

# CHIRALITY 2009

## 21<sup>st</sup> International Symposium on Chirality

### Preliminary Scientific Program

Sunday, July 12, 2009

#### Educational Training / Short Courses

– Must pre-register in order to attend –

##### **Short Course 1: Chiroptical Spectroscopy of Pharmaceuticals and Biomolecules**

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Times: 8:30am – 12:00 pm  
Instructors: Prof. Prasad Polavarapu, Vanderbilt University  
Prof. Nina Berova, Columbia University

Chiral molecules have become invaluable components for drug development and in understanding drug-DNA interactions. To understand these interactions, it is necessary to know the absolute configuration and predominant conformation that a chiral molecule has in its interaction with DNA. To facilitate the structural analysis, pharmaceutical companies have invested, in recent years, a large amount of resources in establishing a facility often termed as “Chiral Tool Box”. This “Tool Box” contains chiroptical spectroscopic equipment and concomitant computational methods for analyzing the chiroptical spectra. Biochemists and synthetic chemists have in the past depended on X-ray crystal structural analysis for determining the absolute configurations of proteins and chiral organic/inorganic molecules synthesized in their labs. However, not all proteins or chiral organic/inorganic molecules can be crystallized, so these chemists are forced to find laborious alternate methods. Chiroptical spectroscopic methods provide a convenient solution to these problems. As chiroptical spectroscopic methods are used for investigating the substances in solution phase, the need for crystallization is completely avoided. As a result, Chiroptical spectroscopy represents the latest trend that is being used increasingly by pharmaceutical companies, biochemists and synthetic chemists. This short course provides the necessary background and practical details for using chiroptical spectroscopic methods. Four chiroptical methods that will be discussed in this short course are: Vibrational circular dichroism (VCD), Vibrational Raman optical activity (VROA), Electronic circular dichroism (ECD/FDCD) and Optical rotatory dispersion (ORD). For each of these methods the experimental methods for measurements will be discussed first. Then the computational methods for analyzing the experimental data will be introduced. Emphasis will be placed on literature examples from pharmaceutical and biological chemistry illustrating the applications of these methods on molecular and supramolecular levels. The advantages (sometimes necessity) of using simultaneously more than one chiroptical method will also be pointed out.

##### **Short Course 2: Introduction to Chiral Separations**

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Times: 8:30 am – 12:00 pm  
Instructor: Prof. Daniel W. Armstrong, University of Texas at Arlington

This introductory short course is designed for researchers faced with separation or analysis of enantiomeric compounds. The goal of the course is to familiarize the participants with the best available options when confronted with the need for chiral separations. The first part of the material to be covered will include a review of the terminology of chirality and a brief overview of the theory behind enantiomeric separations. In addition, new products and techniques will be discussed. Participants should have a basic knowledge of organic chemistry and chromatography and have previous experience with routine HPLC (reverse phase and normal phase).

**Sunday, July 12, 2009**

## **Educational Training / Short Courses**

– Must pre-register in order to attend –

### **Short Course 3: Supermolecular Stereochemistry in Liquid Crystals**

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Times: 1:00 – 4:30 pm

Instructor: Prof. David M. Walba, University of Colorado, Boulder

Stereochemistry in soft materials (liquid crystals, polymers, and gels) is extremely rich, and maintains an aura of complexity due, in part, to the highly “flexible” nature of their structure. With regard to issues of chirality, thermotropic liquid crystals (LCs), which are typically global free energy minima occurring in a large ensemble of small organic molecules, have until recently been quite simple. LCs formed from achiral molecules or racemic mixtures are achiral, while all LCs formed from enantiomerically enriched compounds must be chiral. The latter fact of symmetry (i.e. an ensemble, or phase, of unichiral molecules cannot possess reflection symmetry) led to the theoretical proposal, then experimental realization, of LC phases with polar symmetry driven by chirality combined with layering and tilt. This, in turn, provides measurable and useful, macroscopic electric dipoles in the absence of applied fields. The situation became even more interesting in the late 1990s with the discovery of spontaneous reflection symmetry breaking (and nonpolar symmetry breaking) in LCs – a complex but satisfying story. In this short course, stereochemistry in highly “flexible” systems will be introduced in the context of molecular topological stereoisomerism, (e.g. molecular Mobius strips, knots and links). The basics of LC phase structure, and current thinking about the key free energy terms driving these structures, will then be discussed, followed by a description of the phenomenology and applications of electrically polar LCs, including prospects for utilization of polarity in LCs for high throughput measurement of enantiomeric excess. Finally, the rich stereoisomerism occurring in bent-core, or banana phase materials, including spontaneous reflection symmetry breaking will be discussed. The soft materials community is still divided with regard to the physical reasons for this novel conglomerate formation in fluid phases; models will be explored.

### **Short Course 4: Preparative Chiral Separations**

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Times: 1:00 – 4:30 pm

Instructor: Dr. Christopher J. Welch, Merck & Co., Inc.

This course will present an introduction to modern preparative chiral chromatography. A general introduction to tools and techniques will provide practical background on how to approach small, intermediate, and large scale preparative chromatographic resolutions. Several practical case studies from the pharmaceutical industry will be presented, and general strategies for approaching chromatographic resolutions will be discussed. Attendees are encouraged to bring problems or situations for classroom discussion.

**Sunday, July 12, 2009**

4:00 pm **Symposium Registration Open**

5:30 pm **OPENING REMARKS & PRESENTATION OF CHIRALITY MEDAL**

5:50–6:50 pm **Chirality Medal Award Lecture**

**A Chiral Space Odyssey.** Ben L. Feringa, Stratingh Institute for Chemistry, Zernike Institute for Advanced Materials & Center for Systems Chemistry, University of Groningen, Nijenborgh 4, 9747 AG Groningen, THE NETHERLANDS

7:00–9:00 pm **Chirality Medal Reception**

## Monday, July 13, 2009

8:00 am SYMPOSIUM REGISTRATION OPEN

8:30 am – 5:00 pm **EXPOSITION**

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### **Session 1. SPECTROSCOPY**

**Chair: Nina Berova, Columbia University**

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8:30 am L-101 **Raman Optical Activity and its Applications in Chiral Molecular, Supramolecular and Biomolecular Science.** Laurence D. Barron, Christian Johannessen, Josef Kapitán, Lutz Hecht, WestCHEM, Department of Chemistry, University of Glasgow, Glasgow, UK [PLENARY LECTURE]

9:10 am L-102 **The Application of Vibrational Circular Dichroism (VCD) Spectroscopy to the Determination of the Stereochemistries of Chiral Molecules.** Phillip J. Stephens, University of Southern California, Los Angeles, CA, USA [PLENARY LECTURE]

9:50 am **Coffee Break**

# Monday, July 13, 2009

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## Session 1A. SPECTROSCOPY

Chair: Nina Berova, Columbia University

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- 10:10 am L-103 **Links, Crosslinks, and Tangles on the Way to DNA-directed Assembly of Organic Materials.** James W. Canary, Department of Chemistry, New York University, New York, NY, USA [KEYNOTE LECTURE]
- 10:40 am L-104 **Conformational Sensitivity of Chiroptical Spectroscopic Methods.** Prasad L. Polavarapu, Department of Chemistry, Vanderbilt University, Nashville, TN, USA [KEYNOTE LECTURE]
- 11:10 am **Pause**
- 11:20 am L-105 **Robust Modes in Vibrational Circular Dichroism Spectra.** Valentin Paul Nicu, Evert Jan Baerends, Theoretical Chemistry, Vrije Universiteit Amsterdam, Amsterdam, THE NETHERLANDS
- 11:40 am L-106 **Chiroptical Analysis of Lipids and Glycolipids by Vibrational Circular Dichroism.** Kenji Monde, Masataka Shibata, Atsufumi Nakahashi, Masumi Fukuzawa, Tohru Taniguchi, Nobuaki Miura, Shin-Ichiro Nishimura, Laboratory of Chemical Biology, Graduate School of Advanced Life Science, Frontier Research Center for Post-genome Science and Technology, Hokkaido University, Sapporo, JAPAN
- 12:00 pm L-107 **Two-photon Circular Dichroism: The Experimental Demonstration.** Carlos Toro<sup>1</sup>, Leonardo de Boni<sup>1</sup>, Na Lin<sup>2</sup>, Fabrizio Santoro<sup>3</sup>, Antonio Rizzo<sup>3</sup>, Florencio E. Hernandez<sup>1,4</sup>, <sup>1</sup>Department of Chemistry, University of Central Florida, Orlando, FL, USA; <sup>2</sup>Department of Theoretical Chemistry, Royal Institute of Technology, Stockholm, SWEDEN; <sup>3</sup>Istituto per i Processi Chimico-Fisici del Consiglio Nazionale delle Ricerche (IPCF-CNR), Pisa, ITALY; <sup>4</sup>The College of Optics and Photonics, CREOL, University of Central Florida, Orlando, FL, USA
- 12:20 pm **PAUSE, EXHIBITS, POSTERS, VENDOR SEMINARS** (lunch on own)
- 12:30–1:30 pm **FREE VENDOR SEMINAR Sponsored by Phenomenex**  
“A Welcome Change to the Chiral Industry. How Phenomenex Corporate Capabilities in Chiral Solutions Can Impact Your Work.” (20 mins);  
“Reversed-phase vs. Normal Phase: Which Should Be the Primary Separation Mode Screened in Chiral Method Development?” (25 mins)
- 1:30–3:00 pm **POSTER PRESENTATIONS**

## Monday, July 13, 2009

### Session 1B. SURFACE – SUPRAMOLECULAR

Chair: Daniel Armstrong, University of Texas at Arlington

- 10:10 am L-108 **Aspects of Chirality in Molecular Monolayers.** Karl-Heinz Ernst, Molecular Surface Science, Nanoscale Materials Science Laboratory, Empa – Swiss Federal Laboratories for Materials Testing and Research, Dübendorf, SWITZERLAND [KEYNOTE LECTURE]
- 10:40 am L-109 **Molecule by Molecule Tracking of Chiral Recognition and Self Assembly: A Submolecular Insight by Scanning Tunnelling Microscopy.** Magali Lingenfelder<sup>1</sup>, G. Tomba<sup>2</sup>, G. Costantini<sup>1</sup>, Y. Wang<sup>1</sup>, A. De Vita<sup>2</sup>, K. Kern<sup>1</sup>, <sup>1</sup>Max-Planck-Institute for Solid State Research, Stuttgart, GERMANY; <sup>2</sup>Physics Department, King's College London, London, UK [KEYNOTE LECTURE]
- 11:10 am **Pause**
- 11:20 am L-110 **Synthesis and Structure of Optically Active pi-Stacked Polymers.** Tamaki Nakano, Takeshi Sakamoto, Division of Biotechnology and Macromolecular Chemistry, Graduate School of Engineering, Hokkaido University, Sapporo, JAPAN
- 11:40 am L-111 **Large Effects of Chirality on Deslipping Reactions of Diastereomeric Rotaxanes and Relevant Mechanism Involving Pre-equilibrium.** Keiji Hirose, Yamato Nakamura, Yoshito Tobe, Division of Frontier Materials Science, Graduate School of Engineering Science, Osaka University, Osaka, JAPAN
- 12:00 pm L-112 **Polarity Influence on the Self-assembly of Benzene-1,3,5-tricarboxamides and on Their Role as Physical Crosslinkers in Polymeric Systems.** Tristan Mes, Anja R. A. Palmans, E. W. Meijer, Laboratory of Molecular Science and Technology, Eindhoven University of Technology, Eindhoven, THE NETHERLANDS
- 12:20 pm **PAUSE, EXHIBITS, POSTERS, VENDOR SEMINARS** (lunch on own)
- 12:30–1:30 pm **FREE VENDOR SEMINAR Sponsored by Phenomenex**  
“A Welcome Change to the Chiral Industry. How Phenomenex Corporate Capabilities in Chiral Solutions Can Impact Your Work.” (20 mins);  
“Reversed-phase vs. Normal Phase: Which Should Be the Primary Separation Mode Screened in Chiral Method Development?” (25 mins)
- 1:30–3:00 pm **POSTER PRESENTATIONS**

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**Session 2. ORIGINS**

Chair: Kurt Mislow, Princeton University

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*The Plenary Lectures, and Keynotes and Orals of session 2/2B will probe the latest thinking on nonbiological enantioenrichment and the origins of life. The session, with a special concluding round table discussion, will be moderated by Professor Kurt Mislow, and promises to be controversial and entertaining.*

3:00 pm L-113 **Asymmetric Autocatalysis and Its Role in the Origins of Homochirality.** Kenso Soai, Department of Applied Chemistry, and Chiral Material Research Center, Research Institute of Science and Technology, Tokyo University of Science, Tokyo, JAPAN [PLENARY LECTURE]

3:40 pm L-114 **Did Life Grind to a Start?** Michael McBride, Yale University, New Haven, CT, USA [PLENARY LECTURE]

4:20 pm **Pause**

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**Session 2A. RESOLUTIONS**

Chair: Eiji Yashima, Nagoya University

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4:30 pm L-115 **Preparative Chiral Chromatography in Support of Pharmaceutical Discovery and Development: Recent Progress and Future Directions.** Christopher J. Welch, Merck & Co., Inc., Rahway, NJ, USA [KEYNOTE LECTURE]

5:00 pm L-116 **Production of an Enantiopure Compound 'At Will' from the Corresponding Multi-chiral Racemate by Combining HPLC and Racemisation.** Alexander L. L. Duchateau, Jan van der Lee, Gerard Verzijl, Lyrelle Stacey-Lloyd, DSM Pharmaceutical Products, Innovative Synthesis and Catalysis, Geleen, THE NETHERLANDS

5:20 pm L-117 **A Fluorescent Amino Acid-based Chiral Ionic Liquid for Enantiomeric Discrimination.** David K. Bwambok, Santhosh K. Challa, Mark Lowry, Isiah M. Warner, Department of Chemistry, Louisiana State University, Baton Rouge, LA, USA

5:40 pm L-118 **"Green Chemistry" in Chiral Resolution.** Niteen Vaidya, ChiroSolve, Inc., Santa Clara, CA, USA

6:00 pm **Concluding Remarks and Round Table Discussion**  
Kurt Mislow, Department of Chemistry, Frick Lab, Princeton University, Princeton, NJ, USA  
*The Plenary Lectures, and Keynotes and Orals of session 2/2B probe the latest thinking on nonbiological enantioenrichment and the origins of life. The round table discussion session promises to be controversial and entertaining.*

6:45 pm **Pause**

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**Session 2B. NONBIOLOGICAL ENANTIOENRICHMENT**

**Chair: Kurt Mislow, Princeton University**

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- 4:30 pm L-119 **Thermodynamics of Chiral Asymmetry.** Dilip Kondepudi, Department of Chemistry, Wake Forest University, Winston-Salem, NC, USA [KEYNOTE LECTURE]
- 5:00 pm L-120 **Applications of Attrition Induced Grinding of Racemizable Conglomerates as a Route to Enantiopure Materials.** Richard M. Kellogg<sup>a</sup>, M. Leeman<sup>a</sup>, M. van der Meijden<sup>a</sup>, W. Noorduyn<sup>b</sup>, H. Meekes<sup>b</sup>, W.J.P. van Enckevort<sup>b</sup>, B. Kaptein<sup>c</sup>, Syncom BV, Groningen, THE NETHERLANDS; <sup>b</sup>IMM Solid State Chemistry, Radboud University Nijmegen, Nijmegen, THE NETHERLANDS; <sup>c</sup>Innovative Synthesis and Catalysis, DSM Pharmaceutical Products, Geleen, THE NETHERLANDS
- 5:20 pm L-121 **Studies on the Origin of Homochirality of Peptides.** Meir Lahav<sup>1</sup>, R.A. Illois<sup>1</sup>, I. Weissbuch<sup>1</sup>, G. Bolbach<sup>2</sup>, <sup>1</sup>Weizmann Institute of Science, Rehovot, ISRAEL; <sup>2</sup>Université Pierre and Marie Curie, Paris, FRANCE [KEYNOTE LECTURE]
- 5:50 pm **Pause**
- 6:00 pm **Concluding Remarks and Round Table Discussion**  
Kurt Mislow, Department of Chemistry, Frick Lab, Princeton University, Princeton, NJ, USA  
*The Plenary Lectures, and Keynotes and Orals of session 2/2B probe the latest thinking on nonbiological enantioenrichment and the origins of life. The round table discussion session promises to be controversial and entertaining.*
- 6:45 pm **Pause**

## Tuesday, July 14, 2009

7:15–8:15 am **FREE VENDOR SEMINAR Sponsored by TharSFC, a Waters Company**  
“SFC: New Developments in Isomeric Separation and Purifications”

8:00 am Symposium Registration Open

8:30 am – 5:00 pm **EXPOSITION**

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### **Session 3A. TIDES**

**Chair: James Canary, New York University**

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8:30 am L-201 **Constructing Complex Nanostructures with DNA.** Marvin H. Caruthers,  
Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, USA  
[PLENARY LECTURE]

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### **Session 3B. SYNTHESIS**

**Chair: James Canary, New York University**

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9:10 am L-202 **Enantioselective Synthesis in China - Past, Present, and Future.**  
Albert S. C. Chan, The Hong Kong Polytechnic University, Kowloon, Hong Kong  
[PLENARY LECTURE]

9:50 am **Coffee Break**

**Session 3A. TIDES**

**Chair: James Canary, New York University**

- 10:10 am L-203 **Chiral Peptide Nucleic Acids: Biological Tools and Bio-inspired Materials.** Roberto Corradini, Tullia Tedeschi, Stefano Sforza, Rosangela Marchelli, Dipartimento di Chimica Organica e Industriale-University of Parma, Parma, ITALY [KEYNOTE LECTURE]
- 10:40 am L-204 **Detecting and Following Chirality in Computer Simulations of Liquid Crystals and Biomolecules.** Claudio Zannoni, Dipartimento di Chimica Fisica ed Inorganica, Università, Bologna, ITALY [KEYNOTE LECTURE]
- 11:10 am **Pause**
- 11:20 am L-205 **Control of Dynamic Property and Helicity in a Helically Folded Achiral Peptide through a Side-chain Bridge.** Reiko Kuroda<sup>a,b</sup>, N. Ousaka<sup>b</sup>, N. Tani<sup>a</sup>, T. Sato<sup>b</sup>, <sup>a</sup>Graduate School of Arts and Sciences, The University of Tokyo, Tokyo, JAPAN; <sup>b</sup>Japan Science and Technology Agency, ERATO-SORST Kuroda Chirormorphology Team, Tokyo, JAPAN
- 11:40 am L-206 **Folded Biomimetic Oligomers for Enantioselective Catalysis.** Galia Maayan, Michael D. Ward, Kent Kirshenbaum, Department of Chemistry and Molecular Design Institute, New York University, New York, NY, USA
- 12:00 pm L-207 **L-Oligonucleotide Therapeutics in a D-World. Spiegelmers<sup>®</sup>: From Concept to Realization.** John Turner, NOXXON Pharma AG, Berlin, GERMANY
- 12:20 pm **PAUSE, EXHIBITS, POSTERS, VENDOR SEMINARS** (lunch on own)
- 12:30–1:30 pm **FREE VENDOR SEMINAR Sponsored by Supelco/Sigma-Aldrich**  
"Strategies for Chiral HPLC Method Development"
- 12:30–1:30 pm **FREE VENDOR SEMINAR Sponsored by Chiral Technologies**  
"Comprehensive Solutions for Enantioselective Chromatography"
- 1:30–3:00 pm **POSTER PRESENTATIONS**

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**Session 3B. SYNTHESIS**

**Chair: Jerome LaCour, University of Geneva**

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- 10:10 am L-208 **Synthesis of Stereochemically Complex Natural Products.** Andrew J. Phillips, University of Colorado, Boulder, CO, USA [KEYNOTE LECTURE]
- 10:40 am L-209 **Organocatalytic Epoxidation and Metallocatalytic Diamination of Olefins.** Yian Shi, Department of Chemistry, Colorado State University, Fort Collins, CO, USA [KEYNOTE LECTURE]
- 11:10 am **Pause**
- 11:20 am L-210 **Recent Advances in Enantioselective Phase Transfer Catalysis.** Paul Bulger, Merck & Co., Inc., Whitehouse Station, NJ, USA
- 11:40 am L-211 **A New Approach to Enantioselective Organic Synthesis: Absolute Asymmetric Synthesis of Organometallic Reagents.** Anders Lennartson, Susanne Olsson, Jonas Sundberg, Mikael Hakansson, Department of Chemistry, University of Gothenburg, Gothenburg, SWEDEN
- 12:00 pm L-212 **Synthesis of Cyclophane-type Imidazolium Salts with Planar Chirality and Chirality-Induction Ability of Their Derivative N-Heterocyclic Carbenes.** Kazuhiko Saigo, Yasuhiro Ishida, Yuki Matsuoka, Daisuke Sasaki, Department of Chemistry and Biotechnology, Graduate School of Engineering, The University of Tokyo, Hongo, Tokyo, JAPAN
- 12:20 pm **PAUSE, EXHIBITS, POSTERS, VENDOR SEMINARS** (lunch on own)
- 12:30–1:30 pm **FREE VENDOR SEMINAR Sponsored by Supelco/Sigma-Aldrich**  
"Strategies for Chiral HPLC Method Development"
- 12:30–1:30 pm **FREE VENDOR SEMINAR Sponsored by Chiral Technologies**  
"Comprehensive Solutions for Enantioselective Chromatography"
- 1:30–3:00 pm **POSTER PRESENTATIONS**

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**Session 4A. ANALYTICAL**

Chair: David Walba, University of Colorado at Boulder

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3:00 pm L-213 **New Directions in Enantioselective Analyses.** Daniel W. Armstrong,  
University of Texas at Arlington, Arlington, TX, USA [PLENARY LECTURE]

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**Session 4B. NANO**

Chair: David Walba, University of Colorado at Boulder

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3:40 pm L-214 **The B4 and the Dark Conglomerate: Topologically Disordered Spontaneously Chiral Liquid Crystal Phases Stabilized by Frustrated Intralayer Correlations.**  
Noel A. Clark<sup>1</sup>, L. E. Hough<sup>1</sup>, M.-S. Heberling<sup>1</sup>, M. Spannuth<sup>1</sup>, M. Nakata<sup>1</sup>, M. Glaser<sup>1</sup>, D. Krüerke<sup>2</sup>, C. D. Jones<sup>1</sup>, C. Zhu<sup>1</sup>, G. Heppke<sup>2</sup>, H. Jung<sup>3</sup>, J. Zasadzinski<sup>3</sup>, J. Rabe<sup>4</sup>, W. Stocker<sup>4</sup>, E. Körblova<sup>5</sup>, D. Walba<sup>5</sup>, <sup>1</sup>Department of Physics and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO, USA; <sup>2</sup>Institute of Inorganic and Analytic Chemistry, TU of Berlin, Berlin, GERMANY; <sup>3</sup>Department of Chemical Engineering, University of California, Santa Barbara, CA, USA; <sup>4</sup>Institute for Physics, Humboldt University, Humboldt, GERMANY; <sup>5</sup>Department of Chemistry and Biochemistry and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO, USA [PLENARY LECTURE]

4:20 pm **Pause**

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**Session 4A. ANALYTICAL**

**Chair: Christopher Welch, Merck & Co., Inc.**

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- 4:30 pm L-215 **Separation of Chiral Objects in Achiral Media: What is the Size Limit?** Michal Tencer, Roman Bielski, School of Information Technology and Engineering, University of Ottawa, Ottawa, CANADA
- 4:50 pm L-216 **The Changing Landscape of Chiral Separation and Purification.** Tivadar Farkas, Liming Peng, Swapna Jayapalan, Bezhan Chankvetadze<sup>1</sup>, Phenomenex, Inc., Torrance, CA, USA; <sup>1</sup>Institute of Physical and Analytical Chemistry, Tbilisi State University, Tbilisi, GEORGIA
- 5:10 pm L-217 **Reversed-phase Multichannel Microflow Chiral LC Method Development of Compounds of Pharmaceutical Interest.** Don W. Arnold<sup>a</sup>, David Emlyn Hughes<sup>b</sup>, Phillip H. Pau<sup>a</sup>, <sup>a</sup>Eksigent Technologies, LLC, Dublin, CA, USA; <sup>b</sup>Chromatographic Excellence, LLC, Pennington, NJ, USA
- 5:30 pm L-218 **High-throughput Multiplexing Gas Chromatography for Super High-throughput Measurements of Enantiomeric Excesses.** Oliver Trapp, Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, GERMANY
- 5:50 pm L-219 **Substituent Effects on Chiral Recognition: Chiral HPLC and SFC Separation of Substituted Meldrum's Acid on Amylose and Cellulose Chiral Stationary Phase.** Hong-Xun Guo, Jenny Chen, David Semin, Janet Cheetham, AR&D, Amgen Inc., Thousand Oaks, CA, USA
- 6:10 pm **Pause**
- 7:00 pm **CONFERENCE BANQUET – Western Style US Barbeque Bash (ticket required)**

We invite you to join the Chirality 2009 Permanent International Scientific Committee for Tuesday's Western Style US Barbeque Bash at the foot of the Beaver Run ski lift (includes dinner, music, and open bar).

If you have not purchased your dinner ticket, tickets may be purchased at the Symposium Registration Desk at a cost of \$85 each. Tickets are on sale until Tuesday at 4:00 PM, or until sold out. MUST present ticket in order to attend the BBQ—no exception. Misplaced or lost tickets will not be replaced.

## Tuesday, July 14, 2009

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### Session 4B. NANO

Chair: David Walba, University of Colorado at Boulder

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- 4:30 pm L-220 **Bernauer's Bands.** Bart Kahr, Erica Gunn, John Freudenthal, Department of Chemistry, University of Washington, Seattle WA, USA [KEYNOTE LECTURE]
- 5:00 pm L-221 **Multi-stranded Helical Polymers and Oligomers.** Eiji Yashima, Department of Molecular Design and Engineering, Graduate School of Engineering, Nagoya University, Nagoya, JAPAN [KEYNOTE LECTURE]
- 5:30 pm L-222 **Liquid Chromatographic Separation of Enantiomers with Topologically Chiral Amide-type Trefoil Knots: Chiral Recognition Mediated by a Molecular Scaffold Devoid of Conventional Chirality Elements.** Norbert M Maier<sup>a,b</sup>, Wolfgang Lindner<sup>b</sup>, Jens Brueggemann<sup>c</sup>, Fritz Voegtle<sup>c</sup>, <sup>a</sup>Chiral Technologies, Inc., West Chester, PA, USA; <sup>b</sup>University of Vienna, Institute of Analytical and Food Chemistry, Vienna, AUSTRIA; Kekule Institute for Organic Chemistry and Biochemistry, <sup>c</sup>University of Bonn, Bonn, GERMANY
- 5:50 pm L-223 **Structural Change of Polyacetylene Main Chain Cased by Pendant Rotaxane Mobility.** Toshikazu Takata, Fumitaka Ishiwari, Kei-ichiro Fukasawa, Yasuhito Koyama, Tokyo Institute of Technology, Department of Organic and Polymeric Materials, Tokyo, JAPAN
- 6:10 pm **Pause**
- 7:00 pm **CONFERENCE BANQUET – Western Style US Barbeque Bash (ticket required)**

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**Session 5. NANO – 2**

**Chair: Eiji Yashima, Nagoya University**

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- 8:30 am L-301 **Two-fold Helix Inversion in the Chiral Smectic C Phase in Optically Active Material Derived from (R)-(+)-1-(1-phenyl)ethylamine.** Muto Masakane, Hideyuki Suzuki, Kaoru Fukuda, Seng Kue Lee, Sungmin Kang, Masatoshi Tokita, Junji Watanabe, Department of Organic and Polymeric Materials, Tokyo Institute of Technology, Tokyo, JAPAN [PLENARY LECTURE]
- 9:10 am L-302 **The Detection of Chiral Perturbations in Ferroelectric Liquid Crystals.** Robert P. Lemieux, Chemistry Department, Queen's University, Ontario, CANADA [PLENARY LECTURE]
- 9:50 am **Coffee Break**

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**Session 5A. NANO – 2**

**Chair: Noel Clark, University of Colorado, Boulder**

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- 10:10 am L-303 **New Chiral Geometries.** Elisabetta A. Matsumoto, Gareth P. Alexander, Randall D. Kamien, University of Pennsylvania, Philadelphia, PA, USA [KEYNOTE LECTURE]
- 10:40 am L-304 **Isotropic Ordering and Fast Fluctuation Mode in Isotropic Smectic Blue Phase.** Jun Yamamoto<sup>1</sup>, Isa Nishiyama<sup>2</sup>, <sup>1</sup>Department of Physics, Graduate School of Science, Kyoto University, Kyoto, JAPAN; <sup>2</sup>DIC, Tokyo, JAPAN [KEYNOTE LECTURE]
- 11:10 am **Pause**
- 11:20 am L-305 **Chirality in Mesoporous Materials: The Sergeants and Soldiers Effect in Solid Materials.** Stephanie MacQuarrie, Thomas Blackburn, Steven Dickson, Nicholas Mosey, Robert Lemieux, Cathleen Crudden, Department of Chemistry, Queen's University, Ontario, CANADA
- 11:40 am L-306 **Chiral Amplification in a Dynamic Supramolecular Polymer.** Maarten M. J. Smulders<sup>a</sup>, Paul van der Schoot<sup>b</sup>, Anja R. A. Palmans<sup>a</sup>, Albertus P. H. J. Schenning<sup>a</sup>, E. W. Meijer<sup>a</sup>, <sup>a</sup>Laboratory of Molecular Science and Technology, Eindhoven University of Technology, Eindhoven, THE NETHERLANDS; <sup>b</sup>Theoretical and Polymer Physics Group, Eindhoven University of Technology, Eindhoven, THE NETHERLANDS
- 12:00 pm L-307 **Scanning Tunneling Microscopy Study of a Chiral Amphiphile at a Solid-liquid Interface: Observation of Packing Frustration Leading to Chirality Alternation in a Lamellar Structure.** Wojciech J. Saletta<sup>a</sup>, David B. Amabilino<sup>a</sup>, Hong Xu<sup>b</sup>, Steven De Feyter<sup>b</sup>, <sup>a</sup>Institut de Ciència de Materials de Barcelona (CSIC), Campus Universitari, Bellaterra, SPAIN; <sup>b</sup>Department of Molecular and Nanomaterials, Katholieke Universiteit Leuven, Leuven, BELGIUM
- 12:20–1:30 pm **Pause** (lunch on own)

## Wednesday, July 15, 2009

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### Session 5B. BIO

Chair: John Caldwell, University of Liverpool

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- 10:10 am L-308 **Stereoselective Microbial Transformation of Triadimefon to Triadimenol in Soils: Varying Production Rates of Triadimenol Stereoisomers Could Impact Risk Assessment.** Arthur W. Garrison, Jimmy K. Avants, W. Jack Jones, U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division, Athens, GA, USA [KEYNOTE LECTURE]
- 10:40 am L-309 **Investigations to Elucidate the Enantioselective Biomolecular Recognition Mechanism of Antimony Tartrate.** Kevin A. Schug, Aruna B. Wijeratne, Sandra E. Spencer, Jose Gracia, Peter Kroll, Daniel W. Armstrong, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA [KEYNOTE LECTURE]
- 11:10 am **Pause**
- 11:20 am L-310 **TBD**
- 11:40 am L-311 **Chiral Gas Chromatography – Mass Spectrometry as a Tool for Investigations into Illicitly Produced Ephedrine and Methamphetamine.** Calum Morrison<sup>1</sup>, F. Smith<sup>1</sup>, K. Stawiariski<sup>2</sup>, T. Tomaszewski<sup>2</sup>, M. Biziuk<sup>2</sup>, <sup>1</sup>School of Engineering and Science, University of the West of Scotland, Paisley, UK; <sup>2</sup>Faculty of Chemistry, Gdansk University of Technology, Gdansk, POLAND
- 12:00 pm L-312 **Enantiomer Selective Sorption at Mineral Surfaces. A Case Study with the Organo-phosphorus Pesticide Acephate.** Joe Wilkinson, Martin Preston, Department of Ocean and Earth Sciences, University of Liverpool, Liverpool, UK
- 12:20–1:30 pm **Pause** (lunch on own)

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### Session 6. BIO, NANO, AND PASTEUR

Chair: David Walba, University of Colorado at Boulder

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- 1:30 pm L-313 **Structural Origin of Circularly Polarized Iridescence in Jeweled Beetles.** Vivek Sharma<sup>1-2</sup>, Matija Crne<sup>2-3</sup>, Jung Ok Park<sup>1-2</sup>, Mohan Srinivasarao<sup>1-3</sup>, <sup>1</sup>School of Polymer, Textile and Fiber Engineering, <sup>2</sup>Center for Advanced Research on Optical Microscopy (CAROM) and <sup>3</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, USA [PLENARY LECTURE]
- 2:10 pm L-314 **Does More Stereogenic Centres Mean “More Chiral”?** David B. Amabilino<sup>1</sup>, Patrizia Iavicoli<sup>1</sup>, Hong Xu<sup>2</sup>, Steven De Feyter<sup>2</sup>, <sup>1</sup>Institut de Ciència de Materials de Barcelona (CSIC), Bellaterra, SPAIN; <sup>2</sup>Laboratory of Photochemistry and Spectroscopy, Molecular and Nano Materials, Department of Chemistry, and Institute for Nanoscale Physics and Chemistry, Katholieke Universiteit Leuven, Leuven, BELGIUM [KEYNOTE LECTURE]
- 2:40 pm L-315 **Louis Pasteur and the Language of Chirality.** Joseph Gal, University of Colorado Denver, School of Medicine, Division of Clinical Pharmacology and Toxicology, Aurora, CO, USA [KEYNOTE LECTURE]
- 3:10 pm **Chirality 2009 Closing & Presentation of Best Poster Awards**

# Monday Poster Presentations

Session Times: 1:30 – 3:30 PM

Posters with program numbers in the P-100 series are presented during Monday's Poster Session. All posters will remain up for viewing all day Monday and Tuesday. All posters should be mounted onto the poster boards on Monday between 8:30 AM and 1:30 PM and not removed until Tuesday between 3:00 PM and 4:30 PM (anything remaining after 4:30 PM on Tuesday will be discarded).

P-101 A Tiered Approach to Rapid Chiral Method Development for Supercritical Fluid Chromatography in Drug Discovery. Wesley Barnhart, Kyung H. Gahm, Zheng Hua, Samuel Thomas, Molecular Structure, Discovery Analytical Sciences, Amgen Inc., Thousand Oaks, CA, USA

P-102 Significant Improvements in Chiral Method Development Using an LC-MS-Based Screening Approach. David S. Bell, Jennifer E. Claus, Jay M. Jones, Supelco, Division of Sigma-Aldrich, Bellefonte, PA, USA

P-103 Enzyme Stereospecificity as a Tool for Searching of New Enzymes. Vladimir Wsol<sup>a</sup>, Lucie Skarydova<sup>a</sup>, Adam Skarka<sup>a</sup>, Petr Solich<sup>b</sup>, <sup>a</sup>Department of Biochemical Sciences and <sup>b</sup>Department of Analytical Chemistry, Faculty of Pharmacy, Charles University, Hradec Králové, CZECH REPUBLIC

P-104 Chiral Properties of a New Human Membrane-bound Carbonyl Reductase Playing a Role in Deactivation of Anticancer Drugs. Vladimir Wsol<sup>a</sup>, Lucie Skarydova<sup>a</sup>, Adam Skarka<sup>a</sup>, Petr Solich<sup>b</sup>, <sup>a</sup>Department of Biochemical Sciences and <sup>b</sup>Department of Analytical Chemistry, Faculty of Pharmacy, Charles University, Hradec Králové, CZECH REPUBLIC

P-105 Highly Efficient Enantioresolution of 2,2-Dimethyl-3-hexanol with Cholamide Crystals on the Basis of Intercalation and Bilayer Inversion on the Basis of Intercalation and Bilayer Inversion. Taketoshi Murai, K. Aburaya, I. Hisaki, N. Tohnai, M. Miyata, Department of Material and Life Science, Graduate School of Engineering, Osaka University, Osaka, JAPAN

P-106 Evaluating Memory Effects of Mobile Phase Additives on the Whelk-O<sup>®</sup>1 Chiral Stationary Phase (CSP). Ted Szczerba, Regis Technologies, Inc., Morton Grove, IL, USA

P-107 Advanced Solutions for Preparative SFC (pSFC) Multi-Column Scale-up. Zahid Ali, Regis Technologies, Inc., Morton Grove, IL, USA

P-108 Creating a Solvent Strength Scale for the Prediction of Sample Retentions on the Whelk-O<sup>®</sup>1 Chiral Stationary Phase. Ted Szczerba, Regis Technologies, Inc., Morton Grove, IL, USA

P-109 An Experimental and Theoretical Investigation of the Vibrational Spectra of Eu(tfc)<sub>3</sub> and its Complexes with Chiral Amines. Are shifts Seen in NMR Spectra Also Seen in the VA and VCD Spectra? Christian Merten<sup>a</sup>, Karl J. Jalkanen<sup>b</sup>, Andreas Hartwig<sup>a</sup>, <sup>a</sup>Fraunhofer Institute for Manufacturing Technology and Applied Materials Research, Bremen, GERMANY; <sup>b</sup>Bremen Center for Computational Materials Science, University of Bremen, Bremen, GERMANY

P-110 What can be Learned from the Thousands of Chiral Chromatographic Data in the 2008 Literature? Christian Roussel, Patrick Piras, Nicolas Vanthuyne, UMR 6263, ISM2 Chirosciences, Université Paul Cézanne Marseille, FRANCE

P-111 Stereochemical Studies of Hexylitaconic Acid, An Inhibitor of p53-HDM2 Interaction. Atsufumi Nakahashi<sup>a</sup>, Nobuaki Miura<sup>a</sup>, Kenji Monde<sup>a</sup>, Sachiko Tsukamoto<sup>b</sup>, <sup>a</sup>Graduate School of Advanced Life Science, Frontier Research Center for Post-Genome Science and Technology, Hokkaido University, Sapporo, JAPAN; <sup>b</sup>Graduate School of Science, Chiba University, Chiba, JAPAN

P-112 Stereochemical Study of Chiral Tautomeric Flavorous Furanones by Vibrational Circular Dichroism. Atsufumi Nakahashi<sup>a</sup>, Nobuaki Miura<sup>a</sup>, Kenji Monde<sup>a</sup>, Makoto Emura<sup>b</sup>, Yoshihiro Yaguchi<sup>b</sup>, Daisuke Sugimoto<sup>b</sup>, <sup>a</sup>Graduate School of Advanced Life Science, Frontier Research Center for Post-Genome Science and Technology, Hokkaido University, Sapporo, JAPAN, <sup>b</sup>Corporate Research and Development Division, Takasago International Corporation, Kanagawa, JAPAN

# Monday Poster Presentations

Session Times: 1:30 – 3:30 PM

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- P-113 Discrimination of Cryptochirality in Isotactic Polystyrene by Asymmetric Autocatalysis. Tsuneomi Kawasaki<sup>1,2</sup>, Yuko Araki<sup>1</sup>, Kunihiro Hatase<sup>1</sup>, Jun Okuda<sup>3</sup>, Kenso Soai<sup>1,2</sup>, <sup>1</sup>Department of Applied Chemistry, Tokyo University of Science, Kagurazaka, Tokyo, JAPAN; <sup>2</sup>Chiral Material Research Center, Research Institute of Science and Technology, Tokyo University of Science, Tokyo, JAPAN; <sup>3</sup>Institute for Inorganic Chemistry, RWTH Aachen University, Aachen, GERMANY
- P-114 Formation of Chiral Crystal from Achiral Crystal and Enantioselective Synthesis Induced by Chiral Crystal of Achiral Nucleobase Cytosine in Combination with Asymmetric Autocatalysis. Kenta Suzuki<sup>a</sup>, Yuko Hakoda<sup>a</sup>, Hiroko Mineki<sup>a</sup>, Tsuneomi Kawasaki<sup>a,b</sup>, Kenso Soai<sup>a,b</sup>, <sup>a</sup>Department of Applied Chemistry, Tokyo University of Science, Kagurazaka, Tokyo, JAPAN; <sup>b</sup>Chiral Material Research Center, Research Institute of Science and Technology, Tokyo University of Science, Tokyo, JAPAN
- P-115 Synthesis and Characterization of a New Liquid Crystalline Chiral Single-molecule Magnet. Mathieu Gonidec, David B. Amabilino, Jaume Veciana, Institut de Ciència de Materials de Barcelona, Campus de la Autònoma, Bellaterra, SPAIN
- P-116 Enhancement of IR and VCD Intensities Due to Charge Transfer. Valentin Paul Nicu, Mojgan Heshmat, Evert Jan Baerends, Theoretical Chemistry, Vrije Universiteit Amsterdam, Amsterdam, THE NETHERLANDS
- P-117 Chiral Sensing Polymeric Film. Paola Rizzo, Gaetano Guerra, Dipartimento di Chimica, Università di Salerno, Baronissi (Salerno), ITALY
- P-118 Chiral Separations with Magnetic Silica Nano Particles Modified by a Chiral Selector: Chirality Fishing. Kyu Jung Lee, Hee Jung Choi, Myung Ho Hyun, Department of Chemistry, Pusan National University, Busan, SOUTH KOREA
- P-119 Self-assembly of Symmetrically Tri-deuterated-benzene 1,3,5-tricarboxamides. Seda Cantekin, D. W. R. Balkenende, C. Duxbury, A. R. A. Palmans, E. W. Meijer, Laboratory of Molecular Science and Technology, Eindhoven University of Technology, Eindhoven, THE NETHERLANDS
- P-120 Physical Models for the Origin of Homochirality in Amino Acids. Toshiko Izumi<sup>1</sup>, Martin Klussmann<sup>2,3</sup>, Donna G. Blackmond<sup>1,2</sup>, Cristobal Viedma<sup>4</sup>, <sup>1</sup>Department of Chemical Engineering and <sup>2</sup>Department of Chemistry, Imperial College London, London, UK; <sup>3</sup>Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, GERMANY; <sup>4</sup>Departamento Cristalografía-Mineralogía, Facultad Geología, Universidad Complutense, Madrid, SPAIN
- P-121 Enantiomer-Selective and Helix-Sense-Selective Living Block Copolymerization of Isocyanide Enantiomers and AFM Observations of the Resulting Block Copolymers. Motonori Banno<sup>1</sup>, Zong-Quan Wu<sup>1,2</sup>, Kanji Nagai<sup>1,2</sup>, Kento Okoshi<sup>2</sup>, Kiyotaka Onitsuka<sup>3</sup>, Eiji Yashima<sup>1,2</sup>, <sup>1</sup>Department of Molecular Design and Engineering, Graduate School of Engineering, Nagoya University, Nagoya, JAPAN; <sup>2</sup>Yashima Super-structured Helix Project, ERATO, JST, JAPAN; <sup>3</sup>Osaka University, JAPAN
- P-122 A Simple Bent-core Mesogen Lacking Schiff Base Moieties Exhibiting a B4-like Phase. Ethan Tsai<sup>a</sup>, Jacqueline M. Richardson<sup>b</sup>, Yongqiang Shen<sup>a</sup>, Dong Chen<sup>a</sup>, Michi Nakata<sup>at</sup>, Noel A. Clark<sup>at</sup>, David M. Walba<sup>b</sup>, <sup>a</sup>Department of Physics and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO, USA; <sup>b</sup>Department of Chemistry and Biochemistry and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO, USA
- P-123 Nitrogen Chiral Center Stabilized by Rotaxane Structure. Kazuko Nakazono, Sakiko Suzuki, Toshikazu Takata, Tokyo Institute of Technology, Department of Organic and Polymeric Materials, Tokyo, JAPAN
- P-124 Quantifying the Agreement Between the Experimental and Simulated VCD Spectra. Elke M.S. Debie<sup>1,2</sup>, Rina K. Dukor<sup>1</sup>, Laurence A. Nafie<sup>1,2</sup>, <sup>1</sup>BioTools, Inc., Jupiter, FL, USA; <sup>2</sup>Department of Chemistry, Syracuse University, Syracuse, NY, USA

# Monday Poster Presentations

Session Times: 1:30 – 3:30 PM

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- P-125 An Enantiomerically Pure Allen-ene Acetylenic Macrocyclic: Synthesis and Rationalization of Its Outstanding Chiroptical Response. José Lorenzo Alonso-Gómez<sup>a,b</sup>, Pablo Rivera-Fuentes<sup>b</sup>, Nobuyuki Harada<sup>a,c</sup>, Nina Berova<sup>a</sup>, François Diederich<sup>b</sup>, <sup>a</sup>Department of Chemistry, Columbia University, New York, NY, USA; <sup>b</sup>Laboratorium für Organische Chemie ETH Zurich, SWITZERLAND; <sup>c</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, JAPAN
- P-126 Multi-joint Polymers Composed of Chiral Ferrocene Joints and Rigid Diacetylene Units. Takahiro Fukino, Norifumi Fujita, Takuzo Aida, School of Engineering, The University of Tokyo, Tokyo, JAPAN
- P-127 Gas-phase Enantioselective Association Between Chiral Macrocyclic Hosts and Aminoacid-type Guests: Insights into the Structure and Dynamics of Protonated Three-body Adducts. C. Villani, F. Gasparrini, M. Pierini, M. Speranza, C. Fraschetti, Dipartimento di Chimica e Tecnologie del Farmaco, Università di Roma "La Sapienza", Roma, ITALY
- P-128 Preparative Chiral Purification of Pharmaceutically Compounds Using Axial Compressed Columns. Peter C. Rahn, William Cash, Phenomenex, Inc., Torrance, CA, USA
- P-129 Optimizing Throughput and Purity for Pharmaceutically Active Compounds Using Axial Packed Preparative Chiral Columns. Peter C. Rahn, William Cash, III, Phenomenex, Inc., Torrance, CA, USA
- P-130 Stereochemistry Education on Chiral Polycyclic Hydrocarbons that Belong to Icosahedral Symmetry. Takeshi Iizuka, Gunma University, Setagaya, Tokyo, JAPAN
- P-131 Quinine-immobilized Zirconia for Enantioseparation of Non-acidic Analytes in Reversed-phase Capillary Electrochromatography. Jung Hag Park, Munrak Lee, Yeungnam University, Department of Chemistry, Gyeongsan, SOUTH KOREA
- P-132 Chiral Chemical Absorption Property of a Crosslinked Poly(N-isopropyl acrylamide-Co-Sodium acrylate) Thermoresponsive Gel. Dibyendu S. Bag, Sarfaraz Alam, K.U. Bhasker Rao, Defence Materials and Stores Research and Development Establishment (DMSRDE), Defence Research and Development Organization (DRDO), Kanpur, INDIA
- P-133 Molecular Simulations of Free-Base and Metallo-Porphyrins Appended to 5'-end DNA Scaffold. Ana G. Petrovic<sup>a</sup>, Regina R. Monaco<sup>a</sup>, Warren McGee<sup>a</sup>, Gennaro Pescitelli<sup>b</sup>, Koji Nakanishi<sup>a</sup>, George A. Ellestad<sup>a</sup>, Milan Balaz<sup>c</sup>, Nina Berova<sup>a</sup>, <sup>a</sup>Department of Chemistry, Columbia University, New York, NY, USA; <sup>b</sup>Università degli Studi di Pisa, Dipartimento di Chimica e Chimica Industriale, Pisa, ITALY; <sup>c</sup>Department of Chemistry, University of Wyoming, Laramie, WY, USA
- P-134 Attrition-Enhanced Deracemization in the Synthesis of Clopidogrel - A Practical Application of a New Discovery. Maarten W. van der Meijden<sup>1</sup>, Michel Leeman<sup>1</sup>, Edith Gelens<sup>1</sup>, Wim L. Noorduyn<sup>2</sup>, Bernard Kaptein<sup>3</sup>, Elias Vlieg<sup>2</sup>, Richard M. Kellogg<sup>1</sup>, <sup>1</sup>Syncom B.V., Groningen, THE NETHERLANDS; <sup>2</sup>Radboud University Nijmegen, IMM Solid State Chemistry, Nijmegen, THE NETHERLANDS; <sup>3</sup>DSM Pharmaceutical Products, Advanced Synthesis, Catalysis and Development, Geleen, THE NETHERLANDS
- P-135 Comparison of Chiroptical Properties Between Solid and Solution States. T. Suzuki<sup>1</sup>, T. Osaka<sup>2,3</sup>, T. Asahi<sup>1,3</sup>, <sup>1</sup>Department of Life Science and Medical Bioscience, Waseda University (TWIns), Tokyo, JAPAN; <sup>2</sup>Department of Applied Chemistry, Waseda University, Tokyo, JAPAN; <sup>3</sup>Consolidated Research Institute for Advanced Science and Medical Care, Waseda University (ASMeW), Tokyo, JAPAN
- P-136 Forensic Age Analysis of Teeth Using Amino Acids – Effects of Storage/Extraction Conditions on Aspartic Acid Enantiomers. S. Hendry<sup>1</sup>, C. Morrison<sup>1</sup>, F. Smith<sup>1</sup>, K. Spohr<sup>1</sup>, A. Donaldson<sup>2</sup>, <sup>1</sup>School of Engineering and Science, University of the West of Scotland, Paisley, UK; <sup>2</sup>Glasgow Dental Hospital and School, Faculty of Medicine, University of Glasgow, Glasgow, UK

## Tuesday Poster Presentations

Session Times: 1:30 – 3:30 PM

Posters with program numbers in the P-200 series are presented during Tuesday's Poster Session. All posters will remain up for viewing all day Monday and Tuesday. All posters should be mounted onto the poster boards on Monday between 8:30 AM and 1:30 PM and not removed until Tuesday between 3:00 PM and 4:30 PM (anything remaining after 4:30 PM on Tuesday will be discarded).

P-201 Improved Enantioseparation of a Key Drug Intermediate by Chiral GC Using Hydrogen Carrier Gas. Jian Ning, Tilak Chandrasekaran, Schering Plough Research Institute, Union, NJ, USA

P-202 Calix[4]resorcinarenes and Cationic Cyclodextrins as Water-Soluble Enantioselective NMR Shift Reagents. Ngoc H. Pham, Cora D. Chisholm, T. J. Wenzel, Bates College, Department of Chemistry, Lewiston, ME, USA

P-203 Cyclodextrin-, Cellulose – and Synthetic Polymer-based Chiral Stationary Phases for Enantioseparation of Substituted Binaphthyls. Lucie Loukotková<sup>a</sup>, Zuzana Bosáková<sup>a</sup>, Eva Tesařová<sup>b</sup>, Daniel W. Armstrong<sup>c</sup>, <sup>a</sup>Department of Analytical Chemistry, Charles University in Prague, Faculty of Science, Prague, CZECH REPUBLIC; <sup>b</sup>Department of Physical and Macromolecular Chemistry, Charles University in Prague, Faculty of Science, Prague, CZECH REPUBLIC; <sup>c</sup>Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA

P-204 Calculating Chirality on the Web. Hadassah Elgavi<sup>1</sup>, Chaim Dryzun<sup>1</sup>, Amir Zayit<sup>1</sup>, Mark Pinsky<sup>1,2</sup>, Alex Puschinsky<sup>1</sup>, David Avnir<sup>1</sup>, <sup>1</sup>Institute of Chemistry and the Lise Meitner Minerva Center for Computational Quantum Chemistry; <sup>2</sup>Institute of Earth Sciences, The Hebrew University of Jerusalem, Jerusalem, ISRAEL

P-205 Chiral Silicate Zeolites. Chaim Dryzun<sup>1</sup>, Yitzhak Mastai<sup>2</sup>, Ayelet Shvalb<sup>2</sup>, David Avnir<sup>1</sup>, <sup>1</sup>Institute of Chemistry and the Lise Meitner Minerva Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, Jerusalem, ISRAEL; <sup>2</sup>Department of Chemistry, Bar-Ilan University, Ramat Gan, ISRAEL

P-206 Novel Protic Chiral Ionic Liquids Based on Ephedrine Derivatives. Sergio L. de Rooy, Min Li, David K. Bwambok, Bilal El-Zahab, Santhosh Challa, Isiah M. Warner, Department of Chemistry, Louisiana State University, Baton Rouge, LA, USA

P-207 Molecular Modeling of Enantioselective Adsorption of Chiral Alkan-2-ols in Homochiral Metal-organic Frameworks. Xiaoying Bao, Linda J. Broadbelt, Randall Q. Snurr, Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, USA

P-208 Examples for Fast Chiral Method Development with Parallel LC in Normal Phase and Reverse Phase Mode. Marcel Althaus<sup>a</sup>, Holger Gumm<sup>b</sup>, <sup>a</sup>Hoffmann La Roche, Basel, SWITZERLAND; <sup>b</sup>Sepiatec GmbH, Berlin, GERMANY

P-209 Characterization of Interconversion of Chiral Compounds in Chiral Environment. Jana Svobodová, Pavel Dubský, Eva Tesařová, Bohuslav Gaš, Charles University in Prague, Faculty of Science, Department of Physical and Macromolecular Chemistry, Prague, CZECH REPUBLIC

P-210 Liquid Chromatographic Resolution of  $\alpha$ -amino Acid Derivatives on Two CSPs Based on Diastereomeric Chiral Crown Ethers Incorporating Two Different Chiral Units. Hee Jin Kim, Hee Jung Choi, Yoon Jae Cho, Myung Ho Hyun, Department of Chemistry, Pusan National University, Busan, KOREA

P-211 Preparation and Application of a Crown Ether Based HPLC Chiral Stationary Phase Containing Thioester Linkages. Kyu Jung Lee, Hwan Sun Cho, Hee Jung Choi, Myung Ho Hyun, Department of Chemistry, Pusan National University, Busan, KOREA

P-212 Resolution of Racemic Chiral Drugs Containing a Secondary Amino Group on a Chiral Stationary Phase (CSP) Based on (+)-(18-crown-6)-2,3,11,12- tetracarboxylic Acid. A. Reum Lee, Hee Jung Choi, Myung Ho Hyun, Department of Chemistry, Pusan National University, Busan, KOREA

## Tuesday Poster Presentations

Session Times: 1:30 – 3:30 PM

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- P-213 Performance and Benefits of Macrocyclic Glycopeptide-based CSPs in Enantiomeric Purification Using Bench-top Simulated Moving Bed (SMB) Technology. J.T. Lee<sup>1</sup>, William Campbell<sup>1</sup>, Robert Mierendorf<sup>2</sup>, <sup>1</sup>Supelco, Division of Sigma-Aldrich, Bellefonte, PA, USA; <sup>2</sup>SEMBA Biosciences
- P-214 Enantioselective Synthesis of Fluoro-substituted 1-Chloro-3-phenylpropan-2-ols and 1-Chloro-3-phenylpropan-3-ols as Building Blocks for Biologically Active Compounds. Li-Te Chang, Ling-Wei Hsin, Institute of Pharmaceutical Sciences, College of Medicine, National Taiwan University, Taipei, TAIWAN
- P-215 Speed Up SFC Chiral Method Development with a 8x Parallel System. Holger Gumm, Sepiatec GmbH, Berlin, GERMANY
- P-216 Synthesis and Chiral Recognition of Poly(phenylenevinylene)-Encapsulated Amylose Derivatives. Kazumi Tamura<sup>1</sup>, Eiji Yashima<sup>1</sup>, Tomoyuki Ikai<sup>2</sup>, Yoshio Okamoto<sup>2</sup>, <sup>1</sup>Department of Molecular Design and Engineering, Graduate School of Engineering, Nagoya University, Nagoya, JAPAN; <sup>2</sup>EcoTopia Science Institute, Nagoya University, Nagoya, JAPAN
- P-217 Investigation of Solution Phase Enantioselective Recognition by Continuous Flow Transmission Mode Desorption Electrospray Ionization Mass Spectrometry (CF-TM-DESI-MS). Aruna B. Wijeratne, Samuel H. Yang, Brian Edwards, Kevin A. Schug, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA
- P-218 Sulfoxides in the Enantiospecific Synthesis of [2.2]paracyclophane Derivatives. Rakesh Parmar<sup>a</sup>, Gareth J Rowlands<sup>b</sup>, Richard J. Seacome<sup>a</sup>, <sup>a</sup>Chemistry Division, Department of Chemistry and Biochemistry, University of Sussex, Brighton, UK; <sup>b</sup>Institute of Fundamental Sciences, Massey University, Palmerston North, NEW ZEALAND
- P-219 Synthesis and Chiroptical Properties of Novel Oligopeptides from Achiral Amino Acids. Joon-il Cho<sup>1</sup>, Masahiro Tanaka<sup>1</sup>, Kazushi Kinbara<sup>2</sup>, Takuzo Aida<sup>1</sup>, <sup>1</sup>Department of Chemistry and Biotechnology, School of Engineering, The University of Tokyo, Tokyo, JAPAN; <sup>2</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, JAPAN
- P-220 Towards Enhanced Throughput Screening Using Short Columns Packed with DAICEL 3-Micron CSPs. Norbert M. Maier, Geoffrey B. Cox, Chiral Technologies, Inc., West Chester, PA, USA
- P-221 Operational Pressure Stability of Wide-Pore 3- and 5-Micron Polysaccharide-based Chiral Chromatography Columns. Norbert M. Maier, Geoffrey B. Cox, Chiral Technologies, Inc., West Chester, PA, USA
- P-222 Selectivity Study of New Polysaccharide-based Chiral Stationary Phases. Geoffrey B. Cox, N. Maier, P. Franco, T. Zhang, Chiral Technologies, Inc., West Chester, PA, USA
- P-223 The Utilization of SFC for Achiral Separations Employing a Chiral Column. Eric Pullen, Regis Technologies, Inc., Morton Grove, IL, USA
- P-224 Semi Synthetic Route Towards Therapeutically Active Chiral  $\gamma$ -butyrolactone Based Molecules. I. Ibnusaud, Deenamma Habel, Shubin Chacko, H. Simimole, School of Chemical Sciences, Mahatma Gandhi University, Kottayam, INDIA
- P-225 Synthesis and Examination of Sulfated Cyclofructans as a Novel Class of Chiral Selectors for Capillary Electrophoresis. Man-yung Tong, Chunxia Jiang, Zachary S. Breitbach, Daniel W. Armstrong, University of Texas at Arlington, Arlington, TX, USA
- P-226 Chiral Recognition of (S)-Phenylethylamine and/or (S)-Naphthylethylamine Derived Nickel(II) and Copper(II) Macrocyclic Complexes. Jae Jeong Ryoo<sup>1</sup>, Kil Sik Min<sup>1</sup>, Jong Won Shin<sup>2</sup>, Hwan-Suk Do<sup>1</sup>, Mi Jung Park<sup>1</sup>, <sup>1</sup>Department of Chemistry Education, Kyungpook National University, Taegu, KOREA; <sup>2</sup>Department of Chemistry, Kyungpook National University, Taegu, KOREA

## Tuesday Poster Presentations

Session Times: 1:30 – 3:30 PM

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- P-227 High-throughput Development of Organocatalytic Reactions. Jay C. Conrad, David W. C. MacMillan, Merck Center for Catalysis, Department of Chemistry, Princeton University, Princeton NJ, USA
- P-228 Chiral Synthesis of Mannich Bases and Separation of Racemic Mixtures. Meghal V. Modi<sup>1</sup>, Praful D. Bharadiya<sup>1</sup>, Dhruvo Jyoti Sen<sup>2</sup>, C.N. Patel<sup>2</sup>, <sup>1</sup>Department of Pharmaceutical Chemistry, B. S. Patel Pharmacy College, Gujarat, INDIA; <sup>2</sup>Postgraduate Research Laboratory, Department of Pharmaceutical Chemistry, Shri Sarvajani Pharmacy College, Gujarat, INDIA
- P-229 Analysis of Amino Phosphonic Acids and Their Carboxylic Acid Counterparts Using Crown Ether Columns. Wesley Barnhart, Kyung H. Gahm, Molecular Structure, Discovery Analytical Sciences, Amgen Inc., Thousand Oaks, CA, USA
- P-230 Enantioanalysis of Tertatolol with Immobilized Polysaccharide-derived HPLC Chiral Column at Nano-detection Level. Mohammed Hefnawy, Abdulrhman Al-Majed, Aymen Al-Suwailem, Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh, SAUDI ARABIA
- P-231 Developing Chiral Methods Beyond Chiral Separation in Pharmaceutical Industry. Hong-Xun Guo, Fang Wang, Jenny Chen, Jun Han, David Yeung, Kelly Hu, Steven Wu, David Semin, Janet Cheetham, Amgen Inc., Thousand Oaks, CA, USA
- P-232 About the Role of Affinities and Mobilities in Enantioseparations Using Capillary Electrophoresis. Bezhan Chankvetadze<sup>1</sup>, Ketevan Lomsadze<sup>1</sup>, Ana B. Martinez-Giron<sup>2</sup>, Maria Castro-Puyana<sup>2</sup>, Antonio L. Crego<sup>2</sup>, Maria Luisa Marina<sup>2</sup>, Antonio Salgado<sup>3</sup>, <sup>1</sup>Department of Physical and Analytical Chemistry, School of Exact and Natural Sciences, Tbilisi State University, Tbilisi, GEORGIA; <sup>2</sup>Department of Analytical Chemistry, Faculty of Chemistry, University of Alcalá, Madrid, SPAIN; <sup>3</sup>Department of Medicinal Chemistry, Centro Nacional de Investigaciones Oncológicas (CNIO), Madrid, SPAIN
- P-233 Reversed-phase Chiral Method Development Using Polysaccharide-based Stationary Phases. Liming Peng, Tivadar Farkas, Swapna Jayapalan, Bezhan Chankvetadze<sup>1</sup>, Phenomenex, Inc., Torrance, CA, USA; <sup>1</sup>Institute of Physical and Analytical Chemistry, Tbilisi State University, Tbilisi, GEORGIA
- P-234 Profiling the Isomerization of Biologically Relevant E-Z Isomers by SFC. Jaci Cole, Rui Chen, TharSFC, a Waters Company, Newark, DE, USA
- P-235 The Enantiomeric Separation of 4,5-disubstituted Imidazoles by HPLC using Cyclodextrin-based Stationary Phases. Zachary S. Breitbach, Panduka B. Koswatta, Carl J. Lovely, Daniel W. Armstrong, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA
- P-236 The Use of Cyclofructans as Novel Chiral Selectors for Gas Chromatography. Ying Zhang, Zachary S. Breitbach, Daniel W. Armstrong, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA
- P-237 Development of New LC Chiral Stationary Phases (CSPs) Based on Cyclofructan (CF) and Derivatized Cyclofructans. Ping Sun, Chunlei Wang, Daniel W. Armstrong, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA
- P-238 Synthesis and Evaluation of New Polymeric Chiral Stationary Phase for HPLC-based on *N,N'*-(1S, 2S)-1,2-Bis(2,4,6-trimethylphenyl)ethylenediamine. Eranda Wanigasekara, Tharanga Payagala, Xiaotong Zhang, Daniel W. Armstrong, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA
- P-239 Evaluation of Dalbavancin as Chiral Selector for HPLC and Comparison with Teicoplanin-based Chiral Stationary Phases. Xiaotong Zhang, University of Texas at Arlington, Arlington, TX, USA
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