

## PPXRD-9 Program

22-25 February, Crowne Plaza, Hilton Head Island, SC, U.S.A.  
Workshop and Sessions will be held in the Crystal Ballroom, Salons B & C

### MONDAY WORKSHOP - 22 February 2010

#### UNDERSTANDING AMORPHOUS PHARMACEUTICAL MATERIALS

Organizer: **Shawn Yin**

Bristol-Myers Squibb Company, New Brunswick, NJ, [shawn.yin@bms.com](mailto:shawn.yin@bms.com)

<b>8:30-9:00 am</b>	Introduction – Amorphous Materials and Pharmaceutical Applications	<b>Shawn Yin</b> Bristol-Myers Squibb Company, New Brunswick, NJ
<b>9:00-10:00 am</b>	Amorphous Basics	<b>Ann Newman</b> Seventh Street Development Group, Lafayette, IN
<b>10:00-10:30 am</b>	<b>BREAK</b>	
<b>10:30-12:00 pm</b>	How to Prepare Amorphous API	<b>Michael Pikal</b> University of Connecticut, Storrs, CT
<b>12:00-1:00 pm</b>	<b>LUNCH - Attendees are on their own for lunch</b>	
<b>1:00-2:30 pm</b>	Using PXRD for Amorphous Materials	<b>Simon Bates</b> Aptuit Consulting, West Lafayette, IN
<b>2:30-3:15 pm</b>	Using ssNMR and Other Techniques for Amorphous Materials	<b>Eric Munson</b> University of Kansas, Lawrence, KS
<b>3:15-3:45 pm</b>	<b>BREAK</b>	
<b>3:45-4:30 pm</b>	Using Thermal Techniques for Amorphous Materials	<b>Michael Pikal</b> University of Connecticut, Storrs, CT
<b>4:30-5:30 pm</b>	Optional Panel Discussion	All instructors

## TUESDAY SYMPOSIUM - 23 February 2010

8:30-8:45 am	WELCOMING REMARKS & INTRODUCTIONS	Cyrus E. Crowder International Centre for Diffraction Data, Newtown Square, PA
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### PLENARY SESSION: PATENT AND REGULATORY ISSUES

Chair: **Cyrus E. Crowder**

International Centre for Diffraction Data, Newtown Square,  
PA, [crowder@icdd.com](mailto:crowder@icdd.com)

8:45-10:00 am	<i>INVITED</i> - Patenting Crystalline Forms of Pharmaceuticals – Using Solid State Science to Claim Form & Substance	<b>Jeffrey A. Lindeman</b> J.A. Lindeman & Co. PLLC, McLean, VA
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10:00-10:30 am	BREAK – exhibits open
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### XRPD STRUCTURAL TECHNIQUES (Acquisition and Use of XRPD Data, Indexing, Structure Determination, Rietveld Refinement)

Chair: **Hideo Toraya**

Rigaku Corporation, Tokyo, Japan, [toraya@rigaku.co.jp](mailto:toraya@rigaku.co.jp)

10:30-11:30 am	<i>INVITED</i> - Accurate Powder Structural Study of Pharmaceuticals Using Maximum Entropy Method	<b>Eiji Nishibori</b> Nagoya University, Nagoya, Japan
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11:30-12:00 pm	Ab Initio Crystal Structure Determination of Two Polymorphic Modifications of an Anesthetic Agent, Tetracaine Hydrochloride, Using a Combination of Molecular Modeling and Synchrotron X-ray Powder Diffraction Techniques	<b>Robert Papoular</b> Leon Brillouin Laboratory, Gif-sur- Yvette, France
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12:00-1:15 pm LUNCH – Attendees are on their own for lunch. Exhibits open.

### COMPLEMENTARY TECHNIQUES

Chair: **Shawn Yin**

Bristol-Myers Squibb Company, New Brunswick, NJ [shawn.yin@bms.com](mailto:shawn.yin@bms.com)

1:15-2:15 pm	<i>INVITED</i> - Solid-State Analysis of Pharmaceuticals: Solid-State NMR and PXRD	<b>Eric Munson</b> University of Kansas, Lawrence, KS
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2:15-2:45 pm	PXRD with Raman Spectroscopy, DSC and IR DATA	<b>Chris Gilmore</b> University of Glasgow, Glasgow, UK
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2:45-3:15 pm	Integrated Hyperspectral Imaging for Comprehensive Materials Characterization	<b>Eunah Lee</b> Horiba Jobin Yvon, Inc., Edison, NJ
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3:15-3:45 pm	BREAK - exhibits open	
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#### AMORPHOUS, ACTIVATED AND NANOMATERIALS

Chair: **Cyrus E. Crowder**

International Centre for Diffraction Data, Newtown Square,  
PA, [crowder@icdd.com](mailto:crowder@icdd.com)

3:45-4:45 pm	<i>INVITED</i> - The Amorphous State: A Structural Perspective	<b>Simon Bates</b> Aptuit Consulting, West Lafayette, IN
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#### POSTER SESSION, RECEPTION, EXHIBITS

**6:00-8:00 pm** An evening reception and poster session of submitted papers will be held in the exhibit hall. See "**Guidelines for Preparing Abstracts**" for information on submitting a poster presentation.

## WEDNESDAY SYMPOSIUM - 24 February 2010

#### FORMULATION & PRODUCT DEVELOPMENT

Chair: **Shawn Yin**

Bristol-Myers Squibb Company, New Brunswick,  
NJ [shawn.yin@bms.com](mailto:shawn.yin@bms.com)

8:30-9:30 am	<i>INVITED</i> - Drug Product Characterization: What Form Do I Have?	<b>Ann Newman</b> Seventh Street Development Group, Lafayette, IN
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9:30-10:00 am	Successful Material Identification	<b>Timothy Fawcett</b> International Centre for Diffraction Data, Newtown Square, PA
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10:00-10:30 am	XRPD Characterization of Pharmaceutical Solids - Quantitative Phase Analysis and Lower Limits of Detection	<b>Arnt Kern</b> Bruker AXS, Inc., Karlsruhe, Germany
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10:30-11:00 am	<b>BREAK – exhibits open</b>	
11:00-11:30 am	<b>PXRD Investigation of Changes in Dehydration Behavior of 7-Methoxy-1-Methyl-5-(4-(Trifluoromethyl)Phenyl)-[1,2,4]Triazolo[4,3-A]Quinolin-4-Amine Hydrate After Micronization</b>	<b>Feirong Kang</b> GlaxoSmithKline, King of Prussia, PA
11:30-12:00 pm	<b>X-ray Powder Diffraction Database Tools for the Pharmaceutical Scientist: New Capabilities</b>	<b>Cyrus E. Crowder</b> International Centre for Diffraction Data, Newtown Square, PA
12:00-12:30 pm	<b>Quantification of Indomethacin-Saccharin Cocrystals by Powder X-ray Diffraction</b>	<b>Sitaram Velaga</b> Luleå University of Technology, Luleå, Sweden
12:30-1:30 pm	<b>LUNCH – exhibits open</b>	
	<b>NEW FRONTIERS IN XRD IN PHARMACEUTICAL R&amp;D</b> Chairs: <b>Fangling Needham</b> and <b>Timothy Fawcett</b> International Centre for Diffraction Data, Newtown Square, PA, <a href="mailto:needham@icdd.com">needham@icdd.com</a> ; <a href="mailto:fawcett@icdd.com">fawcett@icdd.com</a> <b>Raj Suryanarayanan</b> University of Minnesota, Minneapolis, MN, <a href="mailto:surya001@tc.umn.edu">surya001@tc.umn.edu</a>	
1:30-2:30 pm	<i>INVITED</i> - <b>The New World of Materials Science &amp; Engineering: Nano &amp; Bio Technology</b>	<b>Robert Snyder</b> Georgia Institute of Technology, Atlanta, GA
2:30-3:30 pm	<i>INVITED</i> - <b>Structure Studies of Disordered Pharmaceutical Materials by High-Energy X-ray Diffraction and Atomic Pair Distribution Function Analysis</b>	<b>Valeri Petkov</b> Central Michigan University, Mt. Pleasant, MI
3:30-4:00 pm	<b>BREAK – last chance to view exhibits</b>	
4:00-4:30 pm	<b>Easy Access to Synchrotron Powder Diffraction on Pharmaceuticals</b>	<b>Brian H. Toby</b> APS, Argonne National Laboratory, Argonne, IL
4:30-5:00 pm	<b>The Use of Field-Portable pXRD for the Rapid Identification of Counterfeit Pharmaceutical Products and Subsequent Excipient Identification and Quantification</b>	<b>David Blake</b> NASA Ames Research Center, Moffett Field, CA

5:00-5:30 pm

**Geometry, Polarization and Absorption  
Corrections for Two-Dimensional XRD**

**Bob B. He**  
Bruker AXS, Inc.,  
Madison, WI

## THURSDAY SYMPOSIUM - 25 February 2010

### POLYMORPH & SALT SCREENING

Chair: Timothy Fawcett

International Centre for Diffraction Data, Newtown Square,  
PA, fawcett@icdd.com

8:30-9:00 am

**Analysis of Amorphous Phase in Highly  
Crystalline API by Powder X-ray  
Diffraction and DSC**

**Beth Sarsfield**  
Bristol-Myers Squibb, New  
Brunswick, NJ

9:00-9:30 am

**Polymorphs in PDF-4/Organics 2010**

**Fangling Needham**  
International Centre for  
Diffraction Data, Newtown  
Square, PA

9:30-11:30 am

**ROUND TABLE & DISCUSSION**

All PPXRD-9 Workshop &  
Symposium participants  
welcome

### Organizing Committee

[Dr. Cyrus Crowder](#), 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, Nottingham, U.K.

[Dr. Arnt Kern](#), Bruker AXS GmbH, Karlsruhe, Germany

[Terry Maguire](#), 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](#), Reading University, Reading, 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. Hideo Toraya](#), Rigaku Corporation, Tokyo, Japan

[Dr. Peter G. Varlashkin](#), GlaxoSmithKline, Durham, NC, U.S.A.

[Dr. Shawn Yin](#), Bristol-Myers Squibb Company, New Brunswick, NJ, U.S.A.