## Programme of the 13th Bologna's convention on Crystal Forms - CF@Bo n. 13 University of Bologna 7-9 September 2025

|             | SUNDAY 7 September  | Aula Prodi Complesso di San Giovanni in Monte<br>University of Bologna  | Abstract |
|-------------|---|---|----------|
| 11:30-14:00 | REGISTRATION  |   |          |
| 13:45-14:00 | Chairing Dario Braga Department of Chemistry G. Ciamician, University of Bologna                                      | Opening of the convention   |          |
| 14:00-14:30 | Fabrizia Grepioni Department of Chemistry G. Ciamician, University of Bologna   | Crystal Forms @ Bo  | 01       |
| 14:30-15:00 | Alfred Lee MSD Research Laboratories Rahway, New Jersey 07065, USA  | Solid Form Discovery: Past, Present and Future.   | 02       |
| 15:00-15:30 | Philippe Fernandes Associate Director at Johnson and Johnson  | Key Insights from Computational Tools in Solid-State Pharmaceutical Development                                   | О3       |
| 15:30-16:00 | Franziska Emmerling Federal Institute for Materials Research and Testing (BAM) Department Materials Chemistry, Berlin | Real-Time Monitoring and Temperature Control for<br>Optimized Polymorph Engineering                               | 04       |
| 16:00-16:30 | Ivo B. Rietveld SMS Laboratory University of Rouen, Normandy, France  | Preparation and stabilisation of metastable polymorphs for the improvement of API bioavailability.                | O5       |
| 16:30-17:00 | Coffee break  |   |          |
|             | Chairing Teresa Duarte Istituto Superior Técnico, Lisbon, Portugal  |   |          |
| 17:00-17:30 | Gareth Williams  Department of Chemistry, University College London, UK   | Accessing new polymorphs via solid solutions  | 06       |
| 17:30-18:00 | Helen Wheatcroft  APS Crystallisation Scientist, AstraZeneca, UK  | Crystallisation and Particle Control of a Multi-<br>component API Crystal Form: From Structure to Process         | 07       |
| 18:00-18:30 | Elena Simone Department of Applied Science and Technology (DISAT) Politecnico di Torino, Torino, Italy                | Can crystal engineers make food? A few examples of crystallization strategies for the design of food formulations | 08       |
| 18:30-19:00 | Gerard Coquerel Laboratoire Sciences et Méthodes Séparatives, University of Rouen, France                             | Interferences between Polymorphism and Solid Solutions  | 09       |

| 19:00       | Aperif in the courtyard                                       | Complesso di San Giovanni in Monte - University of Bologna |     |
|-------------|---|--|-----|
|             | MONDAY 8 September  | Hotel Aemilia  |     |
|             | Chairing Ghazala Sadiq  |  |     |
|             | Senior Scientist, Cambridge Crystallographic Data Centre, UK  |  |     |
| 8:30-9:00   | Jon Steed   | Crystals as Intellectual Property                          | 010 |
| 0.00.0.20   | Department of Chemistry, Durham University, Durham, UK        |  | 011 |
| 9:00-9:30   | Susan Reutzel-Edens   | Turning polymorph challenges into patent opportunities     | 011 |
| 0.00.10.00  | SuRE Pharma Consulting, LLC, Zionsville, Indiana, USA         |  | 040 |
| 9:30-10:00  | Vania André   | Unlocking New Antibiotic Forms: Crystal Engineering        | 012 |
|             | IMS Researcher at CQE-IMS, Istituto Superior Técnico, Lisbon, | and Supramolecular Strategies for Polymorphs,              |     |
|             | Portugal  | Cocrystals, and Beyond                                     |     |
| 10:00-10:30 | Coffee break  |  |     |
|             | Chairing Susan Bourne   |  |     |
|             | University of Cape Town, South Africa                         |  |     |
| 10:30-11:00 | Sarah (Sally) Price   | Pharmaceutical Digital Design: Can we go from              | 013 |
|             | Department of Chemistry, University College London, UK        | Chemical Structure through Crystal Polymorph to            |     |
|             |   | Conceptual Crystallization Process?                        |     |
| 11:00-11:30 | Marcus A. Neumann   | A conceptual framework for the crystallizability of        | 014 |
|             | CEO Avant-garde Materials Simulation Deutschland GmbH,        | organic compounds  | GS1 |
|             | Merzhausen, Germany   |  |     |
| 11:30-12:00 | Doris Braun   | Hybrid Approaches in Solid Form Design: Virtual            | 015 |
|             | Institute of Pharmacy, Christian Doppler Laboratory for       | Screening and Experimental Validation                      |     |
|             | Advanced Crystal Engineering Strategies in Drug Development,  |  |     |
|             | University of Innsbruck, Austria                              |  |     |
| 12:00-12:30 | Joost van den Ende  | Machine Learning within CSP: from one crystal energy       | 016 |
|             | Roche Pharma Research and Early Development, Therapeutic      | landscape to another                                       |     |
|             | Modalities, Basel, Switzerland                                |  |     |
| 12:30-13:00 | Rajni Miglani Bhardwaj  | An integrated approach combining experimental and          | 017 |
|             | Associate research Fellow at Pfizer, New London County,       | computational for solid form design and selection          |     |
|             | Connecticut, USA  |  |     |
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| Poster session   |   | 1  |
|--|---|--|
|  | See conference booklet  | P 1-50   |
| Coffee break and poster session  |   |  |
| Chairing Matteo Daldosso PolyCrystalLine Spa, Medicina, Italy                                    | GOLD sponsor oral presentations   |  |
| Gustavo Santiso-Quinones ELDICO Scientific AG, Allschwil, Switzerland                            | Crystallographic Landscape of Electron Diffraction: Novel Applications for the Pharma and Agrochemical Industry   | GS2  |
| Natalia Dadivanyan  Marketing Manager Pharma & Food Sector Malvern Panalytical Palaiseau, France | Discovering solid forms: new amorphous and crystalline polymorphic forms of sodium naproxen   | GS3  |
| Roman Maag   | Efficient Tools for Solid-State Research  | GS4  |
| Guangxu Sun Executive Director of Solid State Business XtalPi Boston, USA                        | The Synergy of Computation and Experiment in Solid-<br>State R&D  | GS5  |
| Chairing Bill Jones Department of Chemistry, the University of Cambridge, UK                     |   |  |
| Arnaud Grandeury Novartis Leading Scientist, Novartis Pharma AG, Novartis Basel Switzerland      | Solid Form Matters: Microenvironmental Influences on API Stability in Drug Products   | O18  |
| <b>Delia A. Haynes</b> Stellenbosch University, South Africa                                     | Co-crystals, salts and sublimation  | 019  |
| Thomas Rades and Inês Martins Department of Pharmacy Faculty of Health and Medical               | Amorphous forms of drugs: from preparation to polyAmorphism   | O20  |
| Amy Woods-Ryan Durham University (PhD student) and GSK (Investigator), UK                        | HEPES of conformational, multi-zwitterionic polymorphs  | 021  |
|  | Chairing Matteo Daldosso PolyCrystalLine Spa, Medicina, Italy Gustavo Santiso-Quinones ELDICO Scientific AG, Allschwil, Switzerland  Natalia Dadivanyan Marketing Manager Pharma & Food Sector Malvern Panalytical Palaiseau, France Roman Maag Technobis Crystallization Systems Alkmaar, The Netherlands Guangxu Sun Executive Director of Solid State Business XtalPi Boston, USA  Chairing Bill Jones Department of Chemistry, the University of Cambridge, UK Arnaud Grandeury Novartis Leading Scientist, Novartis Pharma AG, Novartis Basel Switzerland Delia A. Haynes Stellenbosch University, South Africa Thomas Rades and Inês Martins Department of Pharmacy Faculty of Health and Medical Sciences University of Copenhagen, Denmark Amy Woods-Ryan | Chairing Matteo Daldosso PolyCrystalLine Spa, Medicina, Italy  Gustavo Santiso-Quinones ELDICO Scientific AG, Allschwil, Switzerland  Natalia Dadivanyan Marketing Manager Pharma & Food Sector Malvern Panalytical Palaiseau, France Roman Maag Technobis Crystallization Systems Alkmaar, The Netherlands Guangxu Sun Executive Director of Solid State Business XtalPi Boston, USA  Chairing Bill Jones Department of Chemistry, the University of Cambridge, UK Arnaud Grandeury Novartis Leading Scientist, Novartis Pharma AG,Novartis Basel Switzerland Delia A. Haynes Stellenbosch University, South Africa Thomas Rades and Inês Martins Department of Pharmacy Faculty of Health and Medical Sciences University of Copenhagen, Denmark Amy Woods-Ryan Durham University (PhD student) and GSK (Investigator), UK |

|             | TUESDAY 9 September  | Hotel Aemilia   |            |
|-------------|--|---|------------|
|             | Chairing Lucia Maini Department of Chemistry G. Ciamician, University of Bologna   |   |            |
| 8:30-9:00   | Anna Slater Department of Chemistry and Materials Innovation Factory, University of Liverpool, UK                                  | Continuous flow chemistry as a tool for crystallisation of porous organic materials   | O22        |
| 9:00-9:30   | Edyta Pindelska Department of Pharmaceutical Chemistry and Biomaterials, Medical, University of Warsaw, Poland                     | Mechanisms of Cocrystal Formation and Coformer Exchange in Ethenzamide Systems – From <i>In Situ</i> Studies to Pharmaceutical Applications | O23        |
| 9:30-10:00  | Matteo Daldosso Chief Scientific and Innovation Officer at PolyCrystalLine, Medicina, Italy  | API: Don't Forget the I. From the Right Molecule to the Right Particle  | O24<br>GS6 |
| 10:00-10:30 | Stephanie Terruzzi Chemessentia Srl (part of Chemo group), Novara, Italy   | Challenges in crystallization scale-up of an API nanocrystalline form   | O25        |
| 10:30-11:00 | Coffee break   |   |            |
|             | Chairing Alessia Bacchi Department of Chemistry, University of Parma   |   |            |
| 11:00-11:30 | Joop ter Horst Tiofarma BV, Oud-Beijerland, Netherlands  | Optimizing complex multicomponent solid form discovery & crystallization process design   | O26        |
| 11:30-12:00 | Irene Bassanetti Senior Scientist in Analytics and Early Formulation Department, Preclinical R&D Chiesi Farmaceutici, Parma, Italy | The Critical Role of 3D Molecular and Biomolecular Structures in Innovative Drug Discovery  | 027        |
| 12:00-12:30 | Martin Viertelhaus Principal Scientist BASF SE - Analytical and Material Science   | Solubility – Easy Parameter with Hurdles in<br>Determination and Interpretation   | O28        |
| 12:30-13:00 | Matteo Lusi Dept of Chemical Science & Bernal Institute, University of Limerick, Ireland   | Crystalline Solutions for Pharmaceutical Problems   | <b>O29</b> |
| 13:00-14:00 | Lunch  |   |            |
|             |  |   |            |

|             | Chairing Simone d'Agostino  |   |     |
|-------------|---|---|-----|
|             | Department of Chemistry G. Ciamician, University of Bologna   |   |     |
| 14:00-14:30 | Luc Aerts Head Solid State Development Sciences, UCB Pharma, Belgium  | Co-crystallisation as a versatile tool in pharmaceutical development  | O30 |
| 14:30-15:00 | Pietro Sacchi Research and Application Scientist, The Cambridge Crystallographic Data Centre, UK                                | Computational approaches for the prediction of particle properties of organic molecular materials.            | 031 |
| 15:00-15:30 | Joe Lubach Distinguished Scientist at Genentech, Inc., department of Synthetic Molecule Pharmaceutics, South San Francisco, USA | Insights into Pharmaceutical Drug Substance and Product Using Multinuclear Solid-State NMR Spectroscopy       | 032 |
| 15:30-16:00 | Helen Blade Principal Scientist - Solid State Computational Pharmaceutics, AstraZeneca, Cambridge, UK                           | Connecting API to product   | O33 |
| 16:00-16:30 | Coffee break and Poster Prizes  |   |     |
| 16:30-17:30 | NICE event: Nature Inspired Crystal Engineering Chairing Fabrizia Grepioni  | Dissemination event of the PRIN 2020 project  |     |
| 16:30-16:45 | Alessia Bacchi University of Parma  | A NICE PoEM: cocrystals from liquid ingredients   | 034 |
| 16:45-17:00 | Giuseppe Resnati Polytechnic of Milan   | Pharmaceutical cocrystals via halogen bond  | O35 |
| 17:00-17:15 | Michele Remo Chierotti University of Torino   | Advanced Solid-State NMR tools for Crystal Engineering: From Structure Elucidation to Phase Purity Assessment | O36 |
| 17:15-17:30 | Pavel Zolotarev University of Milan   | Study of pillared MOFs with Zn-paddlewheel state switching  | O37 |
| 17:30       | Dario Braga   | Closing remarks   |     |

We are grateful to ELDICO, XTALPI, Avant-Garde, TECHNOBIS, Malvern Panalytical, Schrödinger and PolyCrystalLine for sponsoring the convention, and to the journals CrystEngComm and RSC Mechanochemistry for sponsoring poster prizes. We also gratefully acknowledge the companies UCB, GENENTECH, Pfizer and Roche and the Italian crystallographic association AIC for financing the registration of young participants.



























