

PPXRD-11 Program

15 - 18 May 2012

Sanibel Harbour Marriott Resort & Spa, Fort Myers, FL, USA

Exhibition: 16-17 May

TUESDAY

WORKSHOP

15 May

8:30am-5:30pm

UNDERSTANDING AMORPHOUS PHARMACEUTICAL MATERIALS

Organizer: **Dr. Shawn Yin**

Bristol-Myers Squibb Company, New Brunswick, NJ, USA

8:30-9:00am

Introduction – Amorphous Materials and Pharmaceutical Applications

Shawn Yin

Bristol-Myers Squibb Company, New Brunswick, NJ, USA

9:00-10:00am

Amorphous Basics

Lian Yu

University of Wisconsin, Madison, WI, USA

10:00-10:30am

BREAK

10:30-11:30am

Making Amorphous API

Ann Newman

Seventh Street Development Group, Lafayette, IN, USA

11:30-12:30pm

Ultrafast Lasers for the Detection and Quantification of Trace Crystallinity in Amorphous Formulations by SONICC

Garth Simpson

Purdue University, West Lafayette, IN, USA

12:30-1:15pm

LUNCH

1:15-3:15pm

Using PXRD for Amorphous Materials

Simon Bates

Triclinic Labs Inc., West Lafayette, IN, USA

3:15-3:45pm

BREAK

3:45-4:45pm	Using Thermal Techniques for Amorphous Materials	Ann Newman Seventh Street Development Group, Lafayette, IN, USA
4:45-5:30pm	The Strategy for Quantitation of Residual Amorphous in Crystalline API	Peter Varlashkin Physical Properties, GSK Durham, NC, USA

WEDNESDAY
16 May
8:30am-4:30pm

SYMPOSIUM – * asterisk signifies presenter

8:30-8:45am **WELCOMING REMARKS & INTRODUCTIONS FROM THE PROGRAM CHAIR**
Dr. Cyrus E. Crowder
International Centre for Diffraction Data, Newtown Square, PA, USA

AMORPHOUS, ACTIVATED AND NANOMATERIALS
Chair: **Dr. Peter Varlashkin**
Physical Properties, GlaxoSmithKline, Durham, NC, USA

P21	8:45-9:45am	Invited – AMORPHOUS ORGANIC SOLIDS AND THEIR CRYSTALLIZATION	Lian Yu University of Wisconsin, Madison, WI, USA
P14	9:45-10:15am	THE STUDY OF MICRONIZATION INDUCED DISORDER OF ACTIVE PHARMACEUTICAL INGREDIENTS BY XRPD LINE BROADENING ANALYSES	G. Williams*, R. Forcino, J. Brum, F. Vogt GlaxoSmithKline, King of Prussia, PA, USA
	10:15-10:45am	BREAK – exhibits open	
P2	10:45-11:15am	AMORPHOUS QUANTITATION STRATEGY FOR CRYSTALLINE DRUG SUBSTANCE – A GSK PERSECTIVE	P. Varlashkin GlaxoSmithKline, Durham, NC, USA
P13	11:15-11:45am	ADDRESSING THE AMORPHOUS CONTENT ISSUE IN QUANTITATIVE PHASE ANALYSIS: THE CERTIFICATION OF NIST STANDARD REFERENCE MATERIAL 676A	J. Cline*, J. J. Filliben NIST, Gaithersburg, MD, USA R. B. Von Dreele Argonne National Laboratory, Argonne, IL, USA R. Winburn

Minot State University, Minot, ND, USA
P. W. Stephens
State University of New York at Stony
Brook, Stony Brook, NY, USA

P23 11:45-
12:15pm ~~WITHDRAWN - UTILIZING BENCH-TOP PXRD INSTRUMENTATION
FOR QUANTITATIVE ANALYSES OF SPRAY-DRIED SOLID
DISPERSION PHARMACEUTICAL FORMULATIONS: FROM
MANUFACTURING TO PERFORMANCE TESTING~~

J. Gautschi
Agere Pharmaceuticals, Inc., Bend, OR,
USA

P3 12:15-
12:45 pm AN ALTERNATIVE METHOD FOR QUANTITATIVE XRPD ANALYSIS –
PLS REGRESSION TO QUANTIFY AMORPHOUS CONTENT AND
PHASE MIXTURES

D. Beckers
PANalytical B.V., Almelo, The Netherlands

12:45-
2:00pm **LUNCH – Exhibits open.**

FORMULATION & PRODUCT DEVELOPMENT

Chair: **Dr. Detlef Beckers**
PANalytical B.V., Almelo, The Netherlands

P16 2:00-
3:00pm **Invited** – STRUCTURAL CHARACTERIZATION OF SOLID
COMPOSITE MATERIALS AS A TOOL FOR DRUG PRODUCT
FORMULATION AND DEVELOPMENT

Peter Wildfong
Duquesne University, Pittsburgh, PA, USA

3:00-
3:30pm **BREAK – exhibits open**

P4 3:30-
4:00pm PHARMACEUTICAL APPLICATIONS OF TOTAL DIFFRACTION
ANALYSIS TO ASSESS SINGLE AND MULTI-COMPONENT SYSTEMS

**A. Sheikh*, S. Chen, J. Roth, T.
Borchardt**
Abbott Labs, North Chicago, IL, USA

P11 4:00-
4:30pm MATERIAL IDENTIFICATION AND CHARACTERIZATION: 10 YEARS
OF DEVELOPMENTS, THE PDF-4/ORGANICS DATABASE

**T. G. Fawcett*, S.N. Kabbekodu, F.
Needham, C. E. Crowder**
International Centre for Diffraction Data,
Newtown Square, PA, USA

Wednesday
16 May Evening
6:00-8:00pm
POSTER SESSION, RECEPTION, EXHIBITS

P9	STRUCTURE DETERMINATION OF XYLAZINE HYDROCHLORIDE ANHYDROUS CRYSTALLINE FORMS USING POWDER X-RAY DIFFRACTOMETRY DATA	A. Zvirgzdiņš*, A. Actiņš University of Latvia, Rīga, Latvia
P17	NIST STANDARD REFERENCE MATERIALS FOR X-RAY METROLOGY	J. P. Cline*, D. Windover, A. Henins NIST, Gaithersburg, MD, USA
P18	IMIPENEM MONOHYDRATE X-RAY POWDER DIFFRACTION	F. Needham*, C. E. Crowder, T. G. Fawcett International Centre for Diffraction Data, Newtown Square, PA, USA
P26	DIGITAL PATTERN ANALYSES	T. G. Fawcett*, S.N. Kabbekodu, F. Needham, C. E. Crowder International Centre for Diffraction Data, Newtown Square, PA, USA
P7	A THIRD PHASE EFFECT ON THE PHASE TRANSITION OF XYLAZINE HYDROCHLORIDE	K. Krūkle-Bērziņa*, A. Actiņš University of Latvia, Rīga, Latvia

THURSDAY **SYMPOSIUM**
17 May
8:30am-5:45pm

XRPD STRUCTURAL TECHNIQUES
(Acquisition and Use of XRPD Data, Indexing, Structure Determination, Rietveld Refinement)
& CRYSTAL STRUCTURE PREDICTION

Chairs: **Dr. Arnt Kern**, Bruker AXS GmbH, Karlsruhe, Germany
Dr. Timothy Fawcett, International Centre for Diffraction Data, Newtown Square, PA

P10	8:30-9:30am	Invited – CRYSTAL STRUCTURE SOLUTION FROM POWDER MIXTURES: THE PXRD-BTEM-RIETVELD METHOD	Marc Garland*, L.Guo, M. Schreyer, S. Thirunahari ICES, Jurong Island, Singapore
P22	9:30-10:00am	TRIADS XRPD INDEXING ALGORITHM AND ITS USE IN PHARMACEUTICAL DEVELOPMENT	R. B. McClurg SSCI, a Division of Aptuit, West Lafayette, IN, USA
	10:00-10:30am	BREAK – exhibits open	

P25	10:30- 11:30am	Invited – MOLECULAR COCRYSTALS AND SALTS: 'FULL' STRUCTURAL CHARACTERIZATION FROM POWDER DIFFRACTION DATA	Maryjane Tremayne*, L. Thompson, A. Cowell, G. Cutts, D. Bell University of Birmingham, Edgbaston, Birmingham, UK
P12	11:30- 12:30pm	Invited – CRYSTAL STRUCTURE PREDICTION: SYNERGY BETWEEN THEORY AND EXPERIMENT	James A. Kaduk Illinois Institute of Technology, Chicago IL, USA
	12:30- 1:45pm	LUNCH – Exhibits open.	

COMPLEMENTARY TECHNIQUES

Chair: **Dr. Fangling Needham**

International Centre for Diffraction Data, Newtown Square, PA

P20	1:45- 2:45pm	Invited – NUCLEATION AND THE DIFFERING CRYSTALLIZATION BEHAVIOR OF ENANTIOMERS	Gregory A. Stephenson*, C. D. Wolfangel Eli Lilly and Company, Indianapolis, IN, USA
P19	2:45- 3:15pm	SONICC AND TPE-UVF ANALYSIS OF APIS AND COMMON EXCIPIENTS	S. Toth*, G. J. Simpson J. T. Madden, L. S. Taylor, College of Pharmacy, Purdue University, West Lafayette, IN, USA P. Marsac Merck & Co., Inc., West Point, PA, USA
P6	3:15- 3:45pm	DESOLVATION OF DROPERIDOL ISOSTRUCTURAL SOLVATES	A. Bērziņš, A. Actiņš, T. Rēķis, I. Sarceviča University of Latvia, Rīga, Latvia
	3:45- 4:15pm	BREAK – exhibits open	

POLYMORPH & SALT SCREENING

Chair: **Dr. Gregory A. Stephenson**

Eli Lilly and Company, Indianapolis, IN, USA

P15	4:15- 5:15pm	Invited - SOLID-FORM SCREENING AND SELECTION: STRATEGIES AND CHALLENGES OF DIFFICULT MOLECULES	Pingyun (P.Y.) Chen,* J. Bis, S. Carino, R. Couch, D. Igo, L. Katrincic, D. Kinder, B.Norton, S. Sukumar Optiform™ Technologies, Catalent
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Pharma Solutions, Research Triangle
Park, NC, USA

P8 5:15-
5:45pm DETECTING TRACE AMOUNTS OF THE THERMODYNAMICALLY
STABLE POLYMORPH IN A MIXTURE OF POLYMORPHS

R. Bobrovs*, A. Actiņš
University of Latvia, Rīga, Latvia

FRIDAY
18 May
8:30am-
11:30am

SYMPOSIUM

**REGULATORY AND PATENT ISSUES &
NEW FRONTIERS IN XRD IN PHARMACEUTICAL R&D**

Chairs: **Dr. Shawn Yin**, Bristol-Myers Squibb Company, New Brunswick, NJ,
Dr. Cyrus Crowder, International Centre for Diffraction Data, Newtown Square, PA, USA

P24 8:30-
9:30am **Invited** – REGULATORY CONSIDERATIONS ON PHARMACEUTICAL
SOLIDS: POLYMORPHS AND CO-CRYSTALS

Andre S. Raw
FDA, Rockville, Maryland, USA

P5 9:30-
10:00am NEW INSTRUMENTATION FOR PHARMACEUTICAL XRD

B. He
Bruker AXS, Madison, WI, USA

10:00-
10:15am **BREAK**

10:15-
11:30am ROUND TABLE DISCUSSION FOR CONFERENCE ORGANIZERS AND
INTERESTED ATTENDEES

Symposium Adjourned