet three challenges: energy cost, depolymerization selectivity, and depolymerizability/performance tradeoffs.

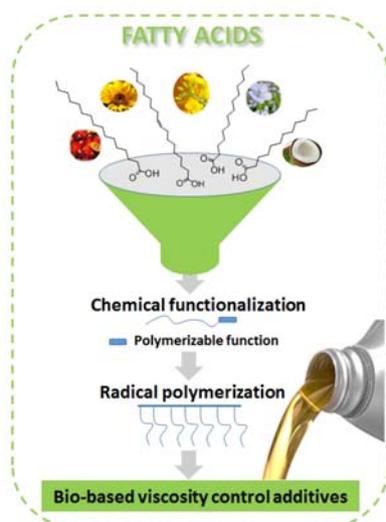
Centering on addressing the above identified challenges, this presentation will describe recent advances made in this field. In particular, the talk will focus on the chemical synthesis of stereoperfect, highly crystalline and high-molecular-weight bacterial polyesters as well as the discovery of infinitely recyclable plastics that are not only thermally and mechanically robust to be useful but also thermally and/or chemically depolymerizable with quantitative selectivity for clean monomer recovery under cost-effective production and deconstruction conditions.

Plant Oil-based Poly(Alkyl Methacrylate) as Viscosity Control Additive for Mineral and Vegetable Oils

Juliette LOMEUGE, Vincent LAPINTE, Claire NEGRELL, Jean-Jacques ROBIN,
Sylvain CAILLOL

¹ Institut Charles Gerhardt, CNRS UMR-5253, Ingénierie et Architectures
Macromoléculaires, 8, rue de l'Ecole Normale, 34296 Montpellier, France
Sylvain.Caillol@enscm.fr

Vegetable oils and their fatty acids (FAs) derivatives have become the most promising alternative solution to design performant bio-based polymers. The increasing success toward these renewable resources is explained by their wide availability, their low toxicity, as well as their reactive sites opening up various possibilities of functionalization. However, considering the poor reactivity of the internal unsaturation of FAs through radical process, most currently available synthesis of monomers reported in literature are limited to polycondensation. Consequently, there is an important challenge in providing monomers from FAs suitable for radical polymerization to provide bio-based vinyl polymers. For instance, poly(alkyl)methacrylate (PMAs) have known a significant widespread since the beginning of the 20th century in various applications and more especially as viscosity modifier additives for mineral oils. However, except some patents reporting the synthesis of acrylic acid from glycerol, the majority of common PMAs are originated from petroleum resources. Therefore, the objective of our work is to synthesize monomers from fatty acids bearing reactive function through radical process and evaluate their resulting methacrylate polymers as viscosity modifiers in various oils such as mineral or vegetable oils.



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Development of New Bio-based Innovative and Responsive Materials Based on Fatty Acid Derivatives

Kim Tremblay-Parrado, Luc Avérous,
BioTeam/ICPEES-ECPM, Université de Strasbourg, Strasbourg, France
khantutta-kim.tremblay-parrado@etu.unistra.fr

Living in an age of increasing environmental and sustainability concern, academics and industries have sought to diverge from fossil-based polymers by increasing the use of renewable resources from biomass.¹ Consequently, in the last quarter century, there have been important developments in oleochemistry. Vegetable oils, fats or even some microalgae are interesting sources of different triglycerides with particular structures. These latter have attractive chemical groups and high functionality allowing them to be used as platform chemicals for polymer synthesis.² For instance, considerable efforts have been made to replace the petrochemical based polyol components by modified oils or fatty acid derived polyols for polymers applications such as polyesters, polyurethane, etc.

The activity of our team (BioTeam) at University of Strasbourg (France) is focused on the development of new bio-based polymer systems for environmental and biomedical applications. Our research group looks at the synthesis of bio-based macromolecular architectures, and goes one step further by adding exclusive properties such as, remendability and recyclability, based on different approaches such as the thermo-reversible Diels-Alder reaction.³⁻⁵ The present work is dedicated to using click chemistry and thermo-reversible covalent bonds as crosslinking points in bio-based polyurethane. We have synthesized unique and novel architectures based on fatty acids of very high oleic sunflower oil (VHOSO) to serve as controlled crosslinking points in polyurethane chains. Derived from VHOSO fatty acids, these architectures are the first of their kind. VHOSO fatty acids were functionalized with furan and maleimide moieties. Insights of the VHOSO based novel structures were obtained by large range of chemical, physicochemical and mechanical characterizations. A short glimpse of the thermo-reversibility of our furan functionalized molecule is depicted in Figure 1. The aim is to vary the polymer architecture and study the subsequent effects on the physical properties, remendability and self-healing ability for a large range of applications (membranes, coating, etc.).

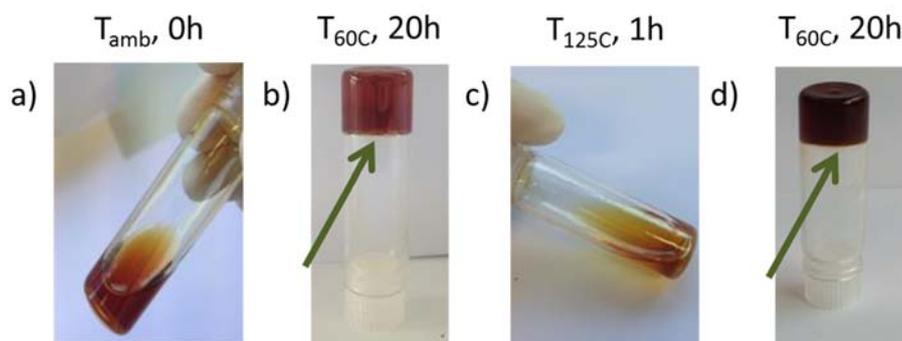


Figure 1: Illustration of the behaviour of the biobased materials with Diels-Alder and retro Diels-Alder reactions according to the temperature: (a) Furan functionalized VHOSO with bis-maleimide in DMSO; (b) Diels-Alder reaction allows for crosslinked architecture at 60°C; (c) retro-Diels-Alder takes place at 125°C with solubility in DMSO; (d) Diels-Alder reaction for re-crosslinked architecture at 60°C.

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Roots towards innovation in sustainable poly(2,5- furandicarboxylate)s polymeric materials

A.F. Sousa¹, M. Matos¹, M.J. Soares¹, A.J.D. Silvestre¹

¹ CICECO - Aveiro Institute of Materials, Departamento de Química, Universidade de Aveiro, 3810-193 Aveiro, Portugal
andreaifs@ua.pt

The issue of plastics is raising serious concern among scientists and the society at large. In fact, it is calculated that since the late 1950s' the total volume of polymers ever produced is 8.3 billion metric tons.¹ A realistic scenario points out that 5 billion metric tons are now accumulated in the landfills or the natural environment because they were prepared under the paradigm of stability, and not to be biodegrade. Additionally, they were/are based on fossil resources. The pollution is a serious issue!

In this context, this study tackles the demand for (bio-)degradable polymers derived from renewable-resources, but still having high-performance thermal and mechanical properties. In this study, 2,5-furandicarboxylic acid (FDCA) (or its di-methyl derivative) and different comonomers (e.g. poly(ethylene glycol) (PEG), poly(lactic acid) (PLA), 1,20-eicosanediol (M20), diglycolic acid), were used to prepare fully renewable polymers, namely the poly(1,4-butylene 2,5-furandicarboxylate)-co-poly((poly(ethylene glycol)) 2,5-furandicarboxylate) (PBF-co-PEGF),² poly(butylene 2,5-furandicarboxylate)-co-(butylene diglycolate)³ copoly(ester(ether))s; poly(ethylene 2,5-furandicarboxylate)-co-poly(lactic acid) (PEF-co-PLAs)⁴ copolyesters; poly(1,20-eicosanediyl 2,5-furandicarboxylate) (PM20F) homopolyester,⁵ among others. These polymers have both stiff aromatic-like units introduced by FDCA and soft aliphatic moieties due to the aliphatic comonomers used, thus modulating, the glass transition and melting temperatures, along with (bio-)degradation and hydrophobicity behaviour of the new materials.

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Sustainable Terpene-Based Biopolymers and Novel Functional Biomaterials

Malte Winnacker, Jacob Sag, Andreas Beringer, Bernhard Rieger
WACKER-Lehrstuhl für Makromolekulare Chemie and Catalysis Research Center,
TU München, Lichtenbergstraße 4, 85747 Garching bei München, Germany
Malte.winnacker@makro.ch.tum.de

Nature can provide a variety of renewable building blocks for the synthesis of sustainable and functional polymers, whose utilization is a key issue in modern polymer chemistry. This natural pool of compounds is interesting in terms of alternative feedstock and green chemistry in general, and especially with regards to significant molecules and structures, that can thus be utilized for the preparation of advanced materials and that are not so easily accessible via fossil-based pathways.^[1,2] In this context, terpenes are very versatile and suitable building blocks for the synthesis of sustainable polymers, due to their abundance, low costs and in terms of their interesting structures comprising e.g. side groups, stereocenters and/or additional functionalities.^[3] Polyamides are very important polymers for applications in many fields (commodities, automotive, biomedicine, ...), and their impact is growing. They are mainly synthesized via polycondensation of dicarboxylic acids and diamines or via ring-opening polymerization (ROP) of lactams. In this context, we investigate the transformation of cyclic biobased terpenoid ketones (e.g. menthone or nopinone (derived from pinene)) to polyamides via their lactams.^[4] This procedure works thus in analogy to the established fossil-based synthesis of polyamide 6 (polycaprolactam, nylon 6, Perlon®) and leads to novel sustainable polyamides with side groups and stereocenters, which have a very important impact on the properties of the resulting polymers.

We also investigate strategies for the utilization of suchlike polymers, their copolymers, blends and bioconjugates as biomaterials for the interactions with living cells.^[5] The properties of the components are thus combined, which results in enhanced features.^[6]

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Renewable polyamides via thiol-ene click' chemistry and long-chain aliphatic segments ^[1]

Phan Huy Nguyen, Steven Spoljaric, Jukka Seppälä

Polymer Technology, Department of Chemical and Metallurgical Engineering, Aalto University School of Chemical Engineering, P.O. Box 16100, 00076 Aalto, Finland

Thiol-ene 'click' chemistry was utilised to prepare dicarboxylic acid monomers containing two sulphur units within the backbone, which subsequently underwent polycondensation to yield a series of renewable, long chain, fatty-acid derived linear polyamides. The linear Sulphur-containing polyamides displayed number average molecular weights of 8000–55,000 g·mol⁻¹ and broad polydispersities biased towards higher weight fractions. Glass transition values were slightly above room temperature (31–35 °C), while melting temperatures ranged from 121 to 170 °C. This novel class of polymers exhibited an impressive property profile, most notably exceptional impact resistance, tear strength, high elasticity, very low water absorption yet high oxygen- and water vapour permeability. The presence of sulphur and the increased aliphatic segment length influenced a wide spectrum of polyamide properties due to the reduced amide linkage (and inter-chain hydrogen bonding) density and less-effective chain packing ability due to the increased atomic radii of the sulphur atoms. The data highlights the technical advantages of these polymers, while also expanding the repertoire and structure-property relationships of both long-chain- and sulphur-containing polyamides, and encouraging further development of polyamide derivatives from renewable sources.

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Sustainable Cellulose modification *via* transesterification using high oleic sunflower in a DBU-CO₂ switchable solvent system

K.N Onwukamike,^{1,2} S. Grelier,² E. Grau,² H. Cramail,² M.A.R. Meier¹

¹ Institute of Organic Chemistry (IOC), Materialwissenschaftliches Zentrum (MZE), Karlsruhe Institute of Technology (KIT), Straße am Forum 7, 76131 Karlsruhe, Germany.

² Laboratoire de Chimie des Polymères Organiques, Université de Bordeaux, UMR5629, CNRS - Bordeaux INP - ENSCBP, 16 Avenue Pey-Berland, 33607 Pessac Cedex France.
kelechukwu.onwukamike@kit.edu

Cellulose, as the most abundant carbon-based polymer in nature, which does not compete with food or feed, is a viable replacement for various un-sustainable fossil-based polymers. However, cellulose faces the challenges that it is not soluble in common organic solvents and also lacks any thermal transition, thereby making direct processing difficult.^[1] To address this insolubility in a sustainable fashion, an optimization of the recently described DBU-CO₂ switchable solvent system was performed.^[2,3] Upon optimization, up to 8 wt.% cellulose could be solubilized at 30 °C under mild CO₂ pressure (2-5 bar).^[4] Since ensuring sustainability during cellulose modification requires a consideration of the entire transformation process,^[5] we successfully carried out a direct transesterification of cellulose with high oleic sunflower oil, without any activating step, in this optimized DBU-CO₂ solvent system to obtain fatty acid cellulose esters (FACEs).^[6] Optimization of the reaction parameters (i.e., concentration, temperature, plant oil equivalents, as well as reaction time) was performed using microcrystalline cellulose (MCC) and followed by infrared spectroscopy (ATR-IR).^[6] Further confirmation of the FACEs structure was achieved via ¹H and ¹³C NMR, and ³¹P NMR revealed DS (degree of substitution) values of up to 1.59. An improved thermal stability after transesterification reactions (up to 30 °C by TGA) and good mechanical properties with an elastic modulus (E) of up to 478 MPa with elongation of about 35% were obtained. In this report, we thus demonstrated a more sustainable approach for the synthesis of FACEs that combines cellulose and plant oil (two renewable resources) directly (i.e. without any chemical modification), resulting in fully renewable polymeric materials with appealing properties.

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Non-isocyanate bio-based polyurethanes through reactive extrusion

Fiona Magliozzi,^{1,2} Etienne Grau^{1,2}, Guillaume Chollet³, and Henri Cramail^{1,2}

¹Univ. Bordeaux, LCPO, UMR 5629, F-33600, Pessac, France

²Bordeaux INP, LCPO, UMR 5629, F-33400, Talence, France

³ITERG, F-33610 Canéjan, France

fiona.magliozzi@enscbp.fr

Polyurethanes (PUs) are specialty polymers found in many markets, such as coatings, paints, elastomers, adhesives and, of course, foams. Nonetheless, the current industrial pathway for the synthesis of conventional polyurethanes involves the use of toxic isocyanates to react with polyols. The combination of fossil resources price variations together with environmental and health concerns pushes scientists to develop green chemistry strategies in the course of polymer synthesis. To that purpose, the development of bio-based monomers and the use of safe chemicals and processes are two main challenges that we tried to tackle in this study.

Indeed, among the routes to non-isocyanate PUs, the polyaddition between a bis-cyclic carbonate (bisCC) and a polyamine, leading to polyhydroxyurethanes, PHUs, bearing pendant hydroxyl groups linked to the polymer skeleton, is quite promising. Nevertheless, this pathway still presents some limitations such as a rather low reaction kinetics and the low PHUs' molecular weight generally obtained.

Herein, the improvements brought by the reactive extrusion, in comparison to bulk conditions, with respect to PHU synthesis were investigated.

The efficiency and main features of this process towards PHUs synthesis, was investigated with different BisCC/diamines systems. The PHUs so-formed were characterized according to the conversion ratios, molar masses, thermal properties and the reaction time needed to reach those values. A comparison with bulk conditions will be presented.

Epoxidized Sucrose Esters as a Platform Technology for High Performance Thermosets

Dean C. Webster

North Dakota State University, Fargo, North Dakota, USA

Dean.webster@ndsu.edu

Epoxidized sucrose esters are unique 100% bio-based epoxy functional vegetable oil-based materials having a compact, star-like molecular structure. Due to the high functionality, these materials lend themselves to the development of thermosets having good strength properties, equivalent to that of petrochemical thermosets. For example, when cured with cyclic anhydrides, thermosets having high modulus and strength are formed. Epoxidized sucrose soyate (ESS) can be cured using bio-based acids to yield thermosets that have fully bio-based content. ESS can also be further functionalized to enable additional crosslinking chemistries. Methacrylated ESS can be cured using free radical chemistry to yield thermosets useful for composites and additive manufacturing. Carbonated ESS can be cured with multifunctional amines to yield non-isocyanate polyurethanes. In all of these cases, the cured thermosets exhibit good hardness and tensile strength as a result of the large number of functional groups and the rigid nature of the sucrose core and have the potential of meeting the material requirements for many applications of thermosets in coatings, composites, and adhesives.

Recent Advances in Hydroformylation, Hydrohydroxymethylation and Hydroaminomethylation of Oleochemicals

Eric Monflier

University of Artois, Unité de Catalyse et Chimie du Solide, UMR CNRS 8181, Faculté des Sciences Jean Perrin, Rue Jean Souvraz, 62307 Lens, France
eric.monflier@univ-artois.fr

To address key sustainability challenges, it is now necessary to develop eco-friendly alternatives to the use of petroleum resources. As such, the valorization of vegetable oils into added-value products has become of major interest. In particular, the direct functionalization of the carbon-carbon double bonds of triglycerides is of major interest to access biosourced building blocks with unique molecular and functional properties.

The hydroformylation, hydrohydroxymethylation or hydroaminomethylation of vegetable fatty compounds are well-known reactions that enable the direct conversion of internal carbon-carbon double bonds into aldehydes, alcohols or amines. These catalytic reactions are atom-economic and can be implemented under homogeneous, heterogeneous, or biphasic conditions. [1-2]

In this presentation, the recent developments in this field will be discussed and commented upon. A special focus will be put on the rhodium catalysed hydroformylation of oleochemicals in an aqueous-organic two-phase system [3] and on cascade reactions such hydrohydroxymethylation [4] or hydroaminométhylation [5] of vegetable oils under homogeneous conditions.

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Renewable building blocks for potential use in coatings

Eva Malmström^{1,3}, Arne Stamm^{1,2}, Linda Fogelström^{1,3}, Per-Olof Syrén^{1,2,3}, Sara Brännström¹, Mats Johansson^{1,3}

¹ KTH Royal Institute of Technology, School of Engineering Sciences in Chemistry, Biotechnology and Health, Dept. of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

² Science for Life Laboratory, Box 1031, SE-171 21 Solna, Sweden

³ Wallenberg Wood Science Center (WWSC), Dept. of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden
mavem@kth.se

Today, 99 % of plastics produced globally are based on fossil-resources. With depleting fossil-resources and increasing environmental awareness it is of utmost importance to identify bio-based resources, available in sufficient amounts, that can be used to produce more sustainable polymers, preferably with properties superior to those of fossil-based counterparts.

Side-streams from the pulp industry may provide sufficient amounts of compounds, however, building blocks from wood, or other plant materials, are not always well suited for polymerization due to an inert structure or presence of several functional groups. Enzyme catalysis may prove very useful in this respect; to equip inert building blocks with sufficient reactivity and/or to effectively perform the polymerization. Enzyme catalysis is particularly interesting where moderate molecular weights are required, such as compounds for coatings.

The scope of the present contribution is to describe some of our recent findings related to our efforts towards renewable monomers suited for UV-curable coatings.

Abstracts

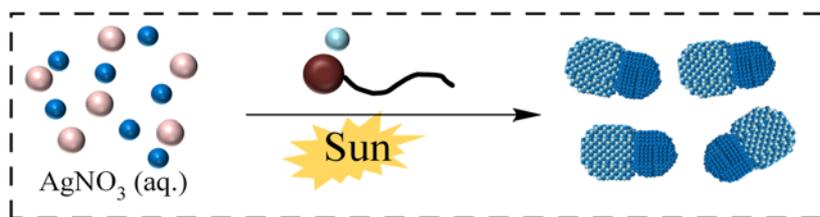
Part 2: Posters

Sustainable Preparation of Catalytically Active Ag/AgBr Janus Nanoparticles Under Sun light using Renewable Surface Active Ionic Liquid

Gurbir Singh, Komal, and Tejwant Singh Kang*

Department of Chemistry, UGC Sponsored Centre for Advanced Studies (CAS-II), Guru Nanak Dev University, Amritsar-143005
 komalchem11@gmail.com; tejwant.chem@gndu.ac.in

The development of photoactive materials sensitive to visible light employing a sustainable approach is highly required due to vast abundance, renewability and non-hazardous nature of visible light. Irradiation of $\text{AgNO}_3(\text{aq.})$ containing nicotinium based ester functionalised renewable surface active ionic liquid (SAIL)¹ having Br⁻ as counter-ion under sunlight results in the formation of Ag/AgBr Janus nanoparticles (JNPs) in less than a minute. The used renewable SAIL have been derived using nicotine (found in the leaves of *Nicotiana rustica*, in the tobacco plant)² and lauryl alcohol (fatty alcohol). The use of renewable sources i.e. sunlight and non-cytotoxic SAIL makes the process a greener and sustainable one for the synthesis of catalytic active Ag/AgBr JNPs. The synthesized NPs have been characterised by X-ray Diffraction spectroscopy (XRD), Energy Dispersive X-ray spectroscopy (EDAX), Transmission Electron Microscopy (TEM) and UV-Visible spectroscopy. The Ag species nucleates and grows from single specific point on the surface of AgBr and results in symmetry breaking growth of Ag. Ag/AgBr JNPs exhibit efficient catalytic activity for photo-degradation of Rhodamine-B under sunlight as well as towards reduction of 4-nitophenol in comparison to other anisotropic Ag/AgBr NPs



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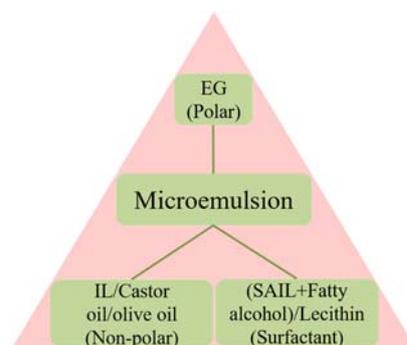
Inherently Green and Thermally stable Microemulsions

Manvir Kaur, Gurbir Singh, Tejwant Singh Kang*

Department of Chemistry, UGC-Centre for Advance Studies – II, Guru Nanak Dev University, Amritsar 143005, India

manvir.chem@gmail.com; tejwant.chem@gndu.ac.in

Thermally stable microemulsions with enhanced environmental sustainability are of great importance as use of organic solvents with high vapor pressure renders the microemulsions as thermally unstable and toxic, and limits their application area. Considering the thermal stability of earlier reported microemulsions (MEs) based on ethylene glycol, surface active ionic liquids and fatty alcohol (decanol as co-surfactant) and hydrophobic ionic liquid (IL),¹ we here in conceptualized and formulated MEs using renewable feed-stocks like castor oil/olive oil (non-polar medium), lipids such as lecithin (surfactant) and ethylene glycol (polar media). The use of renewable feed-stocks not only enhanced the sustainability of MEs but also offered thermal stability to ternary systems. Phase behavior of ternary systems has been characterized and different phases are identified using electrical conductivity measurements. Temperature dependent UV-visible, steady-state fluorescence and DLS supports the thermal stability of formed microemulsions in the temperature range of 25-75 °C. These thermally stable and relatively greener microemulsions along with earlier reported high temperature stable IL-in-Oil microemulsions^{2,3} could be utilized for different applications such as enhanced protein or enzyme stability and high temperature preparation of nanomaterials and drug delivery.⁴



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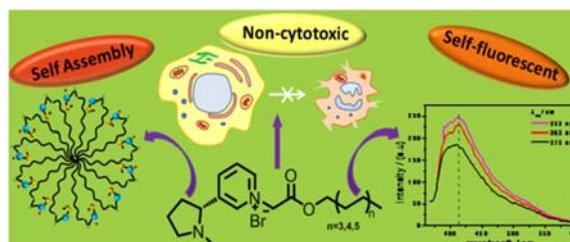
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Nicotine-based Renewable Surface Active Ionic Liquids: Self-assembly and Their Application as Greener Oil Herding Agents

Gurbir Singh,[†] Raman Kamboj, Venus Singh Mithu,[†] Vinay Chauhan, Taranjeet Kaur,[#] Gurcharan Kaur,[#] Sukhprit Singh,^{†,*} Tejwant Singh Kang^{†,*}

[†]Department of Chemistry, UGC-centre for Advance Studies – II, [#]Department of Biotechnology, Guru Nanak Dev University, Amritsar, 143005, India.
gurbirchem.rsh@gndu.ac.in; tejwant.chem@gndu.ac.in

Fatty acids and their respective methyl esters, amines, and alcohols derived from oils and fats of vegetable/animal origin are widely used for the production of important products groups, such as surfactants¹, lubricants, and coatings.² Surface



active ionic liquids (SAILs) have emerged as important class of ionic liquids and have proved to be better surface active agents than the conventional surfactants. Here in ester functionalized nicotine based renewable SAILs, $[C_nENic][Br]$ ($n = 8, 10$ and 12)³ have been synthesized using fatty alcohols (Capryl, Capric and Lauryl alcohol) and nicotine via energy and cost effective synthetic procedure. The critical micelle concentration, cmc , of synthesized SAILs was found to be 2-3 fold lower than homologous SAILs or conventional cationic surfactants. ¹H NMR, spin-lattice (T_1) relaxation time and 2D ¹H-¹H ROESY measurements have been exploited to get detailed account of internal structure of micelle. The size and shape of the micelles have been explored using dynamic light scattering (DLS) and transmission electron microscopy (TEM) measurements. The non-cytotoxic nature of investigated SAILs towards C6-Glioma cell line as well as highly surface activity at air-water interface makes them the potent greener oil herding agents for tackling the global problem of oil spilling into the oceans, which have been investigated.

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Green Initiative to Prepare Glass Fibre Reinforced Composite based on Vegetable Oil Polyester Thermoset Matrices

Abhishek Chowdhury, Prashant Anthony
Sam Higginbottom University of Agriculture, Technology And Sciences,
Allahabad, Uttar Pradesh, India
abhishek.chowdhury2089@gmail.com

Petroleum based plastics, though conventional and economically preferred, remain resistant to biodegradation and constitute a major proportion of non-biodegradable landfills. The world has become increasingly conscious not only about environment but how human activities can lead to negative consequences on the survivability of succeeding generations. Keeping the existing scenario in mind, there have been several researches to explore the synthetic procedures for biodegradable polymers and composites that could be an alternate to conventional polymeric materials. In this paper, FRP composites based on vegetable oil based unsaturated polyester resin (UPRs) is developed as a sustainable alternative material for various industrial application. We have synthesized vegetable oil based polyester resin using the two stage alcoholysis-polyesterification process involving a mixture of propylene glycol and oil with anhydrides in different ratio. The synthesized UPRs were characterized and compared with commercially available products for their thermo-mechanical properties. Thermal stability of the cured UPRs was studied by Thermogravimetric analysis (TGA) and Differential thermal gravimetric (DTG). The onset thermal degradation temperature (T_{onset}) of the synthesized cured resin (CR-2) is at 136°C. Other parameters such as statistic heat-resistant index (T_s) and the integral procedural decomposition temperature (IPDT) were further calculated from TGA plot. The value of T_s and IPDT of CR-2 is 142 °C and 494 °C respectively. Further the comparison of mechanical properties of the synthesized composites with the commercial resin composites reveals that (15-20%) reduction in tensile strength and modulus. Thus, the synthesized composites obtained from raw materials of vegetable origin were biodegradable in nature and had demonstrated compromisable reduction in properties.

Oxidative processes towards 12-OPDA as a precursor of jasmonic acid

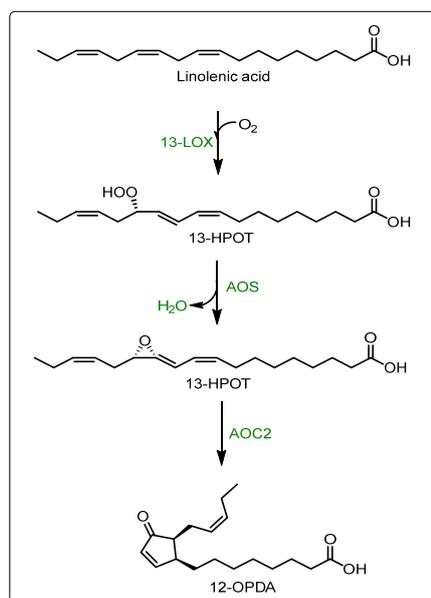
Jana Löwe, Karl-Josef Dietz and Harald Gröger
 Chair of Organic Chemistry I, Faculty of Chemistry, Bielefeld University, Bielefeld,
 Germany
jana.loewe@uni-bielefeld.de

Jasmonic acid is used as a fragrance in perfume industry.^[1] In 2006, 8000 t/a of jasmonate and derivatives were produced.^[2] Because of its high demand and complex chemical synthesis the biocatalytic approach towards jasmonate represents a promising alternative.

The pathway of jasmonic acid synthesis in plants was found in 1984 by Vick and Zimmerman (see figure).^[3]

Jasmonic acid and its precursor *cis*-(+)-12-oxo phytodienoic acid (12-OPDA) are responsible for stress regulation and development.^[4] 12-OPDA also shows pharmacological activity towards mammalian cells.^[5]

The process of jasmonate synthesis starts in the chloroplast by liberation of linolenic acid (α -LA) out of the chloroplast membrane. The lipoxygenase (13-LOX) catalyzes the oxygen insertion at position 13 in the aliphatic unsaturated chain of α -LA. The originated



13-HPOT is converted by an allene oxide synthase (AOS). The unstable peroxide cyclizes without an enzyme to racemic 12-OPDA, whereas in the presence of allene oxide cyclase the reaction is catalyzed to *cis*-(+)-OPDA. The cyclopentenone is then reduced *via* an ene-reductase (OPR3) to cyclopentanone in the peroxisome. Afterwards the aliphatic chain is reduced *via* β -oxidation. In literature, already some enzymatic synthesis of the high cost, low value chemical 12-OPDA on analytical scale are shown^[6], also under participation of our group.^[6d] Due to the pharmacological and industrial relevance we are interested in a biocatalytic production of 12-OPDA on a larger scale, as well as in the formation of 12-OPDA-derivatives through esterification and metathesis reaction.

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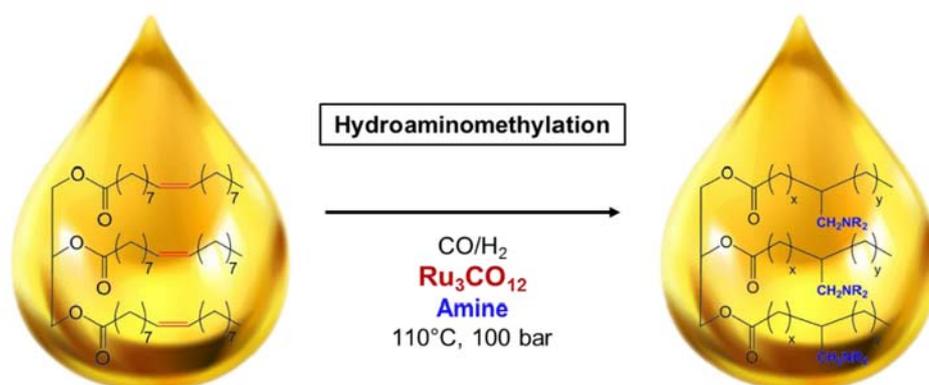
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Ruthenium-catalyzed hydroaminomethylation of vegetable oils

Kévin Cousin, Frédéric Hapiot, Eric Monflier
 Univ. Artois, CNRS, Centrale Lille, ENSCL, Univ. Lille, UMR 8181, Unité de Catalyse et
 Chimie du Solide (UCCS), F-62300 Lens, France
 kevin_cousin1@ens.univ-artois.fr

Amines are important building blocks in the synthesis of chemicals and find a wide range of applications such as polymers, pesticides or the pharmaceutical industry. Hydroaminomethylation (HAM) represents an atom-economic efficient of this class of compounds. HAM are usually carried out HAM reactions in the presence of phosphines,^{1,2,3} or under water gas shift (WGS)⁴ or reverse water gas shift (RWGS)⁵ conditions. Here we have been interested in the ruthenium-catalyzed HAM of triglycerides derived from vegetable oils in the presence of phosphine or amines. Excellent amine selectivities (> 90%) were obtained at 100 °C under 100 bar CO/H₂. The Ru-catalyzed system was compared to a rhodium-based catalytic system. Extension of the studied Ru-based system to other biosourced substrates is also discussed.



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Retardation of lipid oxidation in (o/w) and (w/o) emulsion systems with addition of natural terpene molecules

Olivia Dhara* and Mahua Ghosh

Department of Chemical Technology, University College of Science and Technology, University of Calcutta, Kolkata, West Bengal 700009, India
olivia.dhara@gmail.com

Lipid oxidation is a major cause for deterioration of food quality. In presence of high levels of oxidation prone substances like polyunsaturated fatty acids, control of lipid oxidation becomes a major challenge for the food industry. The present work focused on addition of 1% (w/w) active components of essential oils, namely carene, pinene & linalool with known anti-oxidative behaviour to popular emulsion systems namely, margarine (w/o) and mayonnaise (o/w), prepared using refined rice bran oil. Acid value (AV), peroxide value (PV), and p-anisidine value, were determined periodically to check the status of oxidation. It was found that carene could retard lipid oxidation in both the emulsion systems. However, in margarine (w/o), carene added samples showed more primary oxidation but decreased secondary oxidation with less increase in p-anisidine values. While in mayonnaise(o/w) system it showed overall decrease in oxidation. Hence from the results it can be concluded that carene could successfully prevent lipid oxidation over a considerable time span, where as other two couldnot. Further research in this regards can lead to replacement of synthetic anti-oxidants with bio-renewable terpene molecules for controlling stability of emulsions. It may provide added nutritional benefits also in in-vivo systems.

Functionalized polyurethanes for surface coatings

Philipp Schmidt, Steven Eschig
Fraunhofer Institute for Wood Research Wilhelm-Klauditz-Institut WKI, Braunschweig,
Germany
philipp.schmidt@wki.fraunhofer.de

Click reactions have become more and more prominent in the field of material science. A relevant used example is the [4+2]-cycloaddition of maleimides and furans.^[1] In this work we describe the synthesis of furfurylated polyurethanes, which were functionalized with fatty acid based maleimides to create hydrophobic surfaces. Access to maleimides gives a simple and economic two-step synthesis developed by us.^[2] In the first step, maleic anhydride is reacted with different natural mixtures of bio-based fatty amines to give the corresponding maleamic acids. The formation of the 5-membered maleimide-rings is achieved via acid-catalyzed intramolecular condensation. We achieved the poly-urethane by reacting combinations of 1,6-hexane diisocyanate (HDI), isophorone diisocyanate (IPDI) and 4,4'-methylene diphenyl diisocyanate (4,4'-MDI), polyethylene glycol 400 (PEG 400) and a furan containing diol compound. The diisocyanates and PEG 400 are commercially available. The furan containing diol was obtained via Michael-Addition described by Tseng et al.^[3] Two equivalents of hydroxyl alkyl acrylates were reacted with two equivalents furfurylamine. The furan containing diol was obtained in quantitative yields. For a [4+2]-cycloaddition the furan-functionalized polymer and N-alkyl maleimides were reacted with each other. The use of fatty acid based N-alkyl maleimides allows the introduction of hydrophobic properties. Covalent bonding was proved through ¹H-NMR measurement. Contact angle measurements show the hydrophobic properties of the functionalized polymer. This technique is interesting for the development of new coatings and allows the adaption of surface properties in a wide range.

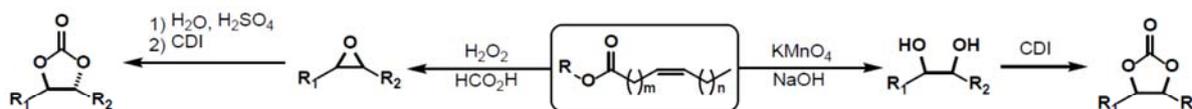
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Stereo selective synthesis of cyclic carbonates based on renewables

Vivian Stefanow, Thomas Werner
 Leibniz Institute for Catalysis at University of Rostock, Rostock, Germany
 vivian.stefanow@catalysis.de

The utilization of renewable resources as an alternative feedstock to petrochemicals has attracted much attention in recent years.^[1] For example readily available and inexpensive vegetable oils derivatives are used in chemical industry as plasticizers and stabilizers.^[2] Fatty acid esters bearing cyclic carbonate functionalities are used directly as plasticizers in PVC and have been shown to be significantly more sustainable than commonly employed alternatives.^[3] For this reason, the synthesis of these compounds is extensively researched and mostly focused on the use of epoxides or diols as intermediates.^[4] Lately, we introduced a bifunctional organocatalytic systems^[5] and an efficient Ca-based catalyst^[6] on the cyclic carbonate synthesis. A drawback of the cyclic carbonate synthesis is the moderate stereo selectivity.^[7] Therefore, we were interested in a stereo selective synthesis cyclic carbonates and hereto found a synthetic route starting from unsaturated fatty acid esters within two or three reaction steps. Four different derivatives with over all yields up to 68% yield for the *cis* carbonates and up to 59% yield for the *trans* carbonates were described.



Scheme 1: Stereo selective synthesis of *cis* and *trans* carbonates derived from fatty acid esters.

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Synthesis of bio-sourced Non-Isocyanate Polyurethanes and their incorporation into water-borne NIPU-Acrylic hybrid systems

Boris Bizet^{1,2}, Étienne Grau¹, José M. Asua², Henri Cramail¹

¹LCPO – UMR 5629, Université de Bordeaux, CNRS, ENSCBP / Bordeaux INP – 16, Av. Pey Berland, F-33607 PESSAC Cedex, France

²POLYMAT, University of the Basque Country UPV/EHU, Centro Joxe Mari Korta – Avda. Tolosa 72 – 20018 Donostia-San Sebastián, Spain
boris.bizet@enscbp.fr, boris.bizet@polymat.eu

Depleting fossil resources as well as fluctuating oil prices have raised scientific concerns about finding more sustainable ways for making consumer goods. This made the concept of biorefinery – a chemical unit processing and transforming biomass into feed, food, energy and chemicals to form value-added products – grow and become a new paradigm.^{1,2}

Moreover, the polyurethane industry is aiming at developing new benign ways of synthesizing the desired products through isocyanate-free routes, yielding Non-Isocyanate PolyUrethanes (NIPUs). In this context, the formation of poly(hydroxy)urethanes (PHUs) through the aminolysis of bis-cyclic carbonates by diamines has gained a lot of interest. Vegetable oils, by their versatility and wide availability, are very often used as sources of monomers.³ However, the industrial implementation of the formed PHUs is often limited due to the low molecular weights obtained as well as the processes at stake in their synthesis. These remain nowadays the most challenging limitations in the field.⁴

In this talk, we introduce a bulk polymerization pathway towards the formation of functional materials from PHUs. The optimization of the reaction conditions allowed for the reaction of a wide range of ester-activated bis-cyclic carbonates as well as diamines. On the one hand, a broad library of NIPUs, exhibiting various degrees of crystallinity and thermal properties was obtained and will be discussed in the specific case of rigid NIPUs. On the other hand, the incorporation of flexible NIPUs into water-borne systems will be described through the example of miniemulsion polymerization of high-solid content PHU-Acrylic formulations.

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P11

Agglomerated stone materials based on acrylated vegetable oils as thermosetting binder

Stefano Zeggio, Fabio Bassetto
Breton SpA, Castello di Godego, Italy
bassetto.fabio@breton.it

Unsaturated polyester resins (UPr), dissolved in styrene, are widely used as binders to aggregate stone and other inorganic raw materials for producing agglomerated stone materials using vibratory compaction in a vacuum environment, patented worldwide as Bretonstone® Technology. The use of UPr involves some technical drawbacks: both resin and styrene monomer are oil-based, hence they come from non-renewable sources and their cost mainly depends on the value of crude oil; due to its high volatility rate, styrene is a dangerous chemical, which involves the designing of complex and expensive intake and burning plants. Many efforts have been dedicated for the development of alternative thermosetting able to overcome these difficulties.

We have found that acrylated epoxidized vegetable oils can be used as alternative resins if they are crosslinked by suitable acrylic monomers/oligomers, initiators and curing conditions. New resins contains more than 50% by weight of renewable raw materials and contains no volatile organic components. The properties of both new thermosetting resin and compound stones produced in this way are even better than traditional ones. In particular, the mechanical properties (such as the flexural strength and the water absorption) and the aesthetic effect (valuated technically by the gloss value) of the industrial slab remain constant, but the resistance to weather conditions (evaluated by QUV panel) is increased. The latter feature permits the use of compound stone in many outdoor applications.

Sustainable synthesis of bio-based surfactants from cashew nutshell liquid (CNSL)

Valentina Bragoni, J. Pollini, R. K. Rit, R. Kirchmann, A. S. Trita and Lukas J. Gooßen
Ruhr Universität Bochum, Universitätsstr 150, 44801, Bochum (Germany)
Valentina.bragoni@rub.de

Cashew nutshell liquid (CNSL) is an inedible waste by-product (1.000.000t/a) of the cashew nut processing. It is an excellent candidate for the synthesis of bio-based synthetically valuable compounds, as its production does not compete with the land use for food production.^[1,2] CNSL is a mixture of phenols bearing a 15-carbon side chain with different degrees of unsaturations.^[3,4]

We have developed an eco-friendly and waste minimised concept for the synthesis of amine-based surfactants from CNSL (Fig. 1).^[5] The key step of the procedure is a reductive amination of CNSL with molecular hydrogen and palladium on charcoal, in water. The resulting cyclohexyl amine derivatives were further converted into *N*-oxide, betaine and quaternary ammonium tensides. Their surfactant properties (surface tension and critical micellar concentration) have been determined and resulted comparable with those of state-of-the-art commercial tensides, opening up a wealth of commercial applications. In the case of the *N*-oxide, a one-pot synthesis with an E-factor of 2 was realized in water as the sole solvent.

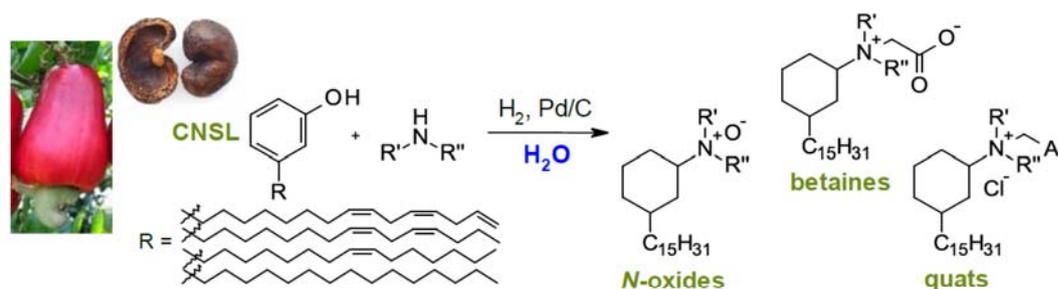


Figure 1. Synthesis of surfactants from CNSL

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Selective product crystallization as a recycling strategy in the methoxycarbonylation of renewable resources

N. Herrmann, D. Vogt, T. Seidensticker, TU Dortmund University, D-44227 Dortmund, Germany
normanherrmann@tu-dortmund.de

Environmental awareness and sustainability are becoming increasingly important in the chemical industry. The use of renewable resources in chemical processes can be a significant contribution in this. Oleo compounds have proven to be promising raw materials in the synthesis of bifunctional monomers for e.g. polycondensates by selectively attaching various functional groups to C=C double bonds. In these transformations, homogeneous transition metal catalysis has a great potential in terms of selectivity and atom-economy. The conversion of renewable resources into polymer precursors can play a major role for the chemical industry both from a sustainability and an economic point of view.

To this end the transformations of renewable feedstocks must become more efficient and competitive to existing routes, especially in view of large scale and continuous operation. In downstream processing, various challenges remain: recovery and recycling of the valuable homogeneous catalyst and efficient product separation and purification. Established industrial processes cannot be adapted one-to-one to the conversion of renewable resources due to significant differences in polarity, boiling points and other properties.

For numerous homogeneously catalyzed transformations of renewable resources for the synthesis of polymer precursors, new solutions for sustainable processes must therefore be developed in order to enable an economic, successful and meaningful transfer to a larger scale.

This poster will present an innovative approach for the Pd-catalyzed methoxycarbonylation of methyl oleate, largely obtained from sunflower oil (Figure 1). By subsequent product crystallization two essential aspects are ensured in this context: The efficient and gentle product separation from the catalyst with the recycling of the latter and the simultaneous recovery of a high-purity monomer for polycondensation.



Figure 1 Methoxycarbonylation of methyl oleate to highly linear dimethyl 1,19-nonadecanedioate

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Castor Oil Based Polyurethane Perlite Composites with Low Thermal Conductivity

Gokhan CAYLI, Milkah Wairimu MURUMI
Istanbul University Cerrahpasa, Istanbul, Turkey
gokhan.cayli@istanbul.edu.tr

Due to the environmental concerns, finding of environmentally friendly and energy saving materials is one of the most interesting subjects [1-2]. In this study, castor oil (CO) was mixed with PMDI (polymeric diphenylmethane diisocyanate) and perlite in order to obtain a building block with low thermal conductivity for construction applications. Castor oil-PMDI mixture contains 78 % CO and 22 % of PMDI that means main body of this mixture is a bio based material. Castor oil is a naturally functionalized plant oil triglyceride and it contains 90 % of ricinoleic acid [3]. Perlite is an amorphous volcanic glass and contains approximately 1-3 % water [4]. If it is exposed to heat, it expands 7-16 times to its original volume. Expanded perlite is a good thermal insulator [5]. This study revealed the thermal and mechanical properties of castor oil-PMDI and perlite composites. Castor oil-PMDI polymer had 700 kg/m³ density and 0,15 W/mK thermal conductivity and showed 3-4 MPa compression strength. Densities of perlite composites of CO-PMDI polymer varied from 700 kg/m³ to 200 kg/m³ and thermal conductivities changed from 0.7 to 0.05 W/mK depending on the perlite amount. The highest compressive strength was observed as 6-7 MPa for the composite that contained 30 % perlite.

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New Series of Epoxidized Sunflower Oil Based Flame Retardant Monomers: Synthesis and Characterization

Gokhan CAYLI, Necla BEKTAS, Demet GURBUZ, Adem CINARLI
Istanbul University-Cerrahpasa, Istanbul, Turkey
gokhan.cayli@istanbul.edu.tr

Plant Oil triglycerides are important materials because they are readily available and many chemicals can be synthesized from those materials [1]. One of the current research topic is the synthesis of flame retardant monomers and polymers from renewable resources. Additionally, there is a great need to synthesize non halogen containing flame retardant compounds [2]. In this study, sunflower oil based phosphorus containing flame retardant monomer is introduced. For this purpose, maleic anhydride was reacted with 2-chloroethanol first. Then, epoxidized sunflower oil was reacted with 2-chloro ethyl maleate. The final product is an orange colored liquid and contains a reactive halogen group and it gave corresponding phosphonates through Arbuzov reaction. Characterization of the materials were performed by FTIR and ¹H NMR spectrum

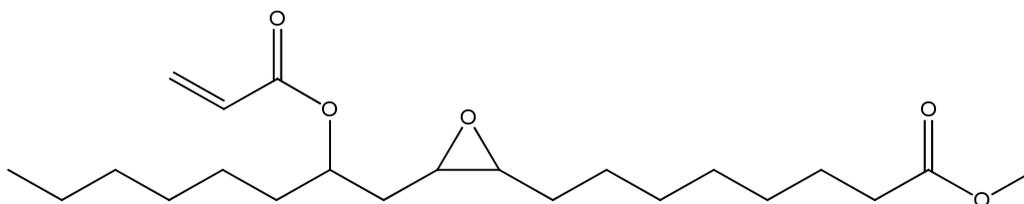
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Synthesis and Characterization of Epoxy Acrylate Derivative of Methyl Ricinoleate

Gokhan CAYLI¹, Pinar CAKIR HATIR²,
¹ Istanbul University Cerrahpasa, Istanbul, Turkey
² Istanbul Arel University, Istanbul, Turkey
gokhan.cayli@istanbul.edu.tr

When considering environmental concerns, it would be necessary to find a versatile monomers from renewable resources with easy synthetic procedures. Our group formerly discovered epoxy acrylate derivatives of castor oil [1-2]. Although they are versatile materials, their functionalities and viscosities are high. Thus, unwanted side reactions such as crack formation and phase separation, during polymerization can be sometimes observed. To solve this problem, fatty acid methyl ester based epoxy acrylate was synthesized in this work. This monomer is small, non-viscous and has low viscosity. Castor oil was transesterified with methanol via base catalyzed two-step transesterification reaction [3]. Methyl ricinoleate, then, acrylated with acryloyl chloride. The obtained acrylated methyl ricinoleate than epoxidized via Prilezhaev reaction. This monomer contains one acrylate and one epoxy groups and polymerization of AMR gave linear polymer.



The structure of epoxidized acrylated methyl ricinoleate

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Polymerization of PEP Resole with Different Types of Oils

Gokhan CAYLI¹, Pinar CAKIR HATIR², Selim KUSEFOGLU³

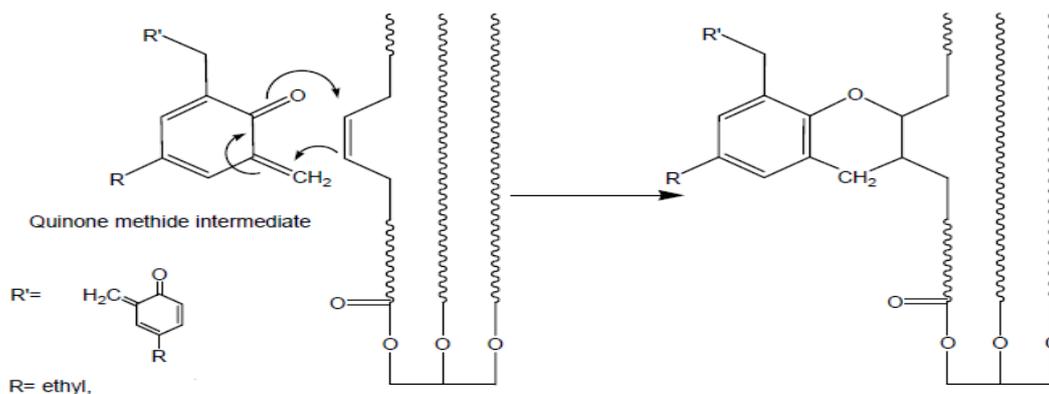
¹ Istanbul University-Cerrahpasa, Istanbul, Turkey

² Istanbul Arel University, Istanbul, Turkey

³ Bogazici University, Istanbul, Turkey

gokhan.cayli@istanbul.edu.tr

Use of the plant oils in chemical industry has three main advantages. Plant oil triglycerides are renewable, they can be used as poly reactive monomers and they usually lead to biodegradable polymers. Due to the resemblance of rubber and plant oil triglyceride double bonds, plant oil triglycerides can be directly polymerized by vulcanizing agents. Many type of vulcanizing agent can be used for this purpose, among them *p.ethyl* phenol based vulcanizing agents were assessed in this study. According to the proposed mechanism, *p.ethyl* phenol resole loose water at elevated temperatures and reactive quinone methide intermediate is produced. Through an Ene reaction, rubbery polymers were obtained. Regaining of the aromatization was the driven force. Thermal and mechanical properties of *p.ethyl* phenol resole adducts of cod liver, linseed and soybean oils were also evaluated in this study.



Proposed reaction mechanism of phenolic vulcanizing agents and plant oil triglycerides

Epoxy Derivative of Maleate Ester of Castor Oil: A New Alternative to Unsaturated Polyesters

Gokhan CAYLI¹, Pinar CAKIR HATIR²

¹ Istanbul University-Cerrahpasa, Istanbul, Turkey

² Istanbul Arel University, Istanbul, Turkey
gokhan.cayli@istanbul.edu.tr

Unsaturated polyesters (UPE) are copolyesters of polyhydric alcohols with saturated and unsaturated polybasic acids. The synthesis of UPE's generally needs high temperatures such as 200 °C and long reaction times such as 16 or 24 hours [1-3]. Those processes consume too much energy. Thus, new compounds with new synthetic routes, which require minimum energy consumptions and reaction times, are desired. For that purpose, a new type of castor oil based monomer is introduced in this study. Castor oil was first esterified with maleic anhydride. Then, the maleinated castor oil was esterified with methanol in the presence of suitable catalyst. The methyl maleate ester of castor oil was epoxidized via Prilezhaev reaction. The synthesized epoxy derivative of maleinated castor oil was then characterized by FTIR, ¹H NMR techniques. The temperature of all the reactions carried out did not exceed 90 °C. Reaction time was less than 12 hours.

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Properties of Epoxidized Maleinated Castor Oil / Hydroxyapatite Composites

Gokhan CAYLI¹, Yesim Muge SAHIN², Erdi BULUS², Demet Sezgin MANSUROGLU²

¹ Istanbul University-Cerrahpasa, Istanbul, Turkey

² Istanbul Arel University, Istanbul, Turkey
gokhan.cayli@istanbul.edu.tr

Hydroxyapatite is a naturally occurring calcium phosphate mineral. The formula is generally written as $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ and it crystallizes in the hexagonal crystal system [1]. Epoxidized maleinated castor oil (EMACO) was synthesized by our group earlier [2]. EMACO contains epoxy groups and free carboxyl groups. When EMACO is synthesized freshly, it is viscous oil. By heating, carboxyl groups react with epoxide groups and a cross-linked material is obtained. In this study, EMACO was filled with hydroxyapatite at different percentages. The mixtures were cured at 90 °C for 24 hours. At the end of polymerization reactions, rubbery and tough polymers were obtained. The properties of the polymers were evaluated by DSC, TGA and DMA techniques. By the aid of this work, sustainable, ecofriendly and low-cost bio-based materials were obtained.

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The Effect of Plant Oil-Based Monomer Unsaturation on Properties of Latexes and Latex Materials with High Biobased Content

Zoriana Demchuk¹, Oleh Shevchuk², Vasylyna Kirianchuk², Ananiy Kohut², Stanislav Voronov², Andriy Voronov¹

¹Coatings and Polymeric Materials Department, North Dakota State University, Fargo, ND, USA

²Organic Chemistry Department, Lviv Polytechnic National University, Lviv, Ukraine
zoriana.demchuk@ndsu.edu

Renewable raw resources, most commonly vegetable oils, have become progressively interesting in making biobased polymers and polymeric materials because of low cost, positive environmental impact and rich application possibilities. Recently, a library of acrylic monomers from variety of plant oils (POBM's) were synthesized using one-step transesterification reaction of vegetable oil triglyceride with N-hydroxyethyl acrylamide. POBM's perform themselves as conventional vinyl monomers in free radical homopolymerization and copolymerization reactions. Using ¹H NMR spectroscopy it was demonstrated the double bonds of fatty acid fragments in monomers remain mostly unaffected during (co)polymerization and can be further used for post-polymerization (crosslinking) reactions. In addition, it was confirmed that unsaturation amount of plant oil-based monomer noticeably impacts the (co)polymerization. The molecular weight and the polymerization rate diminish with increasing unsaturation amount of POBM's. Besides, the experimentally determined chain transfer constants of POBM's linearly depend on the unsaturation amount of the plant oil-based monomer fatty fragment.

Stable latexes with high POBM content were synthesized in copolymerization with styrene using miniemulsion with solid content of 30-40 % and conversion of 85-95 %. The incorporation of plant oil-based fragments into macromolecular chain provides the plasticizing effect to the resulting copolymers. It is demonstrated by glass transition temperature (T_g) noticeable decrease with the increasing amount of POBM in reaction feed and, respectively, in copolymer composition. By establishing the linear dependence of the crosslink density on monomer feed unsaturation, the latex polymer network formation and thermomechanical properties can be adjusted by simply mixing various POBMs at certain ratios in the feed.

Synthesis of novel acrylated cardanol diphenyl phosphate based reactive diluent for UV curable flame retardant coating application

Ganesh Phalak, Shashank Mhaske
Institute of Chemical Technology, Mumbai, India
ganeshphalak1391@gmail.com

Recently, development of sustainable materials from renewable resources has gained tremendous attention for the replacement of fossil reserves. Cashew nut shell liquid (CNSL) is an abundant and low price agricultural non food by-product of cashew nut industry. Cardanol is extracted from the complete distillation of CNSL. A novel acrylated cardanol diphenyl phosphate (ACP) was synthesized via epoxidation of unsaturation in long side chains of cardanol, followed by acrylation of epoxidized cardanol and, phosphorylation of acrylated cardanol. The chemical structure of synthesized products was confirmed using Fourier transform infrared spectroscopy (FTIR), Nuclear magnetic resonance spectroscopy (^1H NMR, ^{13}C NMR and, ^{31}P NMR) and gel permeation chromatography technique (GPC) respectively. The ACP was incorporated as biobased reactive diluent into a urethane acrylate (UA) oligomer with varying ratios for UV curable coating application. The effect of increasing content of ACP into UA oligomer on viscosity of coating formulations was studied using Rheometer analysis. The properties of UV curable coatings were determined by differential scanning calorimetry (DSC), X-ray diffraction analysis (XRD) and, thermo gravimetric analysis (TGA). The flammability of UV cured coatings were analysed by limiting oxygen index (LOI) and UL-94 vertical burning test. TGA result shows that the introduction of ACP into UA oligomer promotes degradation of UA oligomer and enhances the char formation. The structure of obtained char residues was further investigated from scanning electron microscopy (SEM), FTIR and Raman spectroscopy analysis.

Modified Fatty raw materials as PHBV PLASTICIZERS

Hanna Nosal¹, Marek Warzala¹, Kevin Moser², Andrei Holzer², Dorota Stańczyk¹

¹Institute of Heavy Organic Synthesis "Blachownia", Energetyków 9, 47-225
Kedzierzyn-Kozle, Poland

²Fraunhofer Institute for Chemical Technology, Joseph-von-Fraunhofer-Straße 7,
76327 Pfinztal, Germany
e-mail: nosal.h@icso.com.pl

In recent years various publications have shown processing routes for the lab-scale production of PHBV using different carbon sources and strains of bacteria (e.g. *A. latus.*, *C. necator*) [1]. However due to its limited mechanical properties, particularly a high brittleness, the PHBV polymer has not been used for demanding technical applications yet. In the past many publications have reported numerous options to improve the mechanical properties of PHBV by adding petrobased plasticizers e.g. dioctyl adipate, dioctyl phthalate, polyadipate, tri(ethylene glycol) bis(2-ethylhexanoate) [2, 3]. In order to result in fully biobased PHBV-formulations the addition of 100% biobased plasticizers is required. In this poster the use of modified vegetable oils (fatty acids) as plasticizers is investigated. It describes the modification of camelina oil, castor oil, rapeseed oil and selected fatty acids (oleic acid, stearic acid, lauric acid) via chemical processing such as esterification, transesterification and epoxidation with the target to generate and provide functional groups which ensure the compatibility of the plasticizer with the polymer.

Acknowledgments

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Autoxidation of oils according to their composition: Applications to the drying of alkyd paints

Raphael Lebeuf, Laura Dubrulle, Pr. Véronique Rataj
Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181 - UCCS - Unité de
Catalyse et Chimie du Solide F-59000 Lille, France.
raphael.lebeuf@ensc-lille.fr

Kinetic studies of the autoxidation of unsaturated lipids have been undertaken on pure FAMES and on their mixtures. The results were also compared to the ones obtained with the FAMES coming from the transesterification of oils.¹

The autoxidation rate is not proportional to the methyl oleate/linoleate ratio. The addition of methyl linolenate as a third component was also investigated leading to the same observation. A composition of methyl oleate/linoleate/linolenate of $\approx 30:50:20$ looks the best one to get the highest oxidation rate for a lower unsaturation degree.

Also, the effect of metal additives both on the overall autoxidation rate and on the decomposition of the resulting hydroperoxides was studied in order to determine their action mode as dryer for alkyd paints.²

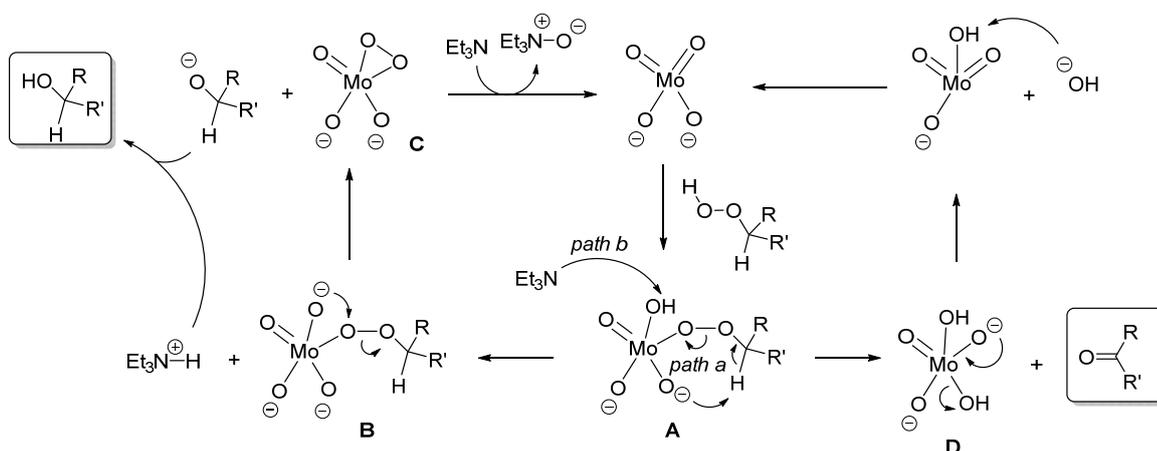
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Oxo-functionalization of unsaturated lipids by a photooxidation / molybdate catalysis sequence

Dr. Raphael Lebeuf, Pr. Véronique Rataj

Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide F-59000 Lille, France.
raphael.lebeuf@ensc-lille.fr

Simple molybdate anion without additional ligands is able to transform with good selectivities the hydroperoxides of FAMES either into their corresponding enone simply by heating at 80°C, or into their allylic alcohol by addition of triethylamine used as a reducer equivalent.¹ The proposed mechanism is the following one:



Other olefins like terpenes also provide the oxygenated products following this sequence.

1 Dual Catalytic Role of Molybdate Ions for Direct Conversion of Photooxidized FAMES into Keto or Hydroxy Derivatives Lebeuf, R., Nardello-Rataj, V. *ACS Sustainable Chem. Eng.* Accepted, 2019 DOI: 10.1021/acssuschemeng.8b04643.

A specific kinetic study to understand better the ring-opening of epoxydes from unsaturated fatty acid systems

Julien Peyrton, Luc Avérous,
BioTeam/ICPEES-ECPM, UMR CNRS 7515, Strasbourg, France
julien.peyrton@etu.unistra.fr

Fossil resources are, by definition, non-renewable and the rarefaction of some oil fractions, focusses industries and academics towards the research for renewable sources. This recent trend is also driven by the development of new molecular architectures which can be extracted from the biomass. A rich chemistry has been developed such as the oleochemistry. In this case, oils and fats from vegetable or animal origin are modified to develop new chemical products. Unsaturated fatty acids contain readily modifiable functions allowing them to be used as platform chemicals for the synthesis of chemicals[1], lubricants[2], polyurethane[3] and biodiesel[4]. With respect to vegetable oils and fats, these transformations often involve the epoxidation of double bonds and the subsequent ring-opening reaction. Triglycerides hold already multiple branches allowing the synthesis of new sustainable macro-molecular architectures.

The activity of the BioTeam at University of Strasbourg (France) is focused on the development of new biobased polymers for environmental and biomedical applications. Our group is always researching the most efficient reaction pathways based on the main green chemistry principles. In this way, epoxy ring opening was investigated using different nucleophiles on a model molecule. A fatty acid methyl ester of very high oleic sunflower oil was epoxidized[5] and then used for the study due to the sole presence of a disubstituted epoxy. Kinetic data including reagent partial orders, reaction rate constant, energy and enthalpy of reaction were determined using pseudo first order conditions. The purpose is to understand the mechanism allowing the ring opening of disubstituted epoxide and to compare the reaction rate of different nucleophiles. This work should help the understanding of the ring opening reaction when this reaction is applied on a more complex oil from different resources (plant, microalgae ...).

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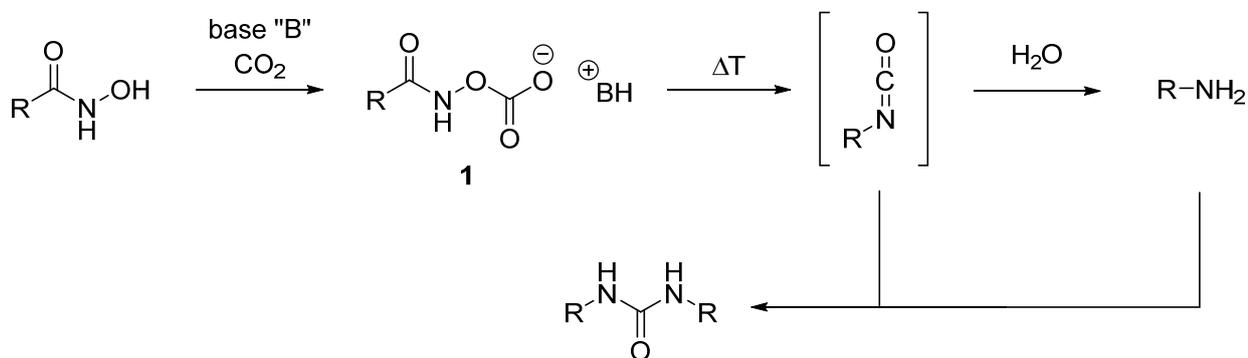
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Sustainable synthesis of ureas and amines *via* CO₂-based Lossen rearrangement

Luca Filippi, Michael a. R. Meier*

Karlsruhe Institute of Technology (KIT), Institute of Organic Chemistry (IOC), Karlsruhe, Germany
m.a.r.meier@kit.edu

CO₂ is one of the most influential causes for the greenhouse effect. The alarming amount of the gaseous substance in the atmosphere originates mainly from fossil fuel burning for energetic purposes. Since the demand for energy is expected to rise even further, the topic of CO₂ capture and its utilization in chemical reactions and processes has gained great interest in the last decades. Herein, we report a CO₂ based modification of the Lossen rearrangement, in which CO₂ is postulated to form the reactive intermediate **1** with the hydroxamic acid derivative and a strong organic base. The rearrangement yielded different ureas, also fatty acid based ones, which could be isolated and characterized by ¹H- and ¹³C-NMR, IR and ESI-MS. Reactions conditions are currently optimized using GC screening.

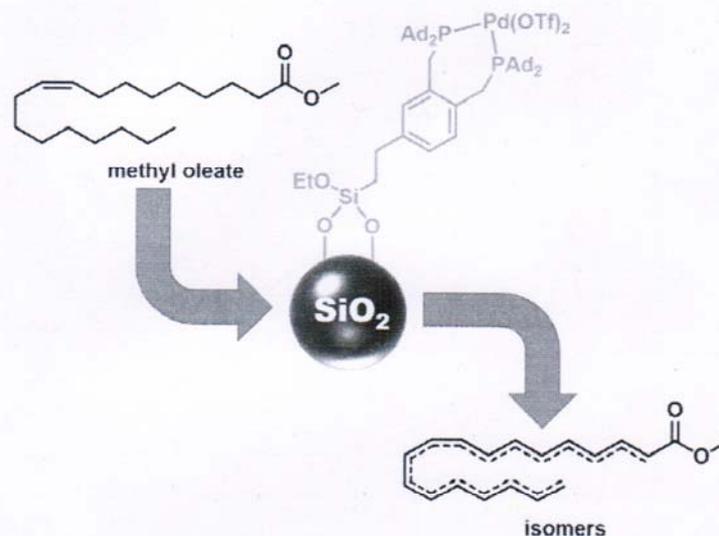


Immobilized Molecular Catalysts for Lipid Isomerization

Felix Einsiedler, Stefan Mecking

Chair of Chemical Material Science University of Konstanz, Konstanz, Germany
Felix.einsiedler@uni-konstanz.de

Comprising long methylene sequences, fatty acids as a renewable resource can serve as raw materials for the production of a broad variety of (functionalized) hydrocarbons. [1] For example, alkenolysis of unsaturated fatty acids leads to mid-chain olefinic compounds. [2] In this context, the product scope is drastically increased by prior isomerization of the double bond. One particular class of catalysts showing high activity in this isomerization are palladium (II) complexes bearing chelating diphosphine ligands. [3] To enable desirable continuous-flow approaches heterogenization of these complexes is necessary. [4] We report on the immobilization of the bis(di-adamantyl phosphino)-*o*-xylene palladium (II) triflate catalyst on mesoporous silica and the isomerization of methyl oleate under mild conditions.



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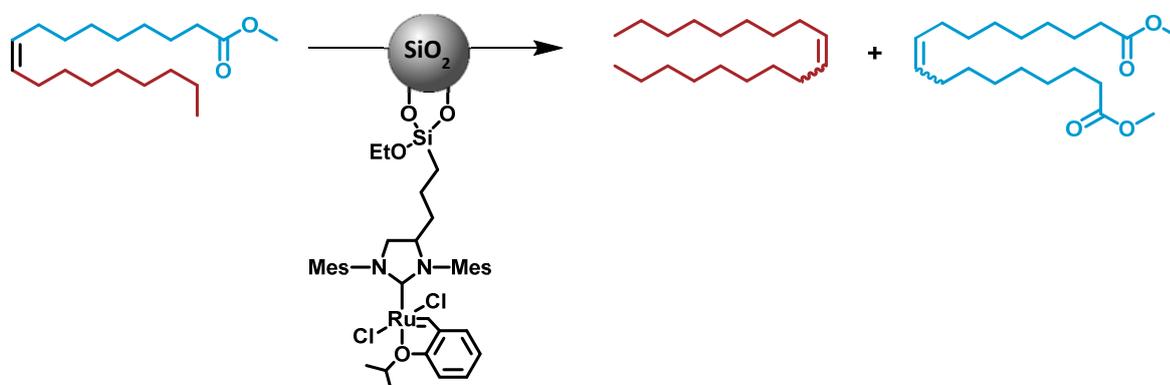
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Immobilized Olefin Metathesis Catalysts for the Conversion of Renewable Raw Materials

Stefanie Kulpa, Natalie Schunck, Stefan Mecking
Chair of Chemical Material Science University of Konstanz, Konstanz, Germany
Stefanie.kulpa@uni-konstanz.de

Due to their molecular structure, fatty acids are attractive renewable feedstocks for the production of otherwise poorly accessible building blocks.¹ Their transformation into value-added chemicals has been expanded significantly by advanced catalytic methods like olefin metathesis.²

To utilize molecular catalysts in continuous flow schemes, and in reaction sequence schemes, an immobilization on solid supports is desirable.^{3,4} We report on the immobilization of the well-defined Hoveyda-Grubbs second-generation catalyst on mesoporous silica and its use in the self-metathesis as well as ethenolysis of methyl oleate as a renewable feedstock.



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Modification of starch via the Biginelli multicomponent reaction

Eren Esen, Michael A. R. Meier

Institute of Organic Chemistry (IOC), Karlsruhe Institute of Technology (KIT), Karlsruhe,
Germany
esen.eren@kit.edu

Starch is one of the most important and abundant renewable polymers with outstanding features (e.g. renewability, biocompatibility, high thermal stability and low cost). Nevertheless, bottlenecks such as low solubility in organic solvents, high hydrophilicity and brittleness makes it not feasible to be processed. Therefore various chemical modifications like esterification, etherification, etc. have been developed to overcome the mentioned problems.[1] Quite recently, multicomponent reactions (MCRs) emerged as a powerful tool to prepare tailor-made, multi-functionalized (bio)polymer architectures offering high molecular diversity in a one-pot synthesis and elegant manner under considerably mild and sustainable conditions. Indeed, the Biginelli Multicomponent Reaction is one of the benchmarks MCRs,[2,3] which facilitates the synthesis of heterocyclic compounds, by using an aromatic aldehyde and a β -keto ester in the presence of urea and a catalyst.

In order to achieve a Biginelli type heterocyclic modification of starch, an acetoacetate derivative of starch is synthesized and further reacted with urea and various (partially) renewable and commercially available aldehyde derivatives to demonstrate the versatility of the method. In-depth analytical characterization via NMR, SEC and FTIR confirms the successful synthesis of Biginelli-starch derivatives. In summary, we demonstrate that it is feasible for starch polymers to be readily functionalized under metal-free and considerably mild conditions, thus yielding otherwise challenging-to-access starch architectures.

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Enzymatic conversions of renewables to tailor-made glycolipid biotensides in uncommon media

André Delavault, Jens Grüninger, Christoph Syldatk

¹ Karlsruhe Institute of Technology (KIT); Institute of Process Engineering in Life Science;
Section II: Technical Biology, Karlsruhe, Germany
andre.delavault@kit.edu

Biotensides is another term designating surface active agents that are also widely known as surfactants. These compounds can be encountered on a daily basis in our cleaning agents, our medicine or even in our food. Because of this wide range of application domains the demand is continuously increasing. The usual chemical synthesis of glycolipids possesses several disadvantages which include lacks of specificity, selectivity and solubility from the substrates. However, it is also possible to enzymatically synthesize those compounds in nearly water free conditions using different biocatalysts and renewable building blocks. Using either a glucosidase or a lipase, one can achieve the synthesis of respectively a glycosidic or an ester bond between a sugar and a fatty alcohol or ester. In order to overcome solubility problems, a deep eutectic solvent (DES) is used to replace an either purely organic or aqueous media. In the systems we use, the DES acts as a solvent and a substrate for the biocatalysed reaction. After reaction, the *de novo* synthesized tensides can be then separated from the media by liquid-liquid extraction and purified by silica-gel chromatography.

Synthesis and Copolymerization of Biginelli-Polycondensates

J. T. Windbiel, M. A. R. Meier

¹Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

julian.windbiel@kit.edu

It is of current and continuous interest to develop new blockcopolymers that offer not only interesting properties, but are also synthesized in a sustainable fashion. Herein, we report a methodology for the synthesis of renewable Biginelli-polycondensates and the subsequent coupling with homopolymers of a different chemical structure.

Terephthalic aldehyde, urea and one of five different *bis*-acetoacetates, respectively, were reacted in a Biginelli-type step-growth polymerization. The *bis*-acetoacetates are derived in good yields from the respective diols and *tert*-butyl acetoacetate. All starting materials can be derived from renewable resources.^[1–4]

Suitable endgroups are introduced by addition of 10-undecenylic-1-acetoacetate to the reaction mixture without significant changes of molecular weight and thermal

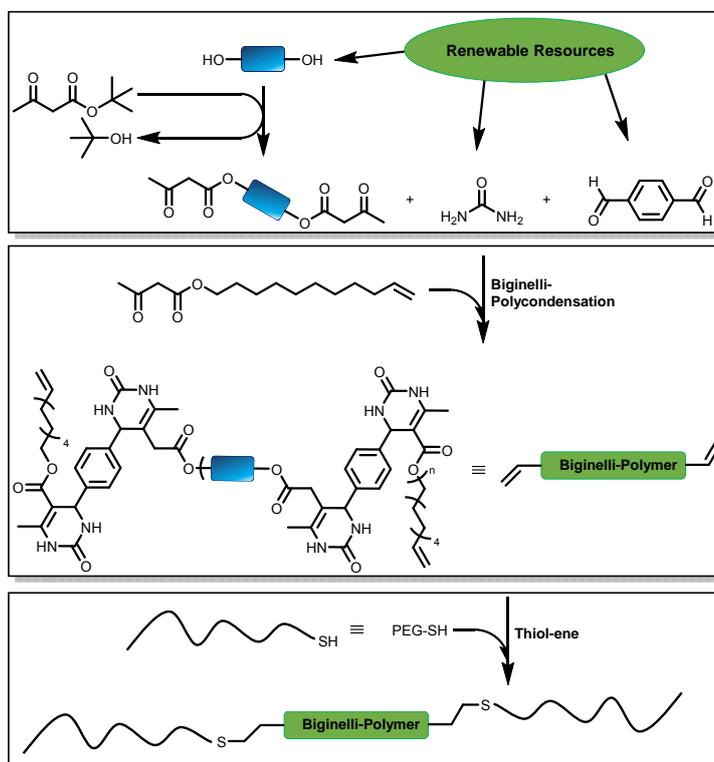
properties of the Biginelli-polycondensate. Subsequently, PEG-thiol is attached to the Biginelli-polymers *via* thiol-ene-reaction, yielding ABA-type blockcopolymers with two distinct thermal transitions.

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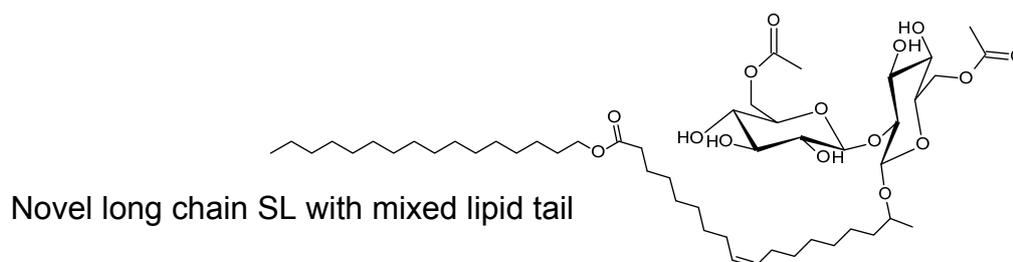


Microbial synthesis of long chain sophorolipids and their potential as emulsifiers

Christian Zerhusen, Timo Bollmann, Birgit Glösen, Ulrich Schörken
TH Köln, Cologne University of Applied Sciences, Leverkusen, Germany
christian.zerhusen@th-koeln.de

Sophorolipids (SLs) are glycolipid biosurfactants synthesized in high yields from sugars and lipids by non-pathogenic yeasts of the clade *Candida*, *Rhodotorula* and *Starmerella* [1,2]. Due to their amphiphilic structure consisting of a hydrophilic β -1-2-diglucoside head and a hydrophobic lipid tail they are mainly used in the cleaning, cosmetic and food industry [3]. The standard lipid substrates for SL production are either triglyceride oils or fatty acids. Utilization of fatty alcohols was originally shown by Tulloch et al [3]. Only a few studies are available up to date with conflicting results regarding the product structures [3,4]. Feeding trials of *Starmerella bombicola* and *Candida kuoi* with several long chain alcohols revealed the production of long chain SLs with esterified fatty alcohols attached to the carboxyl group of the lipid tail. In all cases fatty alcohols were oxidized to their corresponding hydroxyl-fatty acids for initial incorporation into the SL.

Based on these results we were interested to find out, whether a mixed cultivation of *Starmerella bombicola* or *Candida kuoi* with a combination of oleic acid and alcohols of different chain length leads to a SL with mixed lipid tail. Cultivations were done with alcohols from C8 up to C18 and the resulting SLs were purified by preparative HPLC, analyzed via HPLC-MS and NMR. We could clearly identify novel SLs with a long chain tail of mixed lipids. In all cases oleic acid was incorporated as the hydroxylated compound and the free carboxyl group was esterified with the alcohol fed to the cultivation. Initial physicochemical characterization of the hydrophobic SLs revealed a potential use as novel emulsifiers.



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Pheno- and genotypic characterization of three *Yarrowia lipolytica* strains

Silke Hackenschmidt, Stefan Bruder, Felix Bracharz, Johannes Kabisch
Computer-aided Synthetic Biology, TU Darmstadt, Darmstadt, Germany
hackenschmidt@bio.tu-darmstadt.de

Oleaginous yeasts are a promising source for renewable oils. Numerous strains are described in literature. But their capability to accumulate lipids varies between different strains even within one species and highly depends on the cultivation conditions. To reduce the high costs of large-scale production of microbial oil the selection of the microbial strain and identification of its optimal cultivation conditions is one of the first steps to develop a competitive process.

Therefore we screened two hitherto not characterised wild-type isolates strains and the common laboratory strain H222 of the oleaginous yeast *Yarrowia lipolytica* with regard to optimal growth conditions, accumulation of lipids and by-products like citrate and sugar alcohols. Flow cytometry was used to investigate morphological changes during the cultivations. One key finding of the study was the contrary behavior of the wild-type isolates at elevated cultivation conditions. The strain 1889 exhibited robust growth and lipid accumulation at higher cultivation temperature, whereas strain 63 was clearly stressed and lost its oleogenic trait. Furthermore, growth at elevated temperatures promoted sugar alcohol formation independent of the strain and cultivation medium.

Shotgun sequencing was performed for the three strains to gain deeper insight into the genetic background of the different phenotypes. Several polymorphisms have been identified in key proteins of the lipid metabolism and stress response. The variety of polymorphisms makes it difficult to clearly link the phenotypes to single protein variants. But it constitute basis for further studies to develop *Y. lipolytica* to a robust chassis for large-scale production of microbial oil.

Sustainable synthesis of biobased recyclable thermosets

P. S. Löser¹, M. A. R. Meier¹, A. Llevot²

¹ Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

² University of Bordeaux, Bordeaux, France

pia.loeser@kit.edu

Replacing commercial petro-based polymers with bio-based alternatives is an important topic in current research. Amongst the renewable resources, lignin is a valuable source of aromatic compounds.[1] Especially vanillin, already industrially produced from lignin, constitutes a versatile building block for polymer science. Therefore, vanillyl alcohol was selectively allylated on the aromatic hydroxyl group, using catalytic amounts of palladium nanoparticles in water,[2] subsequently coupled with different linkers to form a dimeric compound with a cleavable linker, and then epoxidized in order to mimic and substitute the commercial product diglycidyl ether of bisphenol A (DGEBA). The cleavable linker in the epoxy monomer is introduced to address the lack of recyclability of thermosetting polymers. With this approach, the cured epoxy network can be degraded into smaller polyols that can be reused for the synthesis of another material such as polyurethane. The synthesized monomer was tested in first curing reactions with different diamines and the thermomechanical properties were investigated. In parallel, the sustainable synthesis of diamines from renewable resources is developed. First syntheses were performed using monoterpenes such as dihydrocarvone, which was modified by a series of catalytic reactions.

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Single cell oil production by *Y. lipolytica* for the chemical conversion to hydrocarbons

Eva J. Moldenhauer¹, Stefan Bruder¹, Martin Peters², Andreas Menne², Stefan Junne³,
Johannes Kabisch¹,

¹ Computer-aided synthetic biology, Technical University of Darmstadt, Germany

² Fraunhofer UMSICHT, Oberhausen, Germany

³ Department of Bioprocess Engineering, Technical University of Berlin, Germany
moldenhauer@bio.tu-darmstadt.de

Due to the limitation of fossil fuels, in recent years, many approaches have been developed, to generate alternatives from renewable resources. Yet the microbial production of drop-in biofuels leads to small yields. We chose an alternative approach of microbial production of single cell oil in combination with the chemical conversion to hydrocarbons. With its strong ability for the production of intracellular oils, oleaginous yeast *Y. lipolytica* is an ideal organism for this project. A strain with deletion of the genes responsible for the beta oxidation and deleted lipase gene as well as overexpression of a diglyceride acyltransferase (H222 Δ pox1-6 Δ tg14::Y. lipolytica oil with 250 g maize-germ oil was decarboxylated by Gas-phase Catalytic Cracking (GCC) in the greasoline® process. The product contained 11 % alkanes \leq C11, 18% alkanes \geq C12, 2.4% alkenes, 8.9% alkylated benzenes and 1.4 % polycyclic aromates.

A novel approach on isomerization of long chain carboxylic acids based on inspiration from isomerization of hydrocarbons

Maghrebi Ramin¹, Bondioli Paolo³, Chiaramonti David^{1,2}

¹ Department of Industrial Engineering, University of Florence, Italy

² RE-CORD, Research and Demonstration for R&D, Florence, Italy

³ Innovhub Stazioni Sperimentali per l'Industria S.r.l., Via Giuseppe Colombo 79
20133 Milan, Italy
ramin.maghrebi@unifi.it

Long chain branched fatty acids have been attracting increasing interests due to their widespread applications in cosmetics, lubricant, surfactant, coatings, hydraulic fluids, and biodiesel industries. Since late 1980s, research has been going on towards production of these oleochemical compounds mainly from unsaturated long chain carboxylic acids by porous solid catalysts. Isomerization units will inevitably be important parts of biodiesel production plants, particularly in countries with colder climates. However, few researches have addressed the issue of isomerization of saturated carboxylic compounds by porous solid catalysts doped with non-noble transition metals. Although this approach is interesting, it suffers from low conversions and selectivities. With this in mind we tried to take the advantage of the data available on isomerization of saturated short and long chain hydrocarbons due to the similarities with fatty acids, in order to find the best configuration for our desired process. Then a set of experiments were carried out with palmitic fatty acid under hydrogen atmosphere and HZSM-5 doped with non-noble transition metals in a batch tubular reactor at different temperatures and reaction times (240 – 280 °C; 2 – 6 h). Analysis of the products revealed the presence of iso-palmitic acids as the main products as well as lactones as undesired products. This work proved that hydroisomerization of saturated fatty acids could be done by utilization of porous solid acids doped with non-noble metals. Nevertheless, research into solving low conversions is in progress.

Structural investigation of natural deuterated phospholipid multilayers

Krishna Batchu, Yuri Gerelli, Michael Haertlein, Giovanna Fragneto
Institute Laue-Langevin, 71 avenue des Martyrs F-38000 Grenoble
batchu@ill.fr

Selective deuteration is a useful strategy to highlight specific sample components with different techniques such as NMR, infrared spectroscopy and neutron scattering techniques. More specifically, in the context of biological membranes, phospholipid deuteration is a useful approach to investigate the location of proteins or other lipids, i.e. sterols, in models of cell membranes by means of neutron diffraction or reflection. Nevertheless, the production of deuterated phospholipids in high amounts and as different molecular species (i.e. different headgroup and acyl chain compositions) is currently the limiting factor in the full exploitation of these experiments. In this context, we have been working on the extraction purification of specific deuterated phospholipid classes from *P. Pastoris* cells grown in deuterated culture media. The purified phospholipid fractions in particular phosphatidylcholine (dPC), phosphoethanolamine (dPE), phosphatidylserine (dPS) and Cardiolipin (dCL) were next characterized by means of Neutron Diffraction (ND) measurements. During our last experiment on D16, we prepared a lipid multilayer with the extracted dPC lipids) and the collected experimental data showed the presence of several diffraction orders. Indeed, in order to safely implement the deuterated phospholipids extracted from *P. Pastoris* in experiments involving neutron contrast variation as well as the other above-mentioned techniques, the investigation of their fundamental structural properties is required.

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Optimization of the extraction of glucose monodecanoate synthesized in deep eutectic solvents by response surface modeling

Rebecca Hollenbach, Christoph Syldatk
Karlsruhe Institute of Technology, Karlsruhe, Germany
rebecca.hollenbach@kit.edu

Growing concern about climate change and increasing environmental awareness are leading to a quest for green chemistry with more sustainable circular processes. This also applies to surfactants, which have a wide range of applications: in agrochemicals, food, cosmetics, pharmaceuticals and laundry detergents. Conventional surfactants are based on petroleum and are chemically produced, resulting in product mixtures and by-products. Biosurfactants are based on renewables, biodegradable, non-toxic and are produced by microbial fermentation or selectively synthesized by enzymatic processes. In particular, enzymatic synthesis in deep eutectic solvents avoids harmful solvents and overcomes the problem of dissolving carbohydrates as well as fatty acids.

In addition to the actual synthesis, downstream processing has also a major influence on the sustainability of the overall process. Especially product recovery should be as high as possible and the used solvents need to be biodegradable and non-toxic. Therefore, the influence of the extraction solvent used, the amount of the solvent, the amount of added water and the mixing time on glucose monodecanoate recovery by extraction from deep eutectic solvents was investigated.

Plant Oil-Based Monomers for Reversible Deactivation Radical Polymerisation

P.B.V. Scholten,^{1,2} C. Detrembleur,² M.A.R. Meier¹

¹ Karlsruhe Institute of Technology, IOC, Materialwissenschaftliches Zentrum MZE, Straße am Forum 7, Karlsruhe, Germany; ² Université de Liège, Center for Education and Research on Macromolecules, CESAM Research Unit, Sart-Tilman B6A, Liège, Belgium
pscholten@ulg.ac.be

Renewable monomers have the potential to replace petroleum-derived monomers for reversible deactivation radical polymerisations (RDRP) for a variety of applications, such as adhesives or coatings. Yet, challenges in the polymerisation of non-activated and often internal double bonds found in natural molecules still remain.^{1–4} Moreover, functionalisation pathways attaching renewably-sourced double bonds to natural molecules are rare and sustainable strategies using catalytic or enzymatic reactions are sought after.⁵ Herein we report the sustainable synthesis of several renewable monomers based on glycerol or methyl-10-undecenoate, a ricinoleic acid derivative. These monomers, containing non-activated olefinic double bonds, were copolymerised with vinyl acetate using cobalt-mediated radical polymerisation for the first time. Molecular weights up to 18,000 g mol⁻¹ with an incorporation of up to 49 mol% of renewable monomer were achieved. In addition to the sustainable synthetic pathway, the purification of the polymers was performed by supercritical CO₂ extraction which not only allowed to recover 58% of the unused monomer but also avoided the use of large amounts of solvents. The approach presented herein acts as a blueprint for the synthesis of a whole library of novel renewable monomers for RDRP.

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Progress in homogeneously catalyzed oxidation reactions of fatty acids – sustainability through catalyst recycling

Johanna Vondran, Dieter Vogt, Thomas Seidensticker
Technical University, Dortmund, Germany
Johanna.vondran@tu-dortmund.de

An essential tool for walking along sustainable reaction routes starting from renewables is catalysis. Particularly the application of homogeneous catalysts is beneficial due to relatively mild reaction conditions and high selectivities. However, efficient catalyst recycling strategies are of need to compete on industrial large scale.

Amongst homogeneous catalysis, oxidation reactions have the highest worldwide capacity of 18 million tons per year.^[1] Oleic acid is converted by cleaving its internal double bond to pelargonic acid (PA) and azelaic acid (AA), both of industrial relevance. Whilst the industrial ozonolysis, which implicates disadvantages of energy-demanding production of ozone and the risk of explosion due to unstable intermediates, the homogeneously catalyzed oxidative cleavage is highly selective towards the desired products and involves hydrogen peroxide as a “green” oxidant, forming only water as co-product. In former works, several transition metals were investigated towards their activity,^[2] but combining this high-potential reaction with efficient catalyst separation is challenging for reasons of immiscibility of the fatty acid in an aqueous environment and has thus not been reported so far. In the present project, catalyst recycling is tackled via *thermomorphic multiphase systems* and *membrane technique*. Both concepts are efficient approaches for the conversion of oleo chemicals with homogeneous catalysts in aqueous systems and support the development of a sustainable chemical process.

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List of Participants

List of participants

Dennis Barther

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Fritz-Haber-Weg 6, Geb. 30.42
76131 Karlsruhe, Germany
dennis.barther@kit.edu

Dr. Krishna Chaithanya Batchu

Institut Laue-Langevin
Science
71 avenue des Martyrs, CS 20156
38000 Grenoble, France
batchu@ill.fr

Dr. Ursula Biermann

abiosus e.V.
Bloherfelder Straße 239
26129 Oldenburg, Germany
ursula.biermann@uni-oldenburg.de

Dr. Arno M. Bieser

Freudenberg Technology
Innovation SE & Co. KG
Chemistry and Surface Technologies
Hoehnerweg 2-4
69469 Weinheim, Germany
arno.bieser@freudenberg.de

Benjamin Bitterer

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
benjamin.bitterer@kit.edu

Boris Bizet

LCPO – University of Bordeaux
Biopolymers and Biosourced Polymers
16, Avenue Pey Berland
33607 Pessac, France
boris.bizet@enscbp.fr

Dr. Rolf Blaauw

Wageningen Food & Biobased
Research
Biobased Products
Bornse Weilanden 9
6708 WG Wageningen, Netherlands
rolf.blaauw@wur.nl

Prof. Dr. Uwe Bornscheuer

Greifswald University
Institute of Biochemistry
Department of Biotechnology &
Enzyme Catalysis
Felix-Hausdorff-Str. 4
17489, Greifswald, Germany
uwe.bornscheuer@uni-greifswald.de

Philipp Bohn

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7 Geb. 30.48
76131 Karlsruhe, Germany
philipp.bohn@kit.edu

Dr. Gerhard Brankatschk

OVID e.V.
Am Weidendamm 1A
10117 Berlin, Germany
gebert@ovid-verband.de

Valentina Bragoni

Ruhr University Bochum
Organic Chemistry
Universitätsstr. 150
44801 Bochum, Germany
valentina.bragoni@rub.de

Dr. Sylvain Caillol

ICGM
ENSCM
240 Av Prof Emile Jeanbrau
34296 Montpellier, France
sylvain.caillol@enscm.fr

Michael Carus

nova-Institut GmbH
CEO
Industriestr. 300
50354 Hürth, Germany
michael.carus@nova-institut.de

Dr. Gökhan Cayli

Istanbul University Cerrahpasa
Engineering Sciences
34320 Istanbul, Turkey
gokhan.cayli@istanbul.edu.tr

Prof. Dr. Eugene Chen
Colorado State University
80523 Fort Collins, Colorado
United States
eugene.chen@colostate.edu

Abhishek Chowdhury
Sam Higginbottom University of
Agriculture Technology and Sciences
Chemistry
Mangalam Apartment Flat No E35
Tulsipur Mahmoorganj
221010 Varanasi, India
abhishek.chowdhury2089@gmail.com

Dr. Kevin Cousin
University of Artois
Unité de Catalyse et Chimie du Solide
Faculté des Sciences Jean Perrin
62300 Lens, France
kevin_cousin1@ens.univ-artois.fr

André Delavault
Karlsruhe Institute of Technology (KIT)
Institute of Process Engineering in Life
Sciences-Technical Biology
Fritz-Haber-Weg 4
76131 Karlsruhe, Germany
andre.delavault@kit.edu

Wouter De Weirdt
Tectero
Aannemersstraat 136
9040 Sint-Amandsberg, Belgium
wouter.deweirdt@tectero.com

Zoriana Demchuk
North Dakota State University
Coatings and Polymeric Materials
Department
1735 Research Park Dr N
58102 Fargo, United States
zoriana.demchuk@ndsu.edu

Olivia Dhara
University College of Science and
Technology, University of Calcutta
Department of Chemical Technology
92, Acharya Prafulla Chandra Road,
Rajabazar, Machuabazar, West Bengal
700009 Kolkata, India
olivia.dhara@gmail.com

Prof. Dr. Martino Di Serio
University of Naples Federico II
Department of Chemical Science
Complesso di Monte S. Angelo, via Cintia
80126 Napoli, Italy
diserio@unina.it

Dr. Nicolas Duguet
University Lyon 1
ICBMS
Campus Lyon Tech La Doua, Batiment
Lederer, 1 rue Victor Grignard
69100 Villeurbanne, France
nicolas.duguet@univ-lyon1.fr

Felix Einsiedler
University of Konstanz
Chair of Chemical Material Science
Universitätsstr. 10
78467 Konstanz, Germany
felix.einsiedler@uni-konstanz.de

Dr. Susanna-Carina Engert
BASF SE
RAM – B 1
67056 Ludwigshafen, Germany
susanne-carina.engert@basf.com

Eren Esen
Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
eren.esen@kit.edu

Luca Filippi
Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
luca.filippi@kit.edu

Dr. Verena Goldbach
Covestro Deutschland AG
Technology Scouting
Kaiser-Wilhelm-Allee 60
51373 Leverkusen, Germany
verena.goldbach@covestro.com

Prof. Dr. Karol L. Grela
University of Warsaw
Biological and Chemical Research
Centre, Faculty of Chemistry
Żwirki i Wigury 101
02-089 Warsaw, Poland
prof.grela@gmail.com

Eliane Goossens
Cargill
R&D Centre Vilvoorde
Havenstraat 84
1800 Vilvoorde, Belgium
eliane_goossens@cargill.com

Dr. Adriana Grossmann
Clariant Produkte (Deutschland) GmbH
Industrieparkstraße 1
84508 Burgkirchen, Germany
adriana.grossmann@clariant.com

Prof. Dr. Harald Gröger
University of Bielefeld
Chair of Organic Chemistry I
Faculty of Chemistry
Universitätsstr. 25
33615 Bielefeld, Germany
harald.groeger@uni-bielefeld.de

Jens Grüninger
Karlsruhe Institute of Technology (KIT)
Institute of Process Engineering in Life
Sciences Section II: Technical Biology
Fritz-Haber Weg 4
76131 Karlsruhe, Germany
jens.grueninger@kit.edu

Silke Hackenschmidt
Technische Universität Darmstadt
Computer-aided Synthetic Biology
Schnittspahnstr. 12
64287 Darmstadt, Germany
hackenschmidt@bio.tu-darmstadt.de

Daniel Hahn
Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
daniel.hahn@kit.edu

Norman Herrmann
Technische Universität Darmstadt
Laboratory of Industrial Chemistry
Emil-Figge-Straße 66
44227 Dortmund, Germany
norman.herrmann@tu-dortmund.de

Prof. Dr. Andreas Heise
Royal College of Surgeons in Ireland
(RCSI)
Department of Chemistry
123 St. Stephens Green
2 Dublin, Ireland
andreasheise@rcsi.ie

Jukka Hietala
Neste
Research and Development
Neste Corporation, Technology Centre,
Kilpilahti, POB 310
6101 Porvoo, Finland
jukka.hietala@neste.com

Rebecca J. Hollenbach
Karlsruhe Institute of Technology (KIT)
Institute of Process Engineering in Life
Sciences Section 2 -Technical Biology
Fritz-Haber-Weg 4
76131 Karlsruhe, Germany
rebecca.hollenbach@kit.edu

Dr. Norbert Holst
Fachagentur Nachwachsende
Rohstoffe e.V.
Projektmanagement
Hofplatz 1
18276 Gülzow, Germany
n.holst@fnr.de

Prof. Dr. George John
The City College of New York
Chemistry and Biochemistry
160 Convent Avenue
10031 New York, United States
gjohn@ccny.cuny.edu

Manvir Kaur
Guru Nanak Dev University
Chemistry
143005 Amritsar, India
manvir.chem@gmail.com

Komal Komal

Guru Nanak Dev University
Amritsar Punjab, India
Chemistry
143005 Amritsar, Punjab, India
komalchem11@gmail.com

Dr. Dirk Roland Kuppert

Clariant Produkte (D) GmbH
Group Technology & Innovation
Industriepark Höchst
65926 Frankfurt am Main, Germany

Dr. Raphaël Lebeuf

ENSC-Lille
Cité Scientifique, Avenue Mendeleiev,
Batiment C7
59650 Villeneuve d'Ascq, France
raphael.lebeuf@ensc-lille.fr

Pia S. Löser

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
pia.loeser@kit.edu

Prof. Dr. Johannes Kabisch

Technische Universität Darmstadt
Computer-aided Synthetic Biology
Schnittspahnstr. 12
64287 Darmstadt, Germany
johannes@kabisch-lab.de

Stefanie Kulpa

University of Konstanz
Lehrstuhl für chemische
Materialwissenschaften
Universitätsstr. 10
78464 Konstanz, Germany
stefanie.kulpa@uni-konstanz.de

Dr. Klaus Lorenz

Covestro Deutschland AG
Polyether Process Research
Alte Heerstrasse
41538 Dormagen, Germany
klaus.lorenz@covestro.com

Jana Löwe

University of Bielefeld
Faculty of Chemistry
Universitätstraße Bielefeld 25
33615 Bielefeld, Germany
jana.loewe@uni-bielefeld.de

Dr. Ling Ma

Klüber Lubrication München SE & Co. KG
R&D
Geisenhausenerstraße 7
81379 München, Germany
ling.ma@klueber.com

Ramin Maghrebi

University of Florence
Industrial Engineering
Via Pietro Grocco 15
50134 Firenze, Italy
ramin.maghrebi@unifi.it

Fiona Magliozzi

LCPO University of Bordeaux
Biopolymers and bio-sourced Polymers
16 avenue Pey-Berland
33607 Pessac, France
fiona.magliozzi@enscbp.fr

Prof. Dr. Eva E. Malmström

KTH Royal Institute of Technology
Fiber and polymer technology
Teknikringen 56-58
10044 Stockholm, Sweden
mavem@kth.se

Prof. Dr. Michael A. R. Meier

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
m.a.r.meier@kit.edu

Prof. Dr. Jürgen O. Metzger

abiosus e.V.
Bloherfelder Str.239
26129 Oldenburg, Germany
juergen.metzger@uni-oldenburg.de

Eva J. Moldenhauer

Technische Universität Darmstadt
Computer-aided Synthetic Biology
Schnittspahnstr. 12
64287 Darmstadt, Germany
moldenhauer@bio.tu-darmstadt.de

Prof. Dr. Eric Monflier

University of Artois
UCCS, UMR CNRS 8181
Faculté des Sciences Jean Perrin
Rue Jean Souvraz SP 18
62307 Lens, France
eric.monflier@univ-artois.fr

Dr. Claire Negrell

ICGM (UMR5253) CNRS
IAM
34296 Montpellier, France
claire.negrell@enscm.fr

Huy P. Nguyen

Aalto University
Department of Chemical and
Metallurgical Engineering
Kemistintie 1
2150 Espoo, Finland
phan.nguyen@aalto.fi

Roman Nickisch

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
roman.nickisch@kit.edu

Dr. Hanna Nosal

Institute of Heavy Organic
Synthesis Blachownia
Renewable Raw-Materials Department
Energetyków 9
47-225 Kędzierzyn-Koźle, Poland
nosal.h@icso.com.pl

Dr. Katrin Ochsenreither

Karlsruhe Institute of Technology (KIT)
Technical Biology
Fritz-Haber-Weg 4
76131 Karlsruhe, Germany
katrin.ochsenreither@kit.edu

Kelechukwu N. Onwukamike

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
kelechukwu.onwukamike@kit.edu

Julien Peyrton

ICPEES
BioTeam
25 rue Becquerel
67087 Strasbourg, France
julien.peyrton@etu.unistra.fr

Ganesh Anil Phalak

Institute of Chemical Technology
Mumbai
Department of Polymer & Surface
Engineering
Nathalal Parekh Marg, Matunga
400019 Matunga, India
ganeshphalak1391@gmail.com

Dr. Emanuele Porcellato

Breton SPA
Research Centre
31030 Castello di Godego, Italy
porcellato.emanuele@breton.it

Yasmin S. Raupp

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
yasmin.raupp@kit.edu

Dr. Yann M. Raoul

OLEON SAS
R&D
Rue les rives de l'Oise – Venette
60200 Compiègne, France
yann.raoul@oleon.com

Dr. Marie Reulier

ITERG
Unité RDI Lipochimie
11 Rue Gaspard Monge – ZA
Pessac Canejan
33610 Canejan, France
m.reulier@iterg.com

Michael Rhein

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Fritz-Haber-Weg. 6, Geb. 30.42
76131 Karlsruhe, Germany
michael.rhein@kit.edu

Prof. Dr. Marc Rüschen gen. Klaas

University of Applied Science
Emden Leer
Constantiaplatz 4
26723 Emden, Germany
ruesch.gen.klaas@hs-emden-leer.de

Philipp Schmidt

Fraunhofer Institute for Wood Research
Wilhelm-Klauditz-Institut WKI
Surface Technology
Bienroder Weg 54E
38106 Braunschweig, Germany
philipp.schmidt@wki.fraunhofer.de

Thomas Schmidt

DuPont Nutrition Biosciences
Process Development
Taarnvej 25
7200 Grindsted, Denmark
thomas.schmidt-1@dupont.com

Prof. Dr. Ulrich Schörken

TH Köln - Campus Leverkusen
Faculty of Applied Natural Sciences
Kaiser-Wilhelm-Allee
51368 Leverkusen, Germany
ulrich.schoerken@th-koeln.de

Philip B. V. Scholten

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
pscholten@uliege.be

Natalie Schunck

University of Konstanz
Chemistry
Universitätsstr. 10
78464 Konstanz, Germany
natalie.schunck@uni-konstanz.de

Dr. Thomas Seidensticker

Technische Universität Dortmund
Laboratory of Industrial Chemistry
Emil-Figge-Straße 66
44227 Dortmund, Germany
thomas.seidensticker@tu-dortmund.de

Rebecca Seim

Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
rebecca.seim2@kit.edu

Prof. Dr. Mukund P. Sibi

North Dakota State University
Chemistry and Biochemistry
Dept. 2735, P O Box 6050
58108-6050 Fargo, United States
Mukund.Sibi@ndsu.edu

Gurbir Singh

Guru Nanak Dev University
Department of Chemistry
143005 Amritsar, Punjab, India
gurbirchem.rsh@gndu.ac.in

Dr. Andreia F. Sousa

CICECO - Aveiro Institute of Materials
University of Aveiro
Chemistry
Campus de Santiago
Universidade de Aveiro
3810-193 Aveiro, Portugal
andreiafs@ua.pt

Vivian Stefanow

Leibniz Institute for Catalysis
Catalysis with renewable resources -
organocatalysis
Albert-Einstein-Straße 29b
18059 Rostock, Germany
vivian.stefanow@catalysis.de

Dr. Maeva Subileau

Montpellier SupAgro
UMR IATE
B32, 2 pl Pierre Viala
34060 Montpellier, France
maeva.subileau@supagro.fr

Prof. Dr. Christoph Syldatk
Karlsruhe Institute of Technology (KIT)
Technical Biology
Fritz-Haber-Weg 4
76131 Karlsruhe, Germany
christoph.syldatk@kit.edu

Peter Tollington
Cargill BV
Cargill Bio-Industrials Europe
Evert van de Beekstraat 378
1118CZ Schiphol, Netherlands
peter_tollington@cargill.com

Khantutta-Kim Tremblay-Parrado
ICPEES
Polymers
25 rue Becquerel
67000 Strasbourg, France
khantutta-kim.tremblay-
parrado@etu.unistra.fr

Fabienne Urbanek
Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Fritz-Haber-Weg. 6, Geb. 30.42
76131 Karlsruhe, Germany
fabienne.urbanek@kit.edu

Tanja van Bergen-Brenkman
Croda
R&D
Buurtje 1
2802BE Gouda, Netherlands
tanja.van.bergen@croda.com

Dr. Pierre Villeneuve
CIRAD
SupAgro - 2 Place Pierre Viala
34060 Montpellier, France
pierre.villeneuve@cirad.fr

Johanna Vondran
Technische Universität Dortmund
Laboratory of Industrial Chemistry
Emil-Figge-Straße 66
44227 Dortmund, Germany
johanna.vondran@tu-dortmund.de

Dr. Matthew Walker
TRUMPLER GmbH & Co. KG,
Chemische Fabrik
R&D
Hafenstr. 10
67547 Worms, Germany
Walker.Dr.Matt@trumpler.de

Dr. Marek Warzala
Institute of Heavy Organic
Synthesis Blachownia
Renewable Raw-Materials Department
Energetyków 9
47-225 Kędzierzyn-Koźle, Poland
warzala.m@icso.com.pl

Prof. Dr. Dean C. Webster
North Dakota State University
Coatings and Polymeric Materials
1735 NDSU Research Park Dr N
58102 Fargo, ND, United States
dean.webster@ndsu.edu

Dr. Alfred Westfechtel
KLK EMMERICH GmbH
Research & Development
Henkelstrasse 67 (Tor 1)
40589 Düsseldorf, Germany
alfred.westfechtel@klkoleo.com

Katharina S. Wetzel
Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
katharina.wetzel@kit.edu

Dr. Sophie C.C. Wiedemann
Croda
Process & Analytical Development
Buurtje 1
2800 BE Gouda, Netherlands
sophie.wiedemann@croda.com

Julian Windbiel
Karlsruhe Institute of Technology (KIT)
Institute of Organic Chemistry
Straße am Forum 7, Geb. 30.48
76131 Karlsruhe, Germany
julian.windbiel@kit.edu

Dr. Malte Winnacker

Technische Universität München
Chemistry
Lichtenbergstraße 4
85747 Garching bei München, Germany
malte.winnacker@makro.ch.tum.de

Dr. Stefano Zeggio

Breton SPA
Research Centre
31030 Castello di Godego, Italy
zeggio.stefano@breton.it

Christian Zerhusen

Technische Hochschule Köln
Kaiser-Wilhelm Allee 1
51368 Leverkusen, Germany
Christian.Zerhusen@th-koeln.de

