

PPXRD-4 Event Schedule
21-24 February 2005 - Barceló Hotel Sants, Barcelona, Spain

Monday, February 21

Optional Hands-on Workshop - Indexing Powder Patterns & Rietveld Structural Refinement

Tuesday, February 22

Type	Title of Paper	Speaker & Affiliation
	WELCOMING REMARKS & INTRODUCTIONS	John Faber, International Centre for Diffraction Data, Newtown Square, PA, USA
Formulation, Product Development, Drug Delivery, and Polymorph & Salt Screening Session Chair: Dr. Shawn Yin, Bristol-Myers Squibb, New Brunswick, NJ, USA		
Invited	AN OVERVIEW OF METHODS AND STRATEGIES FOR HIGH-THROUGHPUT POLYMORPH SCREENING: CRYSTALLISATION, DIFFRACTOMETRY AND DATA ANALYSIS	Christian Lehmann, Max-Planck Institut fuer Kohlenforschung, Muelheim an der Ruhr, Germany
Contributed	USING POWDER X-RAY DIFFRACTION ANALYSIS FOR A PHARMACEUTICAL NANOCOMPOSITE	Shawn Yin, Bristol-Myers Squibb Co., New Brunswick, NJ, USA
Contributed	FORMULATION ANALYSES OF COMMON HEALTH SUPPLEMENTS	Timothy G. Fawcett, ICDD, Newtown Square, PA, USA
Contributed	AUTOMATION PLATFORM FOR SALT PRESCREENING AND POLYMORPH SCREENING STUDIES	Werner Zinsser, Zinsser Analytic GmbH, Frankfurt, Germany
Contributed	AN INTEGRATED SYSTEM FOR SOLVENT SOLUBILITY, SINGLE CRYSTAL GROWING, AND POLYMORPH SCREENING OF PHARMACEUTICAL DRUG SUBSTANCES	Ron Chen, Pfizer Global R & D, San Diego, CA, USA

X-rays in Drug Research & Discovery Session Chair: Dr. Daniel Louër, University of Rennes, Rennes, France		
Type	Title of Paper	Speaker & Affiliation
Invited	X-RAY DIFFRACTION APPLIED TO DRUG DEVELOPMENT - AN OVERVIEW	Franck Leveiller, AstraZeneca, Lund, Sweden
Contributed	XRD COMBINATORIAL SCREENING SYSTEM WITH AUTOMATED REFLECTION-TRANSMISSION CONVERSION	Bob He, Bruker AXS, Madison, WI, USA
Contributed	MAPPING DRUG CHEMISTRY USING CLUSTER ANALYSIS AND DIFFRACTION DATABASES	Timothy G. Fawcett, ICDD, Newtown Square, PA, USA

Evening (6:00-9:00)		Poster Session
Title of Paper		Speaker & Affiliation
SAXSESS - A TOOL FOR PHARMACEUTICAL MATERIALS		Detlef Beckers, PANalytical, Almelo, The Netherlands

THE STUDY OF RIGID JOINT THERAPY USING DRY BONE OF PITHUOPHIS MELANOLEUCUS TO OBTAIN A DIFFRACTIONAL CRYSTAL POWDER	Akoma Nwabu Godwin, West Feld Clinic, Serekunda, Banjul, The Gambia
CHIRAL SYMMETRY BREAKING IN THE CRYSTALLIZATION OF 1,1' BINAPHTYL AND POLYMORPHISM	Africa Paz Martin-Islán, Estación Experimental del Zaidín, CSIC, Granada, Spain
THERMAL BEHAVIOUR OF AZITHROMYCIN MONOHYDRATE AND DIHYDRATE FORMS	Jose Montejo-Bernardo, University of Oviedo, Oviedo, Asturias, Spain
POLYMORPHIC ANALYSIS OF TEGAFUR	Fangling Needham, ICDD, Newtown Square, PA, USA
CRYSTAL STRUCTURE DETERMINATION FROM SYNCHROTRON X-RAY POWDER DIFFRACTION DATA BY SIMULATED ANNEALING	Özen Özgen, National Synchrotron Radiation Research Center, Hsinchu, Taiwan, R. O. C.
PARTICLE STATISTICS ENHANCEMENT FOR XRD ANALYSIS USING VIBRATING SAMPLE HOLDERS	Philippe Sarrazin, inXitu, Mountain View, CA, USA
LOD METHOD FOR THE DETECTION OF THE PRESENCE OF ONE POLYMORPHIC FORM IN ANOTHER ONE	Geertrui Schuerman, Johnson & Johnson Pharmaceutical Research & Development, Beerse, Belgium
THE STUDY ON THE STABILITY OF A DRUG. CAN A PRODUCT HAVE LIFE?	Xavier Solans, University of Barcelona, Barcelona, Spain
SOLID-STATE TRANSITIONS OF PHARMACEUTICAL COMPOUNDS STUDIED BY POWDER X-RAY DIFFRACTION.	Elisabeth Theunissen, Johnson and Johnson Pharmaceutical Research and Development, Beerse, Belgium
CHARACTERIZATION OF THE ACTIVE PHARMACEUTICAL INGREDIENT IN FILM-COATED TABLETS AND CALCULATION OF THE DEPTH OF PENETRATION OF X-RAY	Hiroyuki Yamada, Mitsubishi Pharma Co., Kashima, Japan

Wednesday, February 23

XRPD Structural Techniques (Acquisition and Use of XRPD Data, Structure Determination, Indexing, Rietveld Refinement)		
Session Chair: Dr. Detlef Beckers, PANalytical B.V., Almelo, The Netherlands		
Type	Title of Paper	Speaker & Affiliation
Invited	WATCHING THE ACTION AND GETTING THE MOST FROM YOUR DATA	William David, Rutherford Appleton Laboratory, Oxon, UK
Invited	HIGH-THROUGHPUT STRUCTURE DETERMINATION, HIGH-QUALITY STRUCTURE REFINEMENT	Kenneth Shankland, Rutherford Appleton Laboratory, Oxon, UK
Contributed	EFFECT OF HIGH HYDROSTATIC PRESSURE ON THE GAMMA-POLYMORPH OF GLYCINE: A POLYMORPHIC TRANSITION INTO A NEW FORM	Elena Boldyreva, Novosibirsk State University, and Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia
Contributed	RIETVELD STRUCTURAL AND MICROSTRUCTURAL CHARACTERIZATION OF PHARMACEUTICAL PRODUCTS USING THE PROGRAM MAUD	Luca Lutterotti, G.N.R. Analytical Instr., Italstructures X-ray Division, and University of Trento, Riva del Garda, Italy
Contributed	PROTEIN MEASUREMENT ON LABORATORY POWDER DIFFRACTOMETER	Detlef Beckers, PANalytical, Almelo, The Netherlands
Contributed	CLOSE CONTACT PENALTY FUNCTIONS IN DIRECT SPACE METHODS AND ENERGETIC CONSIDERATIONS IN STRUCTURE REFINEMENT	Carlota Conesa-Moratilla, Accelrys Ltd, Cambridge, UK

Complementary Techniques (DSC, TGA, Hot Stage Microscopy, FTIR, Raman, NMR, SEM, AFM, Light Microscopy, XRF, SAXS, SANS)		
Session Chair: Dr. John Faber, International Centre for Diffraction Data, Newtown Square, PA, USA		
Type	Title of Paper	Speaker & Affiliation
Invited	HOW HIGH-RESOLUTION X-RAY POWDER DIFFRACTION SHOULD HELP THE CONSTRUCTION OF TOPOLOGICAL p-T DIAGRAMS LEADING TO THE STABILITY HIERARCHY OF POLYMORPHS	René Céolin, Université René Descartes, Paris, France
Contributed	THE SEARCH FOR POLYMORPHS AND SALTS USING HIGH THROUGHPUT POWDER DIFFRACTION, SPECTROSCOPY AND OTHER TECHNIQUES	Chris Gilmore, University of Glasgow, Glasgow, Scotland, UK
Contributed	POLYMORPH SCREENING: A COMPARISON BETWEEN XRPD AND COMPLEMENTARY TECHNIQUES SUCH AS SOLID STATE NMR, RAMAN AND DSC	Peter van Hoof, Organon NV, Oss, The Netherlands
Contributed	EXAMPLES OF COMPLEMENTARY STUDIES OF THE METASTABLE POLYMORPHS OF PHARMACEUTICALS BY X-RAY POWDER DIFFRACTION, HOT-STAGE MICROSCOPY, THERMAL ANALYSIS AND CALORIMETRY	Elena Boldyreva, Novosibirsk State University, and Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia
Contributed	PHARMACEUTICAL SOLID-STATE CHARACTERIZATION BY SIMULTANEOUS SMALL-AND WIDE-ANGLE X-RAY SCATTERING	Peter Laggner, Austrian Academy of Sciences, Graz, Austria

Thursday, February 24

Patent and Regulatory Issues		
Session Chair: Dr. Julien Giovannini, AstraZeneca R&D, Lund, Sweden		
Type	Title of Paper	Speaker & Affiliation
Invited	A PATENT PRIMER FOR THE PHARMACEUTICAL SCIENTIST	Eyal Barash, Finnegan, Henderson, Farabow, Garrett and Dunner, LLP, Washington, D.C., USA
	ROUND ROBIN XRD	
	Q+A/CLOSING REMARKS	