

PPXRD-5
 The Pharmaceutical Powder X-ray Diffraction Symposium
 14-16 February 2006 - Somerset, New Jersey, U.S.A.
 Sponsored by the International Centre for Diffraction Data

PPXRD-5 Event Schedule

Monday, February 13

Optional Hands-On Workshop - 8:15AM - 5:30PM Characterization of Pharmaceutical Solids: Crystal Studies and XRD Applications
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Tuesday, February 14

Time	Type	Title of Paper	Speaker & Affiliation
9:00-9:30		WELCOMING REMARKS & INTRODUCTIONS	John Faber, International Centre for Diffraction Data, Newtown Square, Pennsylvania, USA
XRPD Structural Techniques (Acquisition and Use of XRPD Data, Indexing, Structure Determination, Rietveld Refinement) Session Chair: Dr. Arnt Kern, Bruker AXS GmbH, Karlsruhe, Germany			
9:30-10:15	Invited	PHARMACEUTICAL POWDER DIFFRACTION: MAKING MOVIES	Bill David, Rutherford Appleton Laboratory, Chilton, Oxfordshire, UK
10:15-10:40	Contributed	STRUCTURE SOLUTION AND QUANTITATIVE X-RAY POWDER DIFFRACTION OF PHARMACEUTICALS	Gregory Stephenson, Eli Lilly & Company, Indianapolis, Indiana, USA
10:40-11:10	Break		
11:10-11:35	Contributed	XRD CHARACTERIZATION OF CRYSTALLINITY AND MICROSTRUCTURE OF PHARMACEUTICAL COMPOSITES	Luca Lutterotti, Dipartimento Ingegneria dei Materiali e Tecnologie Industriali, Universita' di Trento, Trento, Italy
11:35-12:00	Contributed	CLOSE CONTACT PENALTY FUNCTIONS IN DIRECT SPACE METHODS AND ENERGETIC CONSIDERATION IN STRUCTURE REFINEMENT	Cikui Liang, Accelrys, San Diego, CA, USA
12:00-1:30	Lunch		

Time	Type	Title of Paper	Speaker & Affiliation
Complementary Techniques(DSC, TGA, Hot Stage Microscopy, FTIR, Raman, NMR, SEM, AFM, Light Microscopy, XRF, SAXS, SANS) Session Chair: Dr. Gregory Stephenson, Eli Lilly and Company, Indianapolis, Indiana, USA			
1:30-2:15	Invited	COMPLEMENTARY TECHNIQUES FOR THE CHARACTERIZATION OF PHARMACEUTICAL SYSTEMS	Raj Suryanarayanan, University of Minnesota, Minnesota USA
2:15-2:40	Contributed	COMBINED XRD AND RAMAN COMBINATORIAL SCREENING SYSTEM	Bob He, Bruker AXS, Madison, Wisconsin, USA

2:40-3:05	Contributed	CHALLENGES IN DETECTING CRYSTALLINE PHASE IN AN AMORPHOUS MATRIX	Martha Davidovich, Bristol-Myers Squibb, New Brunswick, New Jersey, USA
3:05-3:35	Break		
3:35-4:00	Contributed	NEUTRON POWDER DIFFRACTION WITHOUT RESORT TO DEUTERATION: USE IN MOLECULAR STRUCTURE REFINEMENT	Kenneth Shankland, CCLRC, Rutherford Appleton Laboratory, Chilton, Oxfordshire, UK
4:00-4:25	Contributed	COMBINING MICRO X-RAY FLUORESCENCE AND INFRARED IMAGING SPECTROSCOPES FOR THE UNDERSTANDING OF MODEL AND COMMERCIAL PHARMACEUTICAL TABLET SYSTEMS	Brian Patterson, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

Evening (6:00-9:00)		Poster Session	
Title of Paper		Speaker & Affiliation	
XRPD PATTERN MATCHING: PROBABILITY BASED VERSUS IMAGE COMPARISON		Thomas Degen, PANalytical B.V., Almelo, The Netherlands	
HIGH THROUGHPUT ANALYSIS OF STRUCTURAL GEOMETRIES MINED FROM THE CSD: HOW TO INTERPRET 3000 HITS IN AN AFTERNOON?		Arnt Kern, Bruker AXS, Karlsruhe, Germany	
LOWERING THE LIMITS OF DETECTION OF PHARMACEUTICAL MATERIALS BY POWDER X-RAY DIFFRACTION		Brian Litteer, PANalytical Inc., Natick, Massachusetts, USA	
PDF-4/ORGANICS 2006 REFERENCE POWDER PATTERNS AND THEIR PHARMACEUTICAL APPLICATION		Fangling Needham, ICDD, Newtown Square, Pennsylvania, USA	
CHARACTERIZATION OF THE PHYSICAL FORM OF THE ACTIVE PHARMACEUTICAL INGREDIENT IN INTACT FILM-COATED TABLETS BY X-RAY POWDER DIFFRACTOMETRY		Hiroyuki Yamada, University of Minnesota, Minneapolis, Minnesota, USA	

Wednesday, February 15

Morning	Formulation, Product Development, Drug Delivery and Polymorph & Salt Screening Session Chair: Dr. Shawn Yin, Bristol-Myers Squibb, New Brunswick, New Jersey, USA		
9:00-9:45	Invited	EXPLORING POLYMORPHISM OF MOLECULAR MATERIALS USING HIGH PRESSURE - OPENING UP NEW DIMENSIONS IN POLYMORPH SCREENING	Colin Pulham, University of Edinburgh, Edinburgh, Scotland, UK
9:45-10:10	Contributed	A NOVEL APPROACH OF USING POWDER X-RAY DIFFRACTION FOR HIGH-THROUGHPUT CRYSTALLIZATION/SALT SCREENING	Shawn Yin, Bristol-Myers Squibb Co., New Brunswick, New Jersey, USA
10:10-10:35	Contributed	SIMULATED PXRD PATTERNS AS STANDARD REFERENCES IN PHARMACEUTICAL FORM SELECTION	Dedong Wu, AstraZeneca Pharmaceuticals LP, Wilmington, Delaware, USA
10:35-11:05	Break		
11:05-11:30	Contributed	ADVANCED XRPD SYSTEM FOR THE CHARACTERIZATION OF PHARMACEUTICAL COMPOUNDS	Vladimir Kogan, PANalytical B.V. & DANNALAB, Almelo, The Netherlands
11:30-11:55	Contributed	RESOLVING POLYMORPH CHEMISTRY IN THE CA-O-P-H SYSTEM	Timothy Fawcett, ICDD, Newtown Square, Pennsylvania, USA
11:55-1:25	Lunch		

Afternoon	Con't: Formulation, Product Development, Drug Delivery and Polymorph & Salt Screening		
Time	Type	Title of Paper	Speaker & Affiliation
1:25-1:50	Contributed	USING ANALYTICAL DATA MANAGEMENT SYSTEMS TO ACCELERATE SALT AND POLYMORPH SCREENING	Raeann Wu, Novartis Pharmaceuticals Corp., East Hanover, New Jersey, USA
1:50-2:15	Contributed	MISCELLANEOUS PRACTICAL ISSUES FOR PXRD IN A QC LABORATORY	Peter Varlashkin, Metrics, Inc., Greenville, North Carolina, USA
Patent and Regulatory Issues Session Chair: Dr. Peter Varlashkin, Metrics, Inc., Greenville, North Carolina, USA			
Time	Type	Title of Paper	Speaker & Affiliation
2:15-3:00	Invited	QUESTION-BASED REVIEW - LINKING REGULATORY EVALUATION OF SOLID STATE PROPERTIES TO PHARMACEUTICAL QUALITY	Andre Raw, Food and Drug Administration, Rockville, Maryland, USA
3:00-3:30	Break		
3:30-3:55	Contributed	EQUIPMENT QUALIFICATION	Arnt Kern, Bruker AXS, Karlsruhe, Germany
3:55-4:20	Contributed	PRINCIPLES IN CLAIMING AND ENFORCING SOLID FORM PATENTS	Eyal Barah, SSCI, Inc., West Lafayette, Indiana, USA

Thursday, February 16

Morning	New Frontiers for XRD in Pharmaceutical R&D Session Chair: Dr. John Faber, International Centre for Diffraction Data, Newtown Square, Pennsylvania, USA		
Time	Type	Title of Paper	Speaker & Affiliation
9:00-9:45	Invited	SYNCHROTRON X-RAY POWDER DIFFRACTION: APPLICATIONS IN MACROMOLECULAR CRYSTALLOGRAPHY	Irene Margiolaki, European Synchrotron Radiation Facility(ESRF), Grenoble, France
9:45-10:30	Invited	MICRO-SAMPLE X-RAY POWDER DIFFRACTION. APPLICATIONS IN THE PHARMACEUTICAL SCIENCES.	Joseph Reibenspies, Texas A & M University, College Station, Texas, USA
10:30-10:50	Break		
10:50-11:35	Invited	PAT: ANALYSIS OF PROCESS INDUCED DISORDER OF API BY X-RAY POWDER DIFFRACTION	Simon Bates, SSCI, Inc., West Lafayette, Indiana, USA
11:35-12:15		Q&A/Closing Remarks	



Optional Hands-on Workshop
13 February 2006
Characterization of Pharmaceutical Solids:
Crystal Studies and XRD Applications

Instructors :

Chair: Dr. Jun Han, Novartis Institutes for Biomedical Research, Inc., Cambridge, MA, USA

Dr. Detlef Beckers, PANalytical, Almelo, The Netherlands

Dr. Harry G. Brittain, Center for Pharmaceutical Physics, Milford, NJ, USA
 Dr. John Faber, International Centre for Diffraction Data, Newtown Square, PA, USA
 Dr. Raj Suryanarayanan, University of Minnesota, MN, USA
 Dr. Shawn Yin, Bristol-Myers Squibb Company, New Brunswick, NJ, USA

Morning		
Basic Theories and Concepts (Monday 13 February - 8:15AM - 12PM)		
Time	Workshop	Instructor
8:15 - 9:00	Basics of crystal structure and X-ray diffractometry	Dr. Detlef Beckers
9:00 - 9:45	Techniques of Powder X-ray Diffractometry - Instrumentation and Optimization	Dr. Detlef Beckers
9:45 - 10:00	BREAK	
10:00 - 10:55	Basics of Pharmaceutical Solids	Dr. Harry G. Brittain
10:55 - 12:00	Round table and Q&A for Basic theories and Concepts	All instructors
Afternoon		
Applications and Case Studies (Monday 13 February - 1PM - 5:30PM)		
Time	Workshop	Instructor
1:00 - 1:35	Indexing and structure solution from powder XRD data	Dr. John Faber
1:35 - 2:45	Polymorphs Analysis - Qualitative and quantitative analysis of both API and Finished Products	Dr. Shawn Yin and Dr. Detlef Beckers
2:45 - 3:00	BREAK	
3:00 - 3:50	Application of variable temperature and humidity (environmental) PXRD in Characterizing Pharmaceutical solids	Dr. Shawn Yin and Dr. Jun Han
3:50 - 4:35	Characterization of amorphous and crystalline phases by PXRD	Dr. Harry G. Brittain
4:35 - 5:30	Round table and Q&A for Application and Case Studies	All instructors

Scientific Organizing Committee

Dr. John Faber, Chair, *International Centre for Diffraction Data*, Newtown Square, PA, U.S.A
 Dr. Detlef Beckers, *PANalytical*, Almelo, The Netherlands
 Dr. Harry G. Brittain, *Center for Pharmaceutical Physics*, Milford, NJ, U.S.A.
 Dr. Julien Giovannini, *AstraZeneca*, Lund, Sweden
 Dr. Jun Han, *Novartis Institutes for Biomedical Research*, Inc., Cambridge, MA, U.S.A.
 Dr. Arnt Kern, *Bruker AXS GmbH*, Karlsruhe, Germany
 Dr. Fangling Needham, *International Centre for Diffraction Data*, Newtown Square, PA, U.S.A.
 Dr. Kenneth Shankland, *Rutherford Appleton Laboratory*, Oxon, U.K.
 Dr. Peter W. Stephens, *State University of New York*, Stony Brook, NY, U.S.A.
 Dr. Gregory A. Stephenson, *Eli Lilly and Company*, Indianapolis, IN, U.S.A.
 Dr. Raj Suryanarayanan, *University of Minnesota*, Minneapolis, MN, U.S.A.
 Dr. Peter G. Varlashkin, *Metrics, Inc.*, Greenville, NC, U.S.A.
 Dr. Shawn Yin, *Bristol-Myers Squibb Company*, New Brunswick, NJ, U.S.A.

Location:

Marriott Somerset

110 Davidson Avenue, Somerset, New Jersey 08873