

PPXRD-10 Program

16 - 19 May 2011, Radisson BLU Hotel, Lyon, France

Exhibition: 17-18 May

Workshop and Sessions will be held in the Cordeliers & Tete D'or rooms, 32nd floor

Coffee Breaks, Exhibits, Evening Reception & Poster Session will be held in the Jacobins & Ainay Rooms, 32nd floor

MONDAY
9.00-18.00

WORKSHOP

UNDERSTANDING PHARMACEUTICAL AMORPHOUS MATERIALS

Organizer: **Dr. Shawn Yin**

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

9.00-10.00	Introduction – Amorphous Materials and Pharmaceutical Applications	Shawn Yin Bristol-Myers Squibb Company, New Brunswick, NJ, USA
10.00-10.45	Amorphous Basics	Ann Newman Seventh Street Development Group, Lafayette, IN, USA
10.45-11.15	BREAK	
11.15-12.15	Making Amorphous API	Ann Newman Seventh Street Development Group, Lafayette, IN, USA
12.15-13.15	LUNCH – lunch is included in the workshop fee	
13.15-15.15	Using PXRD for Amorphous Materials	Valeri Petkov Central Michigan University, Mt. Pleasant, MI, USA
15.15-15.45	BREAK	
15.45-16.45	Using ssNMR and Other Techniques for Amorphous Materials	Loren Schieber University of Connecticut, Storrs, CT, USA
16.45-17.30	Using Thermal Techniques for Amorphous Materials	Ann Newman Seventh Street Development Group, Lafayette, IN, USA
17.30-18.00	Optional Panel Discussion	All instructors

TUESDAY
8.30-17.45

SYMPOSIUM – * asterisk signifies presenter

WELCOMING REMARKS & INTRODUCTIONS FROM THE PROGRAM CHAIR

8.30-8.45

Dr. Cyrus E. Crowder

International Centre for Diffraction Data, Newtown Square, PA, USA

AMORPHOUS, ACTIVATED AND NANOMATERIALS

Chair: **Dr. Simon Billinge**

Prof. of Materials Science and of Applied Physics & Mathematics, Columbia University, New York, NY, USA

P31	8.45-9.45	Invited - TOTAL SCATTERING PAIR DISTRIBUTION FUNCTIONS (TSPDF) FOR FINGERPRINTING AMORPHOUS PHARMACEUTICALS	Simon Billinge Columbia University, New York, NY, USA
P10	9.45-10.15	A HIGH PERFORMANCE SMALL ANGLE X-RAY SCATTERING INSTRUMENT	P.U. Pennartz* , L. Fan , L. Jiang , M. Degen , N. Grupido Rigaku Innovative Technologies, Auburn Hills, MI, USA
P18	10.15-10.45	A NOVEL METHOD TO DETERMINE AMORPHOUS PHASE CONCENTRATIONS USING THE RIETVELD REFINEMENT TECHNIQUE	X. Bokhimi Instituto de Física, Universidad Nacional Autónoma de México
	10.45-11.15	BREAK – exhibits open	

XRPD STRUCTURAL TECHNIQUES

(Acquisition and Use of XRPD Data, Indexing, Structure Determination, Rietveld Refinement)

Chair: **Dr. Hideo Toraya**

Rigaku Corporation, Tokyo, Japan

P27	11.15-12.15	Invited - INTERPLAY OF SINGLE CRYSTAL AND X-RAY POWDER DIFFRACTION DATA IN SOLID-STATE PHARMACEUTICS	Gregory A. Stephenson Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, USA
P23	12.15-12.45	STRUCTURE DETERMINATION USING DIRECT METHODS AND CHARGE-FLIPPING ALGORITHM ON HIGH-QUALITY POWDER DIFFRACTION DATA OBTAINED WITH AN IN-HOUSE DIFFRACTOMETER	G. Schuck , A. Iwata Rigaku Europe SE, Germany A. Sasaki Rigaku Corporation, Japan
	12.45-14.15	LUNCH – Symposium Attendees have lunch included in their registration fee. Exhibits open.	

FORMULATION & PRODUCT DEVELOPMENT

Chair: **Dr. Shawn Yin**

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

P32	14.15-15.15	Invited - WHICH API FORM IS IN YOUR DRUG PRODUCT?	Shawn Yin Bristol-Myers Squibb, New Brunswick, NJ, USA
P24	15.15-15.45	INVESTIGATION OF SOLID-STATE STABILITY OF A COCRYSTAL API IN FORMULATION DEVELOPMENT BY XRPD AND SS-NMR SPECTROSCOPY	Z. Jane Li* , V. Abeyta , D. Chen , A. Khawam , T. Offerdahl , J. Park , J.A. Smoliga Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, USA
	15.45-16.15	BREAK - exhibits open	
P7	16.15-16.45	DEGREE OF CRYSTALLINITY BY XRD AS A PROCESS DEVELOPMENT TOOL	I. Adin* , S. Zamir , O. Kurlat , C. Iustain CHEMAGIS LTD, ISRAEL
P13	16.45-17.15	IN SITU MEASUREMENT AND CHARACTERIZATION OF CRYSTAL GROWTH BY X-RAY DIFFRACTION	D. Beckers* , K. Bethke PANalytical B.V., Almelo, The Netherlands
P3	17.15-17.45	STABILITY AND DESOLVATION KINETICS OF DROPERIDOL HYDRATES AND AN ETHANOL SOLVATE, STUDIED BY POWDER X-RAY DIFFRACTOMETRY AND DIFFERENTIAL THERMAL ANALYSIS/THERMOGRAVIMETRY	A. Bērziņš* , A. Actiņš , E. Skarbulis University of Latvia, Rīga, Latvia

Tuesday Evening
18.00-20.00

POSTER SESSION, RECEPTION, EXHIBITS

P4	POWDER X-RAY DIFFRACTOMETRY INVESTIGATION OF XYLAZINE HYDROCHLORIDE SOLID STATE PHASE TRANSITION KINETICS	K. Krūkle-Bērzina* , A. Actiņš University of Latvia, Rīga, Latvia
P5	STRUCTURE DETERMINATION OF MILDRONATE CRYSTALLINE FORMS USING POWDER X-RAY DIFFRACTOMETRY DATA	A. Zvirgzdiņš* , K. Veldre , A. Actiņš University of Latvia, Rīga, Latvia
P8	CRYSTAL STRUCTURE OF TWO POLYMORPHS OF TMC125 (ETRAVIRINE, INTELENCE) FROM SINGLE CRYSTAL AND X-RAY POWDER DIFFRACTION DATA	H. Novoa* , I. Weuts , S. Stokbroekx , R. Leemans , J. Van Gelder Johnson & Johnson Pharmaceutical Research & Development, a division of Janssen Pharmaceutica NV, Beerse, Belgium
P16	POLYMORPHISM AND SOLVATES OF FLECAINIDE BASE <div style="border: 1px solid black; padding: 5px; display: inline-block;">Moved to Polymorph & Salt Screening session.</div>	K. Veldre* , A. Actiņš , A. Zvirgzdiņš , Z. Eglīte , L. Rozenberga , S. Ostrovskā University of Latvia, Rīga, Latvia
P19	OBSERVATIONS OF PHASE TRANSITION USING A SIMULTANEOUS XRD AND DSC MEASUREMENT TECHNIQUE COUPLED WITH HIGH SPEED 1D- AND 2D-DETECTORS	A. Iwata* , A. Ohbuchi , A. Kishi Rigaku corporation, Tokyo, Japan K. Terada TOHO University, Chiba, Japan
P21	THE STUDY OF MICRONIZATION INDUCED DISORDER AND ENVIRONMENTAL STABILITY OF AN ACTIVE PHARMACEUTICAL INGREDIENT (API) USING THERMAL ANALYSIS AND ADENING ANALYSES <div style="border: 1px solid black; padding: 5px; display: inline-block;">WITHDRAWN</div>	G.R. Williams* , J. Brum GlaxoSmithKline, King of Prussia, PA, USA
P25	STANDARD REFERENCE AND TESTING MATERIALS WITHIN THE QUALITY SYSTEM FOR PHARMACEUTICAL PRODUCTION	S. Kononogov , N. Nechaev , B. Kodess* , I. Kommel Federal State Unitary Enterprise, The Russian Research Institute for Metrological Service, Moscow, Russia
P26	PDF-4/ORGANICS 2011 DATABASE HIGHLIGHTS AND ITS APPLICATION	F. Needham* , C.E. Crowder , T.G. Fawcett ICDD, Newtown Square, PA, USA

**WEDNESDAY
8.30-17.30**

SYMPOSIUM

CRYSTAL STRUCTURE PREDICTION

Chair: **Dr. Jamshed Anwar**

Professor of Computational Pharmaceutical Science & Director of Research, Institute of Life Sciences Research,
University of Bradford, West Yorkshire, UK

P15	8.30-9.30	Invited - ADDRESSING THE CHALLENGES FOR APPLYING CRYSTAL STRUCTURE PREDICTION TO PHARMACEUTICAL MATERIALS	Graeme M. Day Department of Chemistry, University of Cambridge, Cambridge, UK
P29	9.30-10.30	Invited - CRYSTAL STRUCTURE PREDICTION OF SMALL ORGANIC MOLECULES; KINETICS VERSUS THERMODYNAMICS	Frank J.J. Leusen* , H.C.S. Chan, J. Kendrick School of Life Sciences, University of Bradford, Bradford, UK
P33	10.30-11.00	PREDICTION OF SOLID STATE PROPERTIES FROM MOLECULAR SIMULATION	Jamshed Anwar University of Bradford, Bradford, UK
	11.00-11.30	BREAK – exhibits open	

POLYMORPH & SALT SCREENING

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

Research Advisor, Eli Lilly and Company, Indianapolis, IN, USA

P17	11.30-12.30	Invited - AN OVERVIEW OF SOLID FORM SCREENING DURING DRUG DEVELOPMENT	Ann Newman Seventh Street Development Group, Lafayette, IN, USA
P6	12.30-13.00	REFERENCE MATERIALS FOR THE STUDY OF POLYMORPHISM AND CRYSTALLINITY OF CELLULOSE	T.G. Fawcett* , C.E. Crowder , S.N. Kabekkodu ICDD, Newtown Square, PA, USA
	13.00-14.30	LUNCH – Symposium Attendees have lunch included in their registration fee. Exhibits open.	J.A. Kaduk Poly Crystallography Inc., Naperville IL, USA
P16	14.30-15.00	POLYMORPHISM AND SOLVATES OF FLECAINIDE BASE	K. Veldre* , A. Actiņš , A. Zvirgzdiņš , Z. Eglīte , L. Rozenberga , S. Ostrovska University of Latvia, Rīga, Latvia

NEW FRONTIERS IN XRD IN PHARMACEUTICAL R&D

Chair: **Dr. Cyrus Crowder**

Principal Scientist, International Centre for Diffraction Data, Newtown Square, PA, USA

P22	15.00-16.00	Invited - EFFECT OF PROCESSING CONDITIONS ON THE PHYSICAL STATE OF EXCIPIENTS IN LYOPHILIZED FORMULATION	Prakash Sundaramurthi* Scientific Affairs, Teva Parenteral Medicines. Inc., Irvine CA, USA
P20	16.00-16.30	MINIMIZING THE X-RAY POWDER D WITHDRAWN RRED ORIENTATION IN BREAK – last chance to view exhibits	R. Suryanarayanan University of Minnesota, Minneapolis, MN, USA
			G.R. Williams* , F. Kang GlaxoSmithKline, King of Prussia, PA, USA
P11	16.30-17.00	NOVEL ELECTRON DIFFRACTION TECHNIQUE FOR TEXTURE ANALYSIS (ORIENTATION & PHASE MAPPING) OF ORGANIC NANOCRYSTALS	M. Veron, E. Rauch* SIMAP/GPM2 lab CNRS-INP, Grenoble, France
			S. Nicolopoulos NanoMEGAS SPRL, Brussels, Belgium
			W.L. Ling, J.M. Otero Inst Biologie Structurale, Grenoble, France
P12	17.00-17.30	VÅNTEC-500 AREA DETECTOR FOR PHARMACEUTICAL XRD	B.B. He Bruker AXS Inc, Madison, WI, USA

THURSDAY
9.00-12.00

SYMPOSIUM

COMPLEMENTARY TECHNIQUES

Chair: **Dr. Julien Giovannini**
AstraZeneca, Nottingham, UK

P30	9.00-10.00	Invited - HR-XRPD, A CRUCIAL FACTOR IN THE DETERMINATION OF THE STABILITY HIERARCHY OF POLYMORPHS BY TOPOLOGICAL AND EXPERIMENTAL PRESSURE-TEMPERATURE DIAGRAMS	I.B. Rietveld* , R. Céolin Université Paris Descartes, Paris, France M. Barrio , J.L. Tamarit Universitat Politècnica de Catalunya, Barcelona, Spain
P28	10.00-10.30	APPLICATION OF AUTOMATED ELECTRON DIFFRACTION TO STRUCTURAL INVESTIGATION OF MOLECULAR CRYSTALS	T.E. Gorelik* , G. Matweeva , U. Kolb , Johannes-Gutenberg University Mainz, Mainz, Germany
P14	10.30-11.00	COMBINED X-RAY DIFFRACTION AND COMPUTED TOMOGRAPHY ANALYSIS OF PHARMACEUTICAL SAMPLES	D. Beckers* , K. Bethke PANalytical B.V., Almelo, The Netherlands

PATENT AND REGULATORY ISSUES

Chair: **Dr. Jeremy K. Cockcroft**
Faculty of Mathematical and Physical Sciences, University College London, London, UK

11.00-12.00 Invited - Speaker to be determined .