

Final Program Chirality 2016

Sunday July 24, 2016

Conference venue opens at 9.00; Posters can be displayed at that time.

Registration opens at 16.00

Short Course 1

Instructors: Nina Berova, Gennaro Pescitelli, Prasad Polavarapu

Time: 10.00 – 16.00 Lecture Hall East

Description: **Basic principles and Recent Advances in Experimental and Theoretical Chiroptical Spectroscopic Methods (ECD, ORD, VCD and ROA) for the Determination of Stereochemical Molecular and Supramolecular Structures**
Chiroptical Spectroscopy

Short Course 2

Instructors: Daniel W. Armstrong, Zachary Breitbach

Time: 10.00 – 16.00 Lecture Hall West

Description: **Chiral Separations**

18.00-18.15 Opening of the Symposium and Presentation of the Chirality Medal
Location: Main Lecture Hall

18.15-19.00 **Chirality Medal Award Lecture by Andreas Pfaltz** L1
Design and Screening of Enantioselective Catalysts

19.00-21.00 Chirality Medal Reception

Monday July 25, 2016

8.15-9.00

Plenary Session 1

Location: Main Lecture Hall Chair: Oliver Trapp		
8.15	Koichi Mikami Achiral but Tropos Ligands for Asymmetric Catalysis	L2

9.00-9.30

Coffee Break, Exhibit and Posters

9.30-12.05

Parallel Session 1

Location: West Chair: Kenso Soai		
Fundamentals		
9.30	<u>Reiko Kuroda</u> , Risa Suzuki, Marina Yamamoto, Hideyuki Tabata What is Happening During the Single Crystal Transformation?	L3
9.55	M. Pitzer, G. Kastirke, M. Kunitski, T. Jahnke, T. Bauer, C. Gohl, F. Trinter, C. Schober, K. Henrichs, J. Becht, S. Zeller, H. Gassert, M. Waitz, A. Kuhlins, H. Sann, F. Sturm, F. Wiegandt, R. Wallauer, L. Ph. H. Schmidt, A. S. Johnson, M. Mazenauer, B. Spenger, J. Kiedrowski, S. Marquardt, S. Marquardt, A. Schießler, M. Reggelin, H. Schmidt-Böcking, J. Stohner, R. Dörner, <u>R. Berger</u> , M. S. Schöffler Absolute Configuration via Light-induced Coulomb Explosion Imaging of Molecules in the Gas Phase	L4
10.20	Melanie Schnell Revealing Structure, Dynamics and Chirality of Molecular Systems	L5
10.45	<u>Oliver Trapp</u> , Golo Storch A by-Design Enantioselective Self-Amplifying Catalyst Based on Non-Covalent Product-Catalyst Interactions	L6
11.10	<u>Simona Rizzo</u> , Serena Arnaboldi, Voichita Mihali, Roberto Cirilli, Alessandra Forni, Armando Gennaro, Abdirisak Ahmed Isse, Marco Pierini, Patrizia Romana Mussini, Francesco Sannicolò Application of the "Inherent Chirality" Concept to Ionic Liquids Design: Effective Chiral Electroanalysis on Achiral Electrodes	L7
11.30	Christopher J. A. Warner, Subrata Dutta, Eefei Chen, <u>Jevgenij A. Raskatov</u> Introduction of D-Glutamate at a Critical Residue of A β 42 Stabilizes a pre-Fibrillary Aggregate with Enhanced Toxicity	L8
11.50	<u>Oleksii Rebrov</u> , Kostiantyn Kulyk, Mauritz Ryding, Mark Stockett, John Alexander, Henning Zettergren, Henning Schmidt, Henrik Cederquist, Richard D. Thomas, Einar Uggerud, Mats Larsson Interaction of Protonated Amino Acids and Amino Acid Inclusive Proton-Bound Diastereomeric Complexes with Chiral and Achiral Molecules	L9

Location: East		Chair: Wolfgang Lindner
Separations		
9.30	Yoshio Okamoto Polysaccharide Derivatives as Powerful Chiral Stationary Phases for HPLC	L10
9.55	Eric Francotte The Impact of Preparative Enantioselective Chromatography on Chiral Drug Development and Pharmaceutical Technology	L11
10.20	<u>Claudio Villani</u> , Alessia Ciogli, Francesco Gasparrini, Omar Ismail Ultra-high-performance liquid chromatography on Pirkle-type chiral stationary phases	L12
10.45	Daniel W. Armstrong D-Amino Acids in Biological Systems: Evaluations using Rapid, High Efficiency Protocols	L13
11.10	<u>Zachary S. Breitbach</u> , Daniel W. Armstrong High Efficiency and Ultra-Fast Chiral Separations in HPLC and SFC	L14
11.30	<u>Jun Shen</u> , Ping Li, Keyi Chi, Geng Li, Yoshio Okamoto Controlled Synthesis of Novel Polysaccharide Derivatives for Enantioseparation by HPLC	L15
11.50	<u>Antonius H.J. Engwerda</u> , Elias Vlieg Speeding up Viedma Ripening	L16

12.05-13.30 Lunch Break

Vendor Seminar 1: **Chiral Technologies**
Main Lecture Hall Pilar Franco: 20 years of Innovation in Enantiomeric Separations
12.15-13.15

13.30-15.30 Parallel Session 2

Location: West		Chair: Thomas Bürgi
Nano		
13.30	Karl-Heinz Ernst Stereochemical Recognition of Chiral Non-Planar Aromatic Hydrocarbons on Surfaces	L17
13.55	Taizo Mori, Anshul Sharma, <u>Torsten Hegmann</u> Significant Enhancement of the Chiral Correlation Length in Nematic Liquid Crystals via Gold Nanoparticles with Axially Chiral Ligands	L18
14.20	Nicholas A. Kotov Chiral Nanoparticles and Their Assemblies	L19
14.40	<u>Anvar S. Baimuratov</u> , Nikita V. Teplyakov, Yurii K. Gun'ko, Alexander V. Baranov, Anatoly V. Fedorov, Ivan D. Rukhlenko Optical Activity of Semiconductor Nanocrystals	L20
15.00	<u>Jihyeon Yeom</u> , Nicholas A. Kotov Inorganic Chiral Nanomaterials: Design Strategies and Origin of Homochirality	L21
15.15	<u>Li Zhang</u> , Minghua Liu Self-Assembled Chiral Nanostructures and their Enantioselective Recognition	L22

Location: East		Chair: Ivo Stary
Supramolecular Chemistry		
13.30	Toshikazu Takata Dynamic Molecular Systems Induced by Rotaxanes Having Mechanical and Axial Chirality	L23
13.55	Eiji Yashima Double-Stranded Helical Foldamers Exhibiting Unique Chiroptical Properties and Functions	L24
14.20	<u>Katsuhiko Maeda</u> , Ryoma Ishidate, Kouhei Shimomura, Tomoyuki Ikai, Shigeyoshi Kanoh, Eiji Yashima Switchable Enantioseparation Based on Switching and Memory of Macromolecular Helicity in Polyacetylene Derivatives in the Solid State	L25
14.40	Zong-Quan Wu Helix-Sense Controlled Polymerization of Achiral Phenyl Isocyanides Using Chiral Pd(II) Initiators	L26
15.00	<u>Gaku Fukuhara</u> , Mami Imai, Denis Fuentealba, Yuki Ishida, Hiroki Kurohara, Cheng Yang, Tadashi Mori, Hiroshi Uyama, Cornelia Bohne, Yoshihisa Inoue Dynamic Hybridization of Glucans with Cationic Polythiophene to Chiral Hetero-Triplex and –Duplexes	L27
15.15	<u>Yuuya Nagata</u> , Tsuyoshi Nishikawa, Michinori Sugimoto Solvent-dependent Abnormal Sergeants-and-Soldiers Effect on Poly(quinoxaline-2,3-diyl) Copolymers Enabling Bidirectional Induction of Single-Handed Helical Sense	L28

15.30-16.00 Coffee Break, Exhibit and Posters

16.00-18.00 Parallel Session 3

Location: West		Chair: Zachary Breitbach
Chirality in Industry		
16.00	<u>Shalini Andersson</u> , Nicolás Marco Arinõ, Emre M. Isin, Fredrik Bergström Enantiospecificity of Fatty Acid Metabolizing Enzymes: Relevance in Drug Discovery	L29
16.30	Rebecca T. Ruck Asymmetric Catalysis for the Synthesis of Active Pharmaceutical Ingredients at MSD	L30
17.00	Jacob Janey Automated Process Development: Robots, Chemistry, and Statistical Design	L31
17.20	Christopher J. Welch Recent Collaborations with Academia on New Enabling Technologies for Stereochemical Analysis in the Pharmaceutical Industry	L32
17.40	<u>Ulrich Mayerhöffer</u> , Christoph Täschler, Ellen Klegraf L-Carnitine at Lonza	L33

Location: East		Chair: Prasad Polavarapu
Spectroscopy		
16.00	<u>Quezia B. Cass</u> , Tiago C. Lourenço, Jau T. Lee, Tiago Venâncio, Juliana C. Barreiro A High-resolution MAS-NMR Study of the Enantiodiscrimination of 3,4 (MDMA) by Immobilized Polysaccharide-based Chiral Phase	L34
16.30	<u>R. Thomas Williamson</u> , Lu Yang, Thomas Wenzel, Melodie Christensen, Wes Schafer, Christopher J. Welch Expedited Selection of NMR Chiral Solvating Agents for Determination of Enantiopurity	L35
17.00	<u>Lucie Habartová</u> , Bohuš Bunganič, Miroslav Zavoral, Vladimír Setnička Chiroptical Spectroscopy of Human Blood Plasma: Revealing the Signature of Degenerative Diseases	L36
17.20	<u>Stefanie Hansmann</u> , Christina M. Thiele NMR Spectroscopy in Homochiral Polyglutamates: Structural Design and Influences on Enantiodifferentiation	L37
17.40	<u>Mira Koeberle</u> , Felix Roth, Volker Schmidts, Christina M. Thiele Homochiral Polyaspartates as a New Alignment Medium in NMR Spectroscopy of Small Organic Molecules	L38

18.00-22.00 Poster Night with BBQ in the Lobby

Tuesday July 26, 2016

8.15 Plenary Session 2

Location: West Chair: Karl-Heinz Ernst Ben Feringa L39 Exploring Chiral Space beyond the Molecule	Location: East Chair: Jeanne Crassous Matthias Bechmann, Norbert Müller, Robert Glaser L40 Crystallization of Platonic-Solid Geometry Hydrocarbons Cubane (C ₈ H ₈) and Dodeca-hedrane (C ₂₀ H ₂₀) Affords Geometrical Changes
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9.00-9.30 Coffee Break, Exhibit and Posters

9.30-12.05 Parallel Session 4

Location: West Chair: James Canary	
Dynamics	
9.30	Rafael Rodríguez, Katherine Cobos, Sandra Arias, Emilio Quiñoá, Ricardo Riguera, <u>Félix Freire</u> L41 Structural Effects of the Aromatic Substitution Pattern in Poly(phenylacetylenes)s
10.00	Sheng Wang, Jie Zhang, <u>Xinhua Wan</u> L42 Optically Active Helical 3,5-Disubstituted Polyphenylacetylenes with Tunable cis-cisoid to cis-transoid Transition
10.30	<u>Lijia Liu</u> , Wenshuai Wang, Yudan Wang, Chunhong Zhang, Toshiki Aoki, Yoshio Okamoto L43 Thermotropic Chiral Amplification in Copolyacetylene Based on Main-chain Conformation Transformation from cis-transoid to cis-cisoid
10.50	<u>Stefano Superchi</u> , Stefania Vergura, Patrizia Scafato L44 Chirality Sensing and Chirality Induction by Flexible Biphenyls
11.10	<u>Wie Zhang</u> , Lu Yin, Yin Zhao L45 Construction of Chiroptical Switches from Achiral Azobenzene-Containing Polymer Systems
11.30	Hiroyuki Miyake L46 Chiral Metal Complexes Exhibiting Multiple Stimuli Responsiveness
11.50	<u>Sandra Arias</u> , Katherine Cobos, Manuel Núñez, Emilio Quiñoá, Ricardo Riguera, Félix Freire L47 Cation- π interaction in PPA through Sergeants and Soldiers Effect and Chiral Nanostructures

Location: East		Chair: Andreas Pfaltz
Synthesis		
9.30	Jerome Lacour Highly Stable Cationic Helicenes as Platforms for Biological, Physical and Chemical Applications	L48
10.00	<u>Shinichi Itsuno</u> , Yuta Endo, Mohammad Shahid Ullah Highly Active Chiral Polymer Catalyst for Asymmetric Reactions	L49
10.30	Jacek Mlynarski Asymmetric Aldol Reaction Promoted by Tertiary Amines	L50
10.50	Kenta Kishi, Yasushi Yoshida, Suman C. Mohanta, Kazuya Sawada, Kazuhiro Takenaka, Shinobu Takizawa, <u>Hiroaki Sasai</u> Catalytic Enantioselective Transformations Using Chiral Spiro Compounds	L51
11.10	<u>Nobuhiro Kanomata</u> , Seiju Komaki, Taku Maeda, Megumi Imada Remote Steric Effects in Planar-chiral Phase-transfer Catalysis for Asymmetric Reactions	L52
11.30	<u>C. Michon</u> , M.-A. Abadie, F. Medina, X. Trivelli, F. Capet, P. Roussel, M. Kouach, N. Duhal, I. Del Rosal, L. Maron, F. Agbossou-Niedercorn Asymmetric Hydroamination of Alkenes: Effects of Silver, Anion and Solvent on Gold(I) Catalysts	L53
11.50	<u>Juliana Manso de O. Silva</u> , Ricardo Almir Angnes, Carlos Roque Duarte Correia Critical Interaction of Substrate Hydroxyl Group with a Cationic Palladium in a Substrate-Directable Heck Arylation	L54

12.05-13.30 Lunch Break

Vendor Seminar 2:	YMC
Main Lecture Hall	<u>Daniel Eßer</u> : Method Scouting and Optimisation Utilising YMC's CHIRAL ART Columns
12.15-13.15	

13.30-15.30 **Parallel Session 5**

Location: West		Chair: Lorenzo Di Bari
Spectroscopy		
13.30	Prasad L. Polavarapu Complete Chiroptical Spectral Analysis for Molecular Structure Determination	L55
13.55	<u>Gennaro Pescitelli</u> , Francesco Zinna, Claudio Resta, Marcin Gorecki, Lorenzo Di Bari Chiral Conjugated Polymers studied by Electronic Circular Dichroism as Solution Aggregates and Thin Films	L56
14.20	Christian Merten Vibrational Circular Dichroism Spectroscopy in Liquid and Solid Rare Gases	L57
14.45	<u>Ludovic Favereau</u> , Jeanne Crassous Helicene and Diketopyrrolopyrrole, a Useful Combination to Obtain Strong Chiroptical Properties in the Near-Infrared Region	L58
15.10	<u>Jochen R. Brandt</u> , Ying Yang, Alasdair J. Campbell, Matthew J. Fuchter Circularly Polarized Phosphorescent Electroluminescence with a High Dissymmetry Factor from Metallahelicene PHOLEDs	L59

Location: East		Chair: Roberto Purrello
Synthesis		
13.30	<u>Kazuhiko Saigo</u> , Yasuhiro Ishida Perfluoroalkyl Group-Incorporated Amino Acids - Asymmetric Synthesis and Application to Protein Engineering	L60
13.55	<u>Takeshi Yamamoto</u> , Ryo Murakami, Michinori Suginome Asymmetric Steglich Rearrangement with Polyquinoxaline-Based Helically Chiral Nucleophilic Catalyst	L61
14.20	<u>James W. Canary</u> , Shahab Mortezaei, Xueyou Duan, Noelle Caterineu Redox-Reconfigurable Stereochemistry and Ambidextrous Catalysis	L62
14.45	<u>Zsolt Szakonyi</u> , Ferenc Fülöp Stereoselective Synthesis and Transformations of Monoterpene-based Aminodiols	L63
15.10	<u>Hongxing Dong</u> , Danxia Zhang, Xiaobo Li, Meixia Zheng, Yiling Ou A Novel Method to Prepare MIPs as Chromatographic Chiral Stationary Phase by In-Situ Polymerization on Silica Surface	L64

15.30-16.00 **Coffee Break, Exhibit and Posters**

16.00-18.00 **Parallel Session 6**

Location: West		Chair Eiji Yashima
Supramolecular Chemistry		
16.00	<u>David M. Walba</u> , Eva Korblova, Lee Foley, Alyssa Scarbrough, Richard Shoemaker, Chenhui Zhu, Alexander Hexemer, Dong Ki Yoon, Hanim Kim, Joseph MacLennan, Dong Chen, Michael Tuchband, Noel A. Clark L65 Host-Guest Chemistry and Chiral Recognition with Liquid Crystal Conglomerate Hosts	
16.30	Jeanne Crassous L66 Chiral Multifunctional Molecules Based on Helicenes	
17.00	Roberto Purrello L67 Supramolecular Chirality: from Memory to Vortexes	
17.20	<u>Thierry Brotin</u> , Delphine Pitrat, Nathalie Calin, Nicolas Vanthuynne, Frank Wien, Nicolas Daugey, Laurent Ducasse, Thierry Buffeteau L68 Understanding the Unusual Chiroptical Properties of the Cryptophane-222 Skeleton	
17.40	Tomoyo Kosaka, Masataka Toyoda, Yoshihisa Inoue, <u>Tadashi Mori</u> L69 Propeller Chirality of Hexaarylbenzenes and Related Molecules	

Location: East		Chair: Nina Berova
This session is dedicated to Ettore Castiglioni, a passionate scientist and engineer in the field of chiroptical spectroscopy and a long standing friend of the Chirality conference series		
Fundamentals/Analytical Techniques		
16.00	Isao Azumaya L70 Chiral Crystallization of Organic Compounds Having No Fixed Chiral Element	
16.30	<u>Masayuki Watanabe</u> , Hiroshi Hayakawa, Ettore Castiglioni L71 Fundamental Requirements of CPL System	
17.00	<u>Francesco Zinna</u> , Lorenzo Di Bari L72 Playing with Lanthanide Circularly Polarized Luminescence	
17.20	<u>Baoliang Wang</u> , Andy Leadbetter, Jacob Wolf, Gary Kitten, John Freudenthal, Chung-Yon Lin, Eric V. Anslyn L73 A Fast CD Spectrometer For Reading Enantiomeric Excess Directly From The Micro-well Plate	
17.40	<u>Paola Rizzo</u> , Giovanna Longhi, Sergio Abbate, Ettore Castiglioni, Gaetano Guerra L74 Vibrational Circular Dichroism and Circular Polarized Luminescence of Achiral Guest Molecules	

19.30-22.00 **Conference Dinner**

– Reservations must be made in advance, ask at the conference office for remaining tickets and a shuttlebus reservation

Wednesday July 27, 2016

8.45 Plenary Session 3

Location: West	Chair: David Walba	Location: East	Chair: Yitzhak Mastai
Ron Naaman	L75	Yingying Duan, Yuanyuan Cao, Ben Liu, Shunai Che	L76
The Miraculous of Chirality – The Electron's Spin and Molecular Chirality - How are they Related?		Chiral Inorganic Mesostructured Films with Multi-Optical Activity	

9.30-10.00 Coffee Break, Exhibit and Posters

10.00-12.30 Parallel Session 7

Location: West		Chair: Gennaro Pescitelli	
Spectroscopy			
10.00	Laurence A. Nafie		L77
	Vibrational Circular Dichroism in Protein Amyloid Fibrils		
10.30	Anja R.A. Palmans		L78
	Elucidation of the self-assembly behaviour of benzene-1,3,5-tricarboxamides by circular dichroism spectroscopy		
11.00	<u>Steffen Lüdeke</u> , Anja Rüter, Aurelien Forget, Anjan Roy, Carolina Carballo, Rina K. Dukor, Lawrence A. Nafie, Christian Johannessen, V. Prasad Shastri		L79
	Studying Higher Order Structure in Polysaccharide Hydrogels by Raman Optical Activity		
11.25	<u>Arkadii V. Tarasevych</u> , Valeriy N. Snytnikov, Alexander A. Rastoguev, Mark G. Baronskiy, Anton I. Kostyukov		L80
	Luminescent Probing of Enantiopure and Racemic α -Amino Acid		
11.50	<u>Monika Michaelis</u> , Nina Wurzler, Christian Perl, Nils Hildebrand, Robert Meißner, Lucio Colombi Ciacchi		L81
	Assessment of Secondary Structures of Oligopeptides via a Combined Approach of Circular Dichroism and Advanced Sampling Methods		
12.15	<u>Alexander Kastner</u> , Stefanie Züllighoven, Tom Ring, Cristian Sarpe, Christian Lux, Arne Senftleben, Thomas Baumert		L82
	Wavelength dependence of Photoelectron Circular Dichroism in Femtosecond Multiphoton Ionization		

Location: East		Chair: Ron Naaman
Nano		
10.00	<u>Yitzhak Mastai</u> , Ortal Lidor-Shalev Chiral Thin Films of Metal Oxides by Atomic Layer Deposition on Biological Fibers	L83
10.30	Thomas Bürgi Chirality of Nanoscale Gold Particles and Clusters	L84
11.00	<u>Ignacio L. Garzón</u> , J. Jesús Pelayo, Robert L. Whetten Geometric Quantification of Chirality in Ligand-Protected Metal Clusters	L85
11.25	<u>Andrew J. Gellman</u> , Aaron Rienicker, Mathew Payne Mapping Enantioselectivity across Surface Structure Space	L86
11.50	<u>N. Shukla</u> , D. Yang, Y. Zhao, A.J. Gellman Enantiomeric Separations of Chiral Pharmaceuticals using Chiral Tetrahedral Au Nanoparticles	L87
12.15	<u>Rafael Rodríguez-Riego</u> , Zulema Fernández, Esteban Suarez, Mohammad Alzubi, Emilio Quiñoá, Ricardo Riguera, Félix Freire Chiral Amplification in Langmuir-Schaefer Monolayers	L88

12.30-13.30 **Lunch Break**

Vendor Seminar 3: **BioTools**
 Main Lecture Hall Rina Dukor: BioTools Update: VCD, ECD & ROA
 12.40-13.25

Location: Main Lecture Hall		Chair: Jerome Lacour
13.30	Kenso Soai The Origin of Homochirality and Asymmetric Autocatalysis	L89
14.15	<u>Uwe J. Meierhenrich</u> , Cornelia Meinert, Iuliia Myrgorodska, Pierre de Marcellus, Thomas Buhse, Laurent Nahon, Søren V. Hoffmann, Louis d'Hendecourt Organic Molecules Detected in Cometary Ice Analogs and in Comet 67P by the Rosetta Philae Lander	L90
14.45	<u>Wolfgang Lindner</u> , Michal Kohout, Antal Péter, István Ilisz Combinatorial Aspects of Chiral Zwitterionic Ion Exchangers Probed for the Enantiomer Separation of Ampholytes by LC	L91
15.15	<u>I. Starý</u> , I. G. Stará, J. Vacek, J. Vacek Chocholoušová, A. Jančařík, J. Rybáček, O. Stetsovych, M. Švec, K. Kosmider, P. Jelínek, B. Such Helicenes at Nanoscale: Their Synthesis and Properties	L92
15.45	Presentation of Awards	
16.00	Invitation to Chirality 2017 , Closing of Symposium	