



2016 PPXRD Program



ICDD Customer Newsletter

PPXRD PROGRAM APRIL 2016

MONDAY OPTIONAL WORKSHOP 9:00 AM – 5:30 PM

Organizer & Instructors:

A. Kern, Bruker AXS GmbH,
Karlsruhe, Germany,
arnt.kern@bruker.com

F. Gozzo, Excelsus Structural
Solutions SPRL, Brussels, Belgium,
fabia.gozzo@excelsus.us

Quantitative Phase Analysis by XRPD

This workshop will discuss the basis of quantitative phase analysis (QPA) for both single peak and whole pattern approaches. The focus will be on how to select and apply these methods, particularly in the context of the derivation of absolute phase abundances. The presence of poorly crystalline or amorphous content requires extension of the basic methods, but once these are established, they can be shown to produce QPA to the similar lower limits of detection and accuracy as for crystalline phases.

TUESDAY SESSIONS

*Indicates Presenter

- 8:45 **Welcoming Remarks from PPXRD-14 Organizing Committee Chairman**
T. Blanton, International Centre for Diffraction Data, Newtown Square, PA, USA
- New Frontiers in XRD for Pharmaceutical R&D**
Chair: **D. Beckers**, PANalytical, Almelo, The Netherlands, detlef.beckers@panalytical.com
- 9:00 Invited - Characterization of Spatial Phase Heterogeneity in Tablets by X-ray Diffractometry
R. Suryanarayanan*, University of Minnesota, Minneapolis, MN, USA
- 9:45 P4 Invited - Instrumentation and Applications of 2D XRD for Pharmaceuticals
B.B. He*, Bruker AXS, Madison, WI, USA
- 10:30 Break
- 11:00 P6 Large-Area CdTe Pixel Detectors for High-Energy X-ray Diffraction Applications
D. Sisak Jung*, **T. Donath**, DECTRIS Ltd., Switzerland
J. Bednarcik, Deutsches Elektronen-Synchrotron, Germany
M. Di Michiel, European Synchrotron Radiation Facility, France
S. Jacques, School of Materials, University of Manchester, UK
- 11:30 P52 Crystal Structure Determination from Beam Sensitive Organic Materials using Electron Diffraction
P.P. Das*, **S. Nikolopoulos**, NanoMEGAS SPRL, Brussels, Belgium
- 12:00 Lunch
- Patent Issues**
Chair: **T. Blanton**, International Centre for Diffraction Data, Newtown Square, PA, USA, tblanton@icdd.com
- 1:30 P22 Invited – Using X-ray Powder Diffraction and Other Solid-State Data to Protect Pharmaceutical Inventions
E.H. Barash*, Barash Law LLC, Lafayette, IN, USA
- PXRD Techniques/Rietveld Refinement/Crystal Structure Prediction/Crystal Structure Verification**
Chair: **R. Suryanarayanan**, University of Minnesota, Minneapolis, MN, USA
- 2:30 P7 Invited - Crystal Structures of Large-Volume Commercial Pharmaceuticals
J. Kaduk*, Illinois Institute of Technology, Chicago, IL and North Central College, Naperville IL, USA
- 3:15 Break
- 3:45 P14 Invited – Transmission Non-ambient X-ray Powder Diffraction as a Means to Study Liquid-solid Transformations
S. Bates*, Triclinic Labs, Lafayette, IN, USA
- 4:30 P15 Humidity Induced Phase Transitions in HEWLYSOZYME Investigated By Microcrystalline Powder Diffraction
D. Beckers*, **T. Degen**, **G. Nénert**, PANalytical B.V., Almelo, The Netherlands
S. Saslis, **S. Logotheti**, **F. Karavassili**, **A. Valmas**, **I. Margiolaki**, University of Patras, Greece
S. Trampari, Kapodistrian University of Athens, Greece
- 5:00 End

TUESDAY EVENING POSTER SESSION 5:30 – 7:00 PM

*Indicates Presenter

- P8 Unraveling the Solid State of MK-8970: A Racemic Acetal Carbonate Prodrug of Altegravir
N. Tsou*, **C. Scott Shultz**, **R.J. Varsolona**, Department of Process & Analytical Chemistry, Merck Research Laboratories, Rahway, NJ, USA
- P9 Monitoring Solid Forms and Solid-State Transformations of Drugs by X-ray Powder Diffraction
K. Xu*, **X. Xiong**, **H. Li**, Sichuan University, Chengdu, Sichuan, China
- P10 Evaluation of Dehydration Mechanism of Ondansetron Hydrochloride with Crystal Structure Analysis
R. Mizoguchi*, **H. Uekusa**, Department of Chemistry and Materials Science, Tokyo Institute of Technology, Tokyo, Japan
- P12 STOE InSitu HT2 – A New In-situ Reaction Chamber in Debye-Scherrer Geometry
J. Richter*, **S. Correll**, **T. Hartmann**, Stoe & Cie GmbH, Darmstadt, Germany
- P13 Estimation of Grain Size by Two-Dimensional X-ray Diffractometry: Applications to Powders and After Compression into Tablets
S. Thakral*, **R. Suryanarayanan**, Department of Pharmaceutics, University of Minnesota, Minneapolis, MN, USA
N.K. Thakral, Eli Lilly and Company, Indianapolis, IN, USA
- P27 ICDD Full Diffraction Pattern Polymer Project – New Entries for PDF-4+ 2016 and PDF-4/Organics 2017
T. Blanton*, **S. Gates-Rector**, ICDD, Newtown Square, PA, USA
S. Misture, Kazuo Inamori School of Engineering, Alfred University, Alfred, NY, USA
- P29 Incorporation of Pharmaceutical API's into the PDF[®] Databases
A. Gindhart, **T. Blanton***, International Centre for Diffraction Data, Newtown Square, PA, USA
J. Kaduk, Illinois Institute of Technology, Chicago, IL, USA
- P30 Crystal Structures of New Group 2 Citrate Salts
J.A. Kaduk, Illinois Institute of Technology, Chicago IL and North Central College, Naperville IL, USA
A. Rammohan, Atlantic International University, Honolulu, HI, USA
- P31 Crystal Structures of Large-Volume Commercial Pharmaceuticals
J.A. Kaduk, Illinois Institute of Technology, Chicago, IL and North Central College, Naperville IL, USA
R.J. Papoular, IRAMIS/CEA-Saclay, Leon Brillouin Laboratory, Gif-sur-Yvette Cedex, France
A.M. Gindhart, **T.N. Blanton**, International Centre for Diffraction Data, Newtown Square, PA, USA

WEDNESDAY SESSIONS

*Indicates Presenter

Formulation & Product Development/Polymorph, Salt & Co-crystal Screening

Chairs: **T. Fawcett**, International Centre for Diffraction Data, Newtown Square, PA, USA, fawcett@icdd.com

K. Saito, Rigaku Europe SE, Ettlingen, Germany, Keisuke.Saito@rigaku.com

- 9:00 P24 Invited – Strategies to Expand Solid-state Landscapes of Drugs to Enable Successful Tablet Formulation Development
C. Sun*, Department of Pharmaceutics, University of Minnesota, Minneapolis, MN, USA
- 9:45 P5 Invited - Two-Dimensional X-ray Diffractometry in Pharmaceutical Product and Process Development
N.K. Thakral*, Eli Lilly and Company, Indianapolis, IN, USA
- 10:30 Break
- 11:00 P32 Invited – Capturing the Significance of X-ray Crystallography in Pharmaceutical Field: The Application to Characterize New Salt, Co-Crystal and Co-Amorphous
E. Yonemochi*, Hoshi University, Tokyo, Japan
- 11:45 P20 Which Form? Which Formulation? A Case Study on the Impact of Form to Bioavailability and Formulation Development
A. Patel*, Bristol-Myers Squibb, New Brunswick, NJ, USA
- 12:15 Lunch
- Amorphous, Activated and Nanomaterials**
Chair: **F. Gozzo**, Excelsus Structural Solutions SPRL, Brussels, Belgium, fabia.gozzo@excelsus.us
- 1:45 P19 Invited - Total Scattering Characterization of Amorphous and Nanostructured Pharmaceuticals
A. Prodi*, Excelsus Structural Solutions sprl, Brussels, Belgium
P.M. Mazzeo, Excelsus Structural Solutions (Swiss) AG
A. Cervellino, SLS, Paul Scherrer Institut (CH)
F. Gozzo, Excelsus Structural Solutions sprl, Brussels, Belgium and Excelsus Structural Solutions (Swiss) AG
- 2:30 P18 The Analysis of Non-Crystalline Materials in Pharmaceutical Formulations
T. Fawcett*, **S.N. Kabekkodu**, **S. Gates-Rector**, **A.M. Gindhart**, **J.R. Blanton**, **T.N. Blanton**, International Centre for Diffraction Data, Newtown Square, PA, USA
- 3:00 Break
- 3:30 P53 X-ray Scattering Studies on Nano Crystalline and Amorphous Materials
D. Beckers*, **M. Gateshki**, PANalytical B.V., Almelo, The Netherlands
A. Adibhatla, PANalytical Inc., Westborough MA, USA
- 4:00 P26 Quantification of Multiple Amorphous Phases
A. Adibhatla*, PANalytical Inc., Westborough MA, USA
T. Degen, **D. Beckers**, PANalytical B.V., Almelo, The Netherlands
- 4:30 Ends

THURSDAY SESSIONS

Qualitative and Quantitative Analysis

Chair: **T. Blanton**, International Centre for Diffraction Data, Newtown Square, PA, USA, tblanton@icdd.com

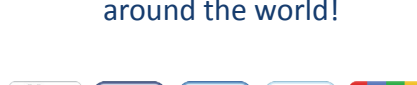
- 8:30 P28 Invited - Characterization of Active Pharmaceutical Ingredients and Excipients in Commercial Formulations and Preparation of New Forms by Crystallization and Heat Treatment
G. Díaz De Delgado*, **R.A. Toro**, **A.J. Dugarte**, **Y.W. Escalante**, **R.C. López**, **J.A. Trejo**, **J.E. Contreras**, **J.M. Delgado**, Laboratorio de Cristalografía-LNDRX, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida, Venezuela
- 9:15 P11 Absolute Quantification of Pharmaceuticals: The Search of Suitable Internal Standards
M.L. Reine-Schmitt*, Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland
P.P. Mazzeo, Excelsus Structural Solutions (Swiss) AG, Switzerland
A. Prodi, Excelsus Structural Solutions SPRL, Belgium
F. Gozzo, Excelsus Structural Solutions (Swiss) AG, Switzerland and Excelsus Structural Solutions SPRL, Belgium
- 9:45 Break
- 10:00 P25 Excipient Reference Data in the Powder Diffraction File™ (PDF™) for Phase Identification in Pharmaceutical Formulations
J. Quagliarello, **K. Drishnan**, **S. Gates-Rector**, **T. Fawcett**, **T. Blanton***, International Centre for Diffraction Data, Newtown Square, PA, USA
- 10:30 P21 Recent Developments in the Powder Diffraction File™
S. Kabekkodu*, **S. Gates-Rector**, **A. Gindhart**, **J. Blanton**, **T. Blanton**, **T. Fawcett**, International Centre for Diffraction Data, Newtown Square, PA, USA
- 11:00 Closing Comments
- 11:15 Symposium Ends

For more information visit www.icdd.com/ppxrd
Email: ppxrd@icdd.com

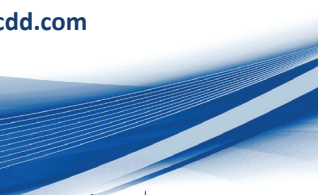


Have you connected with ICDD yet?

Stay informed with information about upcoming exhibits, meetings, workshops, product tutorials, and pictures from events we've attended around the world!



International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, PA 19073-3273
Phone: 610-325-9814 / Fax: 610-325-9823
Toll Free: 866-378-9331 (U.S. & Canada Only)
info@icdd.com sales@icdd.com
Registration Support: registration@icdd.com
www.icdd.com www.dxcicdd.com



ICDD, the ICDD logo, PDF and Denver X-ray Conference and design are registered in the U.S. Patent and Trademark Office. Powder Diffraction File is a trademark of the JCPDS—International Centre for Diffraction Data.
©2016 JCPDS—International Centre for Diffraction Data