

PPXRD-07

25-28 February 2008

The Florida Hotel and Conference Center

Orlando, Florida

The International Centre for Diffraction Data is pleased to announce The 7th Pharmaceutical Powder X-ray Diffraction Symposium in Orlando, FL, U.S.A..

Optional Workshop Exercises in Quantitative Phase Identification Monday, 25 February 8:30 a.m.-6:00 p.m.	
Practical Aspects of Quantitative PXRD in the Pharmaceutical Industry	Peter Varlashkin, GlaxoSmithKline, Durham, NC, USA
Data Collection Strategies for X-ray Transparent Materials	Detlef Beckers, PANalytical, Almelo, The Netherlands
An Overview of QPA and Rietveld Methods for X-ray Powder Diffraction	John Faber, Scientist Emeritus, ICDD, Newtown Square, PA, USA
Sample Preparation for Rietveld Analyses	Fangling Needham, ICDD, Newtown Square, PA, USA
Hands-On Exercises in Quantitative Phase Identification	Detlef Beckers, John Faber, Fangling Needham, Peter Varlashkin

Tuesday, 26 February - 8:30 a.m.-5:00 p.m.

Type	Title of Paper	Speaker & Affiliation
	WELCOMING REMARKS & INTRODUCTIONS	John Faber, International Centre for Diffraction Data, Newtown Square, Pa, USA

	XRPD Structural Techniques (Acquisition and Use of XRPD Data, Indexing, Structure Determination, Rietveld Refinement)	
Invited	CRYSTALS STRUCTURES OF MODERATELY COMPLEX ORGANIC MOLECULES ARE PREDICTABLE	Marcus A. Neumann, Avant-garde Materials Simulation, St-Germain-en-Laye, France
Contributed	CRYSTALLITE VOLUME, AREA, SPECIFIC AREA AND MORPHOLOGY OBTAINED VIA RIETVELD REFINEMENT	Xim Bokhimi, Insituto de Fisica, Universidad Nacional Autónoma de México, D. F., Mexico
Contributed	AUTOMATED ANALYSIS OF POWDER X-RAY DATA USING SCRIPTING AND DATA PIPELINING TECHNIQUES	Max Petersen, Accelrys, Inc., San Diego, CA, USA
Contributed	THE ANALYSIS OF NANOMATERIALS, AMORPHOUS MATERIALS AND SEMICRYSTALLINE MATERIALS	Timothy Fawcett, ICDD, Newtown Square, PA, USA
Contributed	SDPD: A KEY COMPONENT IN POPULATING THE CARBAMAZEPINE CRYSTAL STRUCTURE LANDSCAPE	Kenneth Shankland, STFC Rutherford Appleton Laboratory, Oxon, U.K

Tuesday Afternoon	Complementary Techniques & PAT	
Type	Title of Paper	Speaker & Affiliation
Invited	QUANTITATIVE PXRD: IMPROVING RESOLUTION FOR MULTI-COMPONENT SYSTEMS USING CONTEMPORARY CHEMOMETRIC METHODS	Peter Wildfong, Duquesne University, Pittsburgh, PA, USA
Contributed	EDXRD PROBE FOR PHAMACEUTICAL VERIFICATION	Noureddine Anibou, Xstream Systems Inc., Sebastian, Florida, USA

Contributed	HYDRATES PRODUCED BY CONTROLLING WATER ACTIVITIES IN	Shan-Ming Kuang, Roche Carolina, Florence, SC, USA
Contributed	IDENTIFICATION OF GUMS AND SCREENING FOR CATALYST RESIDUES IN PHARMACEUTICAL END PRODUCTS USING XRF SPECTROMETRY	Lieven Kempnaers, PANalytical, Almelo, The Netherlands

Tuesday Evening (6:30-9:00)		Poster Session
Title of Paper	Speaker & Affiliation	
DETERMINATION OF SPECIFIC SURFACE AND PARTICLE SIZE DISTRIBUTION BY SMALL ANGLE X-RAY SCATTERING	Detlef Beckers, PANalytical, Almelo, The Netherlands	
A NEW HIGH-THROUGHPUT SAXS SCREENING TOOL FOR ACCELERATED COMBINATORIAL MEASUREMENTS	Gerd Langenbucher, Anton Paar USA, Ashland, VA, USA	
PHARMACEUTICAL REFERENCE APPLICATIONS OF PDF-4/ORGANICS 2008	Fangling Needham, ICDD, Newtown Square, PA, USA	
WWW.POWDERDATA.INFO: A RELIABLE SOURCE OF FREELY AVAILABLE, HIGH-QUALITY EXPERIMENTAL XRPD DATA	Kenneth Shankland, STFC Rutherford Appleton Laboratory, Oxon, U.K	
QUANTITATIVE MULTIVARIATE APPLICATIONS IN PXRD OF INTACT MULTI-COMPONENT CONSOLIDATED PHARMACEUTICAL SYSTEMS	Peter Wildfong, Duquesne University, Pittsburgh, PA, USA	
CHEMOMETRICS AS A TOOL FOR COMPARING DIFFERENT GEOMETRICAL MODES IN MULTI-COMPONENT QUANTITATIVE PXRD ANALYSIS OF INTACT COMPACTS	Peter Wildfong, Duquesne University, Pittsburgh, PA, USA	

Wednesday, 27 February - 9:00 a.m. – 5:00 p.m.

Wednesday Morning	Formulation, Product Development, Drug Delivery and Polymorph and Salt Screening
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Type	Title of Paper	Speaker & Affiliation
Invited	TWO-DIMENSIONAL XRD FOR PHARMACEUTICAL	Bob He, Bruker AXS, Madison, WI, USA
Contributed	PXRD ANALYSIS OF THE MECHANICALLY INDUCED INTER-CONVERSION BETWEEN TWO NEAT POLYMORPHIC FORMS OF BMS-XYZ HAVING SIMILAR LAYERED CRYSTAL STRUCTURES	Denette Murphy, Bristol-Myers Squibb, New Brunswick, NJ, USA
Contributed	AUTOMATION SOLUTIONS FOR SALT PRESCREENING AND POLYMORPH SCREENING STUDIES	Clifford Olson, Zinsser NA, Northridge, CA, USA
Contributed	POLYMORPH ANALYSES: TOOLS AND RESULTS	Timothy Fawcett, ICDD, Newtown Square, PA, USA
Contributed	TWO POSSIBLE VARIANTS OF A SINGLE CRYSTAL FORM OF AN API AND HOW TO FILE SUCH A PRODUCT	Peter Varlashkin, GlaxoSmithKline, Durham, NC, USA

Wednesday Afternoon		
New Frontiers for XRD in Pharmaceutical R&D (Cocrystals & Crystallization)		
Type	Title of Paper	Speaker & Affiliation
Invited	THE NEW GOLDEN AGE OF PHARMACEUTICAL PATENTS: COCRYSTALS AND THE SOLID STATE - SPECIAL THANKS TO THE SUPREME COURT OF THE UNITED STATES	Eyal Barash, Aptuit Consulting, West Lafayette, IN, USA
Invited	X-RAY DIFFRACTION ANALYSIS OF COCRYSTALS EXHIBITING A DISORDERED GUEST MOLECULAR ARRANGEMENT WITHIN A CRYSTALLINE HOST LATTICE	Simon Bates, Aptuit Consulting, West Lafayette, IN, USA

Contributed	X-RAY SOURCE, OPTICS AND DETECTORS FOR PHARMACEUTICAL XRD	Bob He, Bruker AXS, Madison, WI, USA
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Thursday, 28 February - 9:00 a.m. – 12:30 p.m.

An Invitation to Participate in an XRD Round Robin	
Title of Paper	Speaker & Affiliation
AN INVITATION TO PARTICIPATE IN AN XRD ROUND ROBIN	John Faber, Scientist Emeritus, ICDD, Newtown Square, PA, USA
SAMPLES FOR ROUND ROBIN	Fangling Needham, ICDD, Newtown Square, PA, USA

Poster Session

26 February 2008

An evening reception and poster session of submitted papers will be held at the The Florida Hotel and Conference Center. See guidelines for submission of abstracts for information on submitting a poster.

Exhibition

26-27 February 2008

Concurrent with the symposium and evening poster session and reception will be a commercial exhibition of analytical instrumentation and related products and services. Exhibitors are invited to inquire about exhibit reservations and sponsorship opportunities.

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

Terry Maguire, *International Centre for Diffraction Data*, Newtown Square, PA, U.S.A.

Leah Mooney, *International Centre for Diffraction Data*, Newtown Square, PA, U.S.A.

Dr. Fangling Needham, *International Centre for Diffraction Data*, Newtown Square, PA, U.S.A.

Dr. Kenneth Shankland, *Rutherford Appleton Laboratory*, Oxon, U.K.

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, *GlaxoSmithKline*, Durham, NC, U.S.A.

Dr. Shawn Yin, *Bristol-Myers Squibb Company*, New Brunswick, NJ, U.S.A.

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