

# PPXRD-8

The 8th Pharmaceutical Powder X-ray Diffraction Symposium  
Sponsored by the International Centre for Diffraction Data  
4-7 May 2009  
Glasgow, Scotland, U.K.

## Optional Workshop

Characterization of Pharmaceutical Solids

**Monday, 4 May**

9.00-17.00

Workshop instructors are scientists from academia, industry and the International Centre for Diffraction Data. In order to facilitate the participation of postgraduate students and young scientists, the workshop will begin with a talk on the fundamentals of XRD, followed by an introduction to pharmaceutical materials science. The topics to be covered in the workshop are:

- Instrumental and software advances
- Direct analysis of pharmaceutical dosage forms
- Quantitative phase analyses
- Use of XRD in the characterization of nanomaterials and amorphous phases
- Effective use of databases
- Applications of high intensity X-radiation
- Regulatory applications of XRD (including QbD)

### Workshop Instructors:

**Dr. Raj Suryanarayanan**, Workshop Chair, University of Minnesota, U.S.A.

**Dr. Detlef Beckers**, PANalytical, The Netherlands

**Dr. Cyrus Crowder**, ICDD, Newtown Square, PA, U.S.A.

**Dr. Tim Fawcett**, ICDD, Newtown Square, PA, U.S.A.

Dr. Geert Vanhoyland, Bruker-AXS GmbH, Germany

## Tuesday, 5 May - 8.30-17.20

Type	Title of Paper	Speaker & Affiliation
	WELCOMING REMARKS & INTRODUCTIONS	<b>Cyrus Crowder</b> , ICDD, Newtown Square, PA, U.S.A.

<b>Morning</b>	<b>Organic Crystal Structure Prediction</b> <b>Session Chair: Dr. Detlef Beckers</b> , PANalytical, Almelo, The Netherlands	
Invited	<b>COMPUTED CRYSTAL ENERGY LANDSCAPES AS AN AID TO UNDERSTANDING POLYMORPHISM</b>	<b>Sarah (Sally) L. Price</b> , University College London, London, U.K.
Contributed	<b>POWDER DIFFRACTION AND CRYSTAL STRUCTURE PREDICTION: A TWO-WAY RELATIONSHIP</b>	Maryjane Tremayne, University of Birmingham, Birmingham, U.K.
	<b>XRPD Structural Techniques (Acquisition and Use of XRPD Data, Indexing, Structure Determination, Rietveld Refinement)</b> <b>Session Co-chairs: Dr. Ken Shankland</b> , Reading University, Reading, U.K. and <b>Dr. Arnt Kern</b> , Bruker AXS GmbH, Karlsruhe, Germany	
Invited	<b>ADVANCES IN CRYSTAL STRUCTURE SOLUTION BY EXPO2008</b>	<b>Angela Altomare</b> , IC-CNR, Bari, Italy
Contributed	<b>TRANSFORMATIONS AND CRYSTAL STRUCTURES OF A SUBSTITUED TRIAZINE AND ITS SALT FORMS: A VT-XRPD, SDPD AND CASTEP STUDY</b>	Julie Bardin, University of Strathclyde, Glasgow, Scotland, U.K.
Contributed	<b>SOLVING ORGANIC STRUCTURES FROM POWDER DATA AT LOW RESOLUTION USING CHARGE FLIPPING COMBINED WITH MAXIMUM ENTROPY TECHNIQUES</b>	Christopher Gilmore, University of Glasgow, Glasgow, Scotland, U.K.
Contributed	<b>A NEW HIGH PERFORMANCE HIGH-RESOLUTION POWDER DIFFRACTION SYSTEM AND ITS APPLICATIONS TO CRYSTAL STRUCTURE ANALYSIS</b>	Paul Ulrich Pennartz, Rigaku European Headquarters, Eschweiler, Germany
<b>Afternoon</b>	<b>Formulation, Product Development, Drug Delivery and Polymorph &amp; Salt Screening</b> <b>Session Chair: Dr. Shawn Yin</b> , Bristol-Myers Squibb Company, New Brunswick, NJ, U.S.A.	

Invited	<b>SCREENING FOR SOLID-STATE TRANSFORMATIONS DURING SALT SELECTION</b>	<b>Gregory Stephenson</b> , Eli Lilly and Company, Indianapolis, IN, U.S.A.
Contributed	<b>ANALYSIS OF BLISTER PACKED TABLETS</b>	<b>Detlef Beckers</b> , PANalytical, Almelo, The Netherlands
Contributed	<b>MANY PATTERNS AND MANY METHODS: NEW METHODS UTILISING MULTIPLE ANALYSIS TECHNIQUES IN POLYMORPH AND SALT SCREENING SYSTEMS</b>	Gordon Barr, University of Glasgow, Glasgow, Scotland, U.K.
Contributed	<b>DETERMINATION OF THE EUTECTIC TEMPERATURE OF TREHALOSE-WATER BINARY SYSTEM BY X-RAY DIFFRACTOMETRY</b>	Prakash Sundaramurthi, University of Minnesota, Minneapolis, MN, U.S.A.
Contributed	<b>PARTICLE SIZE ANALYSIS BY TWO-DIMENSIONAL XRD</b>	Bob He, Bruker-AXS, Inc., Madison, WI, U.S.A.
Contributed	<b>MATERIAL IDENTIFICATION: THE DESCRIPTIVE STATISTICS OF PHASE IDENTIFICATION</b>	<b>Timothy Fawcett</b> , ICDD, Newtown Square, PA, U.S.A.

<b>Tuesday Evening (18.30-20.30)</b>		<b>Poster Session</b>
<b>Title of Paper</b>	<b>Speaker &amp; Affiliation</b>	
<b>QUANTITATIVE PHASE ANALYSIS OF ISOTIBOLONE IN TIBOLONE RAW MATERIAL USING THE SCARLETT-MADSEN METHOD</b>	Selma Gutierrez Antonio, Institute of Chemistry - UNESP, Araraquara, São Paulo, Brazil	
<b>STRUCTURE DETERMINATION OF A NEW POLYMORPH OF RACEMIC IBUPROFEN FROM LAB XRPD DATA</b>	Jean-Baptiste Arlin, University of Strathclyde, Glasgow, Scotland, U.K.	

<b>X-RAY SCATTERING STUDIES ON NANO CRYSTALLINE AND AMORPHOUS MATERIALS USING HIGH-ENERGY X-RAYS ON A LABORATORY SYSTEM</b>	<b>Detlef Beckers</b> , PANalytical, Almelo, The Netherlands
<b>APPLICATION OF HIGH-THROUGHPUT CLUSTER ANALYSIS TO MULTIPLE DATA TYPE – COMBINING DATASETS</b>	Gordon Cunningham, University of Glasgow, Glasgow, Scotland, U.K.
<b>METROLOGICAL ASSURANCE OF QUALITY CONTROL OF PHARMACEUTICAL PRODUCTION USING POWDER XRD METHODS</b>	Boris Kodess, VNIIMS, ICS&E, Moscow, Russia
<b>CHARACTERIZATION OF PHARMACEUTICALS BY XRPD AND THERMAL ANALYSIS: BUPROPION HYDROCHLORIDE</b>	Elisabetta Maccaroni, Università dell'Insubria, Como, Italy
<b>THE ROLE OF XRPD IN ACCELERATING PHARMACEUTICAL PHASE IDENTIFICATION AND SELECTION</b>	A. E. McKeown, Merck & Co. Inc, Rahway, NJ, U.S.A.
<b>STUDYING STRUCTURAL ASPECTS OF SALT HYDRATION BY VT-PXRD</b>	Gary Miller, University of Strathclyde, Glasgow, Scotland, U.K.
<b>COMPARISON OF SPECIMEN PREPARATION TECHNIQUES FOR X-RAY POWDER DIFFRACTION DATA OF ALPHA TEGAFUR</b>	<b>Fangling Needham</b> , ICDD, Newtown Square, PA, U.S.A.
<b>X-RAY POWDER DIFFRACTION IN QUANTIFYING POLYMORPHIC MIXTURES OF PHARMACEUTICAL SOLIDS: A CASE STUDY OF FAMOTIDINE</b>	Zoltán Németh, Gedeon Richter Plc, Budapest, Hungary
<b>CRYSTALLIZATION OF LYOPROTECTANT IN THE FROZEN SYSTEM AND ITS PHASE TRANSITION DURING DRYING</b>	Prakash Sundaramurthi, University of Minnesota, Minneapolis, MN, U.S.A.
<b>CRYSTAL STRUCTURES OF PHARMACEUTICALLY ACCEPTABLE CARBAMAZEPINE COCRYSTALS FROM SYNCHOTRON DATA</b>	Ryan Taylor, University of Strathclyde, Glasgow, Scotland, U.K.

Wednesday, 6 May - 8.30 – 17.35

<b>Morning</b>	<b>Amorphous, Activated and Nanomaterials</b> Session Chair: Dr. Julien Giovannini, AstraZeneca, Nottingham, U.K.	
<b>Type</b>	<b>Title of Paper</b>	<b>Speaker &amp; Affiliation</b>
Invited	<b>PHYSICAL STABILITY OF AMORPHOUS SOLID DISPERSIONS: XRPD AND COMPUTATIONAL STUDIES OF 'MISCIBILITY'</b>	<b>Igor Ivanisevic</b> , SSCI, a division of APTUIT Inc., West Lafayette, IN, U.S.A.
Invited	<b>CRYSTALLITE SIZES AND MICROSTRAINS DETERMINED BY RIETVELD REFINEMENT: APPLICATION TO MILLED LACTOSE</b>	<b>Vincent Caron</b> , Trinity College Dublin, Dublin, Ireland
Contributed	<b>XRPD, EXAFS, AND SAXS FOR CHARACTERIZATION OF NANOPARTICLES FOR PHARMACOLOGY</b>	Michael Boiko, Ioffe Physical-Technical Institute, Saint-Petersburg, Russia
Contributed	<b>CHARACTERISATION AND PREDICTION OF STABILITY OF AMORPHOUS MATERIALS DURING PHARMACEUTICAL DEVELOPMENT: PAIR-WISE DISTRIBUTION FUNCTION</b>	Helen Blade, AstraZeneca, Macclesfield, Cheshire, U.K.
Contributed	<b>DIFFRACTION, NON-CRYSTALLINITY, AND THE PDF DATABASE</b>	<b>Cyrus Crowder</b> , ICDD, Newtown Square, PA, U.S.A.
Contributed	<b>STUDYING AMORPHOUS PHARMACEUTICAL MATERIALS BY POWDER X-RAY DIFFRACTION AND OTHER SOLID-STATE TECHNIQUES</b>	<b>Shawn Yin</b> , Birstol-Myers Squibb, New Brunswick, NJ, U.S.A.
Contributed	<b>QUANTITATIVE ANALYSIS OF PHASES WITH PARTIAL OR NO KNOWN CRYSTAL STRUCTURE</b>	Geert Vanhoyland, Bruker AXS GmbH, Karlsruhe, Germany
<b>Afternoon</b>	<b>New Frontiers in XRD in Pharmaceutical R&amp;D</b> Session Co-chairs: Dr. Cyrus Crowder, ICDD, Newtown Square, PA, U.S.A., and Dr. Harry Brittain, Center for Pharmaceutical Physics, Milford, NJ, U.S.A.	

Invited	<b>TOWARD A RATIONALIZATION OF THE HYDRATION-DEHYDRATION MECHANISM OF SODIUM DICLOFENAC</b>	Christopher Frampton, SAFC Pharmorphix Ltd., Cambridge, Cambridgeshire, U.K.
Invited	<b>PROTEIN POWDER DIFFRACTION AT THE ESRF</b>	<b>Jonathan Wright</b> , ESRF, Grenoble cedex, France
Contributed	<b>NEW POSSIBILITIES FOR X-RAY DIFFRACTOMETRY</b>	Bernd Hasse, Incoatec GmbH, Geesthacht, Germany
<b>Complementary Techniques</b> <b>Session Chair: Dr. Raj Suryanarayanan</b> , University of Minnesota, Minneapolis, MN, U.S.A.		
Invited	<b>ENVIRONMENTAL ATOMIC FORCE AND CONFOCAL RAMAN MICROSCOPES IN PHARMACEUTICAL SCIENCE</b>	<b>Greg Haugstad</b> , University of Minnesota, Minneapolis, MN, U.S.A.
Contributed	<b>APPLICATION OF X-RAY SPECTROMETRY AT X-RAY ABSORPTION EDGES FOR INVESTIGATION OF HUMAN ALBUMIN</b>	Konstantin Pogrebitsky, Ioffe Physical-Technical Institute, Saint-Petersburg, Russia

**Thursday, 7 May - 8.30 – 12.00**

<b>Morning</b>	<b>Patent and Regulatory Issues</b> <b>Session Co-chairs: Dr. Peter Varlashkin</b> , GlaxoSmithKline, Durham, NC, U.S.A., <b>Dr. Fangling Needham</b> , ICDD, Newtown Square, PA, U.S.A., and <b>Dr. Philip G. Lake</b> , GlaxoSmithKline, Leigh, U.K.	
<b>Type</b>	<b>Title of Paper</b>	<b>Speaker &amp; Affiliation</b>
Invited	<b>BUILDING A STRONG PATENT PORTFOLIO WITH COCRYSTALS AND DISORDERED SOLIDS – A LIFECYCLE MANAGEMENT APPROACH</b>	<b>Eyal Barash</b> , SSCI, a division of Aptuit Inc., West Lafayette, IN, U.S.A.

<b>Round Robin Results from PPXRD-7</b> Session Chair: Dr. Fangling Needham, ICDD, Newtown Square, PA, U.S.A.	
<b>Title of Paper</b>	<b>Speaker &amp; Affiliation</b>
<b>ROUND ROBIN for PHARMACEUTICAL COMPOUNDS</b>	<b>Fangling Needham, Cyrus Crowder, Timothy Fawcett, ICDD, Newtown Square, PA, U.S.A.</b>
<b>Q&amp;A/Closing Remarks</b>	

	<b>Early Registration Fee</b>	<b>Registration Fee</b>
<b>Symposium &amp; Workshop 4-7 May</b>	\$1,199 USD	\$1,500 USD
<b>Symposium Only 5-7 May</b>	\$899 USD	\$1,200 USD
<b>Symposium &amp; Workshop Student fee</b>	\$499 USD (must fax registration form along with student identification to +610.325.9823)	\$499 USD (must fax registration form along with student identification to +610.325.9823)
<b>Symposium Only Student fee</b>	\$299 USD (must fax registration form along with student identification to +610.325.9823)	\$299 USD (must fax registration form along with student identification to +610.325.9823)

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