

## The 13th Conference of the Asian Crystallographic Association

05th - 08th Dec 2015 | Science City, Kolkata, India

## **Conference Program**





International Union of Crystallography



Indian Crystallographic Association



|                      | Plenary Speakers                                                                                                                                                  |  |  |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| Day-1,<br>December 5 | <b>Petra Fromme,</b> Arizona State University, USA "Serial femtosecond crystallography: The dawn of a new era in structural Biology" #PL-1                        |  |  |
| Day-2,<br>December 6 | Mohamed Eddaoudi, King Abdullah University of Science and Technology, Saudi Arabia "Metal-organic frameworks from design strategies to applications" #PL-2        |  |  |
| Day-3,<br>December 7 | <b>Kenneth Harris,</b> Cardiff University, UK "New experimental techniques for exploring crystallization pathways and structural properties of solids"#PL-3       |  |  |
| Day-4,<br>December 8 | Mamannamana Vijayan, Indian Institute of Science, Bangalore, India<br>"Structural diversity and ligand specificity in lectins. From plants to Mycobacteria" #PL-4 |  |  |
|                      | Keynote Speakers                                                                                                                                                  |  |  |
| Day-2,<br>December 6 | Michelle Dunstone, Monash University, Australia "Packing a giant punch: The MACPF/CDC pore forming protein superfamily" #KN-1                                     |  |  |
| Day-2,<br>December 6 | Sue-Lein Wang, National Tsing Hua University, Taiwan "Recent developments and prospects in porous inorganic framework materials" #KN-2                            |  |  |
| Day-2,<br>December 6 | Michi Suga, Okayama University, Japan "Mechanism of photosynthetic water-splitting based on the atomic structure of photosystem II" #KN-3                         |  |  |
| Day-4,<br>December 8 | <b>Haitao Li,</b> Tsinghua University, China "Mark the "readership" for transcription control" #KN-4                                                              |  |  |
| Day-4,<br>December 8 | Parimal Bharadwaj, Indian Institute of Technology Kharagpur, India "Studies on metal organic frameworks through chemical crystallography" #KN-5                   |  |  |

| Lunch Time Meetings  |                                                                                                                                         |  |  |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------|--|--|
| Day-2,<br>December 6 | AsCA Council Meeting (only for Council Members)                                                                                         |  |  |
| Day-3,<br>December 7 | <b>Mitchell Guss:</b> New initiatives of IUCr Commission on Biological Macromolecules (for macromolecular crystallography participants) |  |  |
| Day-4,<br>December 8 | Meeting of the International Program Committee for AsCA 2016                                                                            |  |  |
|                      | Evening Programs                                                                                                                        |  |  |
| Day-1,<br>December 5 | Welcome Mixer & Cultural Program                                                                                                        |  |  |
| Day-2,               | Roger Durst (Bruker)                                                                                                                    |  |  |
| December 6           | Dr. Ashwani Kumar (BARC, India)                                                                                                         |  |  |
| Day-2,<br>December 6 | Dinner (Sponsored by Bruker)                                                                                                            |  |  |

|               | DAY-1: SATURDAY, DECEMBER 5, 2015                                                                                                             |  |  |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------|--|--|
|               | Registration                                                                                                                                  |  |  |
| 09:00 - 18:00 | Pre-Function Area, Main Hall                                                                                                                  |  |  |
|               | Crystallographic Software Session I                                                                                                           |  |  |
| 10:00 - 12:00 | Main Hall                                                                                                                                     |  |  |
| Chair:        | K. Suguna, Indian Institute of Science, Bangalore, India                                                                                      |  |  |
| 30 minutes    | Pavel Afonine, Lawrence Berkeley National Lab, USA "Structure refinement and validation tools in Phenix" #CS-1                                |  |  |
| 30 minutes    | <b>Sanotsh Panjikar,</b> Australian Synchrotron, Australia "Automated crystal structure determination using multiple data sets" #CS-2         |  |  |
| 30 minutes    | Jon Agirre, CCP4, York University, UK "CCP4i2: a new graphical interface for the CCP4 suite" #CS-3                                            |  |  |
| 30 minutes    | <b>Thomas Terwilliger,</b> Los Alamos National Laboratory, USA "X-ray structure determination using weak anomalous data" #CS-4                |  |  |
|               | Crystallographic Software Session II                                                                                                          |  |  |
| 10:00 - 12:00 | Hall-1                                                                                                                                        |  |  |
| Chair:        | Brendan Kennedy, University of Sydney, Australia                                                                                              |  |  |
| 30 minutes    | <b>Dylan Jayatilaka,</b> University of Western Australia, Australia "CrystalExplorer and the Tonto library for quantum crystallography" #CS-5 |  |  |

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| 30 minutes    | Benoit Guillot, Universite de Lorraine, France                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |  |  |
|               | "The MoPro software package for electron density analysis of small compounds and biological macromol-                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |  |  |
|               | ecules" #CS-6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |  |  |
| 30 minutes    | Horst Pushmann, Durham University, UK                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |  |  |
|               | "The many faces of Olex2" #CS-7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |  |  |
| 30 minutes    | Max Avdeev, Australian Nuclear Science and Technology Organisation, Australia                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |  |  |
|               | "Recent trends in neutron powder diffraction data analysis software" #CS-8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |  |  |
|               | Lunch                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |  |  |
| 12:00 - 14:00 | Food Court                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |  |  |
|               | Opening Ceremony                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |  |  |
| 14:00 - 14:30 | Main Hall                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |  |  |
|               | Plenary Session - I                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |  |  |
| 14:30 - 15:30 | Main Hall                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |  |  |
| Chair:        | Gautam Desiraju, Indian Institute of Science, Bangalore, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |  |  |
| Speaker:      | Petra Fromme, Arizona State University, USA                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |  |  |
|               | "Serial femtosecond crystallography: The dawn of a new era in structural biology" #PL-1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |  |  |
| Afternoon Tea |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |  |  |
| 15:30 - 16:00 | Pre Function Area, Main Hall                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |  |  |

|                                                        | General Interest Session - Pharmaceuticals                                                            |  |
|--------------------------------------------------------|-------------------------------------------------------------------------------------------------------|--|
| 16:00 - 18:00                                          | Main Hall                                                                                             |  |
| Co-Chairs:                                             | Ashwini Nangia, University of Hyderabad, India                                                        |  |
|                                                        | <b>Srinivasulu Aitipamula,</b> Institute of Chemical and Engineering Sciences A*STAR, Singapore       |  |
| 30 minutes                                             | <b>Tong-Bu Lu</b> , Sun Yat-Sen University, China                                                     |  |
|                                                        | "The improvement of unfavorable physicochemical properties of APIs via pharmaceutical cocrystals"     |  |
|                                                        | #GIS-1                                                                                                |  |
| 30 minutes                                             | Parthasarathi Dastidar, Indian Association for the Cultivation of Science, Kolkata, India             |  |
|                                                        | "Pharmaceutical gels: A crystal engineering approach towards developing drug delivery systems" #GIS-2 |  |
| 30 minutes                                             | <b>Peter Czabotar,</b> Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia      |  |
|                                                        | "Targeting cell death pathway proteins with small molecule therapeutics" #GIS-3                       |  |
| 30 minutes                                             | Colin Groom, Cambridge Crystallographic Data Centre, UK                                               |  |
|                                                        | "Structural chemistry in drug design: Affinity, properties and solubility" #GIS-4                     |  |
| Welcome Mixer & Cultural Program (by Tanusree Shankar) |                                                                                                       |  |
| 18:00 – 20:00                                          | Mini Hall                                                                                             |  |

|                    | DAY-2: SUNDAY, DECEMBER 6, 2015                                                                                                                                     |  |
|--------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| Plenary Session II |                                                                                                                                                                     |  |
| 09:00 - 10:00      | Mini Hall                                                                                                                                                           |  |
| Chair:             | Yuji Ohashi, Tokyo Institute of Technology, Japan                                                                                                                   |  |
| Speaker:           | Mohamed Eddaoudi, King Abdullah University of Science and Technology, Saudi Arabia "Metal-organic frameworks from design strategies to applications" #PL-2          |  |
|                    | Morning Coffee                                                                                                                                                      |  |
| 10:00 - 10:30      | Pre Function Area, Mini Hall                                                                                                                                        |  |
|                    | Microsymposium 1 – Membrane Proteins                                                                                                                                |  |
| 10:30 - 12:30      | Mini Hall                                                                                                                                                           |  |
| Co-Chairs:         | Jacqui Gulbis, Walter and Eliza Hall Institute of Medical Research, Australia Rajesh Ghai, University of New South Wales, Australia                                 |  |
| 30 minutes         | Arun Shukla, Indian Institute of Technology, Kanpur, India "Structural insights in to GPCR-arrestin interaction" #MS1-1                                             |  |
| 30 minutes         | Janesh Kumar, National Centre For Cell Science, Pune, India "The twists and turns of glutamate receptor activation and desensitization" #MS1-2                      |  |
| 20 minutes         | Alice Vrielink, University of Western Australia, Australia<br>"Combating multidrug resistance in Neisseria: Structure of an endotoxin modifying enzyme" #MS1-3      |  |
| 20 minutes         | Adeline Robin, Walter and Eliza Hall Institute of Medical Research, Australia "Direct activation and structural insights into the pro-apoptotic protein Bax" #MS1-4 |  |

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| 20 minutes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Chacko Jobichen, National University of Singapore, Singapore                                              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | "Structure of AcrH-AopB chaperone-translocator complex reveals a role for membrane-hairpins in type III   |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | secretion system translocon assembly" #MS1-5                                                              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Microsymposium 2 – Engineering of Crystalline and Non-Crystalline Solids                                  |
| 10:30 - 12:30                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Hall-1                                                                                                    |
| Co-Chairs:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Kumar Biradha, Indian Institute of Technology, Kharagpur, India                                           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | <b>Peng Cheng,</b> State Key Lab, Nankai U. China                                                         |
| 30 minutes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Kazuki Sada, Hokkaido University, Japan                                                                   |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | "Crystal crosslinking of metal-organic frameworks as the third kind of crystalline polymerization"        |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | #MS2-1                                                                                                    |
| 30 minutes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | <b>J. Narasimha Moorthi,</b> Indian Institute of Technology, India                                        |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | "De novo approaches to the development of crystalline porous materials (MOFs) and amorphous organic       |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | light emitting diodes (OLEDs)" #MS2-2                                                                     |
| 20 minutes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Suryanarayan Cherukuvada, Indian Institute of Science, India                                              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | "On the headaches of resolving a low melting combination as a definite eutectic or an elusive cocrystal", |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | #MS2-3                                                                                                    |
| 20 minutes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Partha Jana, Indian Institute of Technology, India                                                        |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | "Structure determination of ?-brass related composite structures by a (3+1)-dimensional space descrip-    |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | tion"#MS2-4                                                                                               |
| 20 minutes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | lan Williams, Hong Kong University of Science and Technology, Hong Kong                                   |
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| Microsymposium 3 – Diffraction Imaging and XFELS                     |                                                                                                 |  |
|----------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|--|
| 10:30 - 12:30                                                        | Hall-2                                                                                          |  |
| Co-Chairs:                                                           | Yoshinori Nishino, Hokkaido University, Japan                                                   |  |
|                                                                      | <b>Changyong Song,</b> Pohang University of Science and Technology, Korea                       |  |
| 30 minutes                                                           | Kensuke Tono, Japan Synchrotron Radiation Research Institute, Japan                             |  |
|                                                                      | "Imaging and crystallography platforms at SACLA" #MS3-1                                         |  |
| 30 minutes                                                           | <b>Kyung Hwan Kim,</b> Korea Advanced Institute of Science and Technology, Korea                |  |
|                                                                      | "Capturing the formation of chemical bond with femtosecond X-ray solution scattering" #MS3-2    |  |
| 20 minutes                                                           | Shin-ichi Adachi, High Energy Accelerator Research Organization (KEK), Japan                    |  |
|                                                                      | "Visualizing bond formation in solution with femtosecond X-ray scattering" #MS3-3               |  |
| 20 minutes                                                           | Daewoong Nam, Pohang University of Science and Technology, Korea                                |  |
|                                                                      | "Fixed target single-shot imaging of nanostructures using thin solid membranes at SACLA" #MS3-4 |  |
| 20 minutes                                                           | Yoshinori Nishino, Hokkaido University, Japan                                                   |  |
|                                                                      | "Live cell nano-imaging free from radiation damage by using X-ray free-electron laser", #MS3-5  |  |
| Lunch                                                                |                                                                                                 |  |
| 12:30 - 13:30                                                        | Food Court                                                                                      |  |
| Lunch Time Meeting - AsCA Council Meeting (only for Council Members) |                                                                                                 |  |
| 12:30 - 13:30                                                        | Board Room                                                                                      |  |

|               | Microsymposium 4 – Macromolecular Complexes and Assemblies                                                                                                                                 |  |
|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| 13:30 - 15:30 | Mini Hall                                                                                                                                                                                  |  |
| Co-Chairs:    | Jayaraman Sivaraman, National University of Singapore, Singapore Satoshi Murakami, Tokyo Institute of Technology, Japan                                                                    |  |
| 30 minutes    | Yonggui Gao, Nanyang Technological University, Singapore "Structural insight into translational GTPase in protein synthesis and its regulation" #MS4-1                                     |  |
| 30 minutes    | <b>Udo Heinemann</b> , Max Delbruck Center for Molecular Medicine, Berlin, Germany "Structural and biochemical studies of adaptor protein binding to AAA ATPases: p97 and CDC48" #MS4-2    |  |
| 20 minutes    | Michi Suga, Photosynthesis Research Center, Okayama University, Japan "Structural basis for energy transfer pathways in the plant PSI-LHCI supercomplex" #MS4-3                            |  |
| 20 minutes    | <b>Kakoli Bose</b> , ACTREC, Tata Memorial Centre, Kharghar, India "Molecular basis of DISC assembly and procaspase-8 activation in a novel adaptor-independent cell death pathway" #MS4-4 |  |
| 20 minutes    | <b>Veendra Kumar</b> , Institute of Molecular and Cell Biology, Singapore "Structure of ribosome bound to BipA" #MS4-5                                                                     |  |
|               | Microsymposium 5 – Structure and Properties of Functional Materials                                                                                                                        |  |
| 13:30 - 15:30 | Hall-1                                                                                                                                                                                     |  |
| Co-Chairs:    | Rahul Banerjee, CSIR-National Chemical Laboratory, India David Turner, Monash University, Australia                                                                                        |  |
| 30 minutes    | C. Malla Reddy, Indian Institute of Science Education and Research, India "Understanding mechanically reconfigurable organic single crystals" #MSS-1                                       |  |

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| Chris Sumby, University of Adelaide, Australia  Matrix isolation in MOFs: towards catalysis by understanding reactivity" #MSS-2  Neeraj Sharma, University of New South Wales, Australia  Using in situ synchrotron X-ray diffraction to understand the Na insertion/extraction reactions in the la <sub>3</sub> V <sub>2</sub> O <sub>3</sub> x(PO <sub>4</sub> )2F <sub>3-3x</sub> family" #MSS-3  Prasado Rao, National University of Singapore, Singapore  "Ion migration pathway studies in lithium based compounds for rechargeable batteries" #MSS-4 |
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| Using in situ synchrotron X-ray diffraction to understand the Na insertion/extraction reactions in the $(a_sV, O_sx(PO_a)2F_{3.2x}$ family" #MS5-3 Prasado Rao, National University of Singapore, Singapore                                                                                                                                                                                                                                                                                                                                                 |
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| Debrati Das, Indian Institute of Technology, Kharagpur, India<br>Structural Adaptation of Ni <sub>2</sub> O <sub>4</sub> units to form cubane, open Dicubane, dimeric cubane, and one-dimen-<br>ional polymeric cubanes: Magnetostructural Correlation of Ni <sub>4</sub> Clusters" #MS5-5                                                                                                                                                                                                                                                                  |
| ymposium 6 – Synchrotron and Neutron Sources, Instrumentation and Application                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| lall-2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Richard Garrett, Australian Synchrotron, Australia<br>e-Geun Park, Seoul National University, Korea                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Di-Jing Huang, National Synchrotron Radiation Research Centre, Taiwan<br>Scientific opportunities of a low-emittance synchrotron light source‴ #MS6-1                                                                                                                                                                                                                                                                                                                                                                                                       |
| Takashi Kamiyama, J-PARC Center & Neutron Science Laboratory (KEK), Japan  Current and future of crystallography with high intensity neutron beams" #MS6-2                                                                                                                                                                                                                                                                                                                                                                                                  |
| iji Nishibori, University of Tsukuba, Japan<br>Structural studies using multiple powder diffraction dataset" #MS6-3                                                                                                                                                                                                                                                                                                                                                                                                                                         |
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| 20 minutes    | Suman Mandal, Shiv Nadar University, India                                                                                                                                                                                 |
|               | "Scanning the resolution limit in neutron protein crystallography" #MS6-4                                                                                                                                                  |
| 20 minutes    | Stefan Brandstetter & Clemens Schulze-Briese, Dectris Ltd, Switzerland "Novel Hybrid Photon Counting detectors for advanced X-ray studies" #MS6-5                                                                          |
|               | Afternoon Tea                                                                                                                                                                                                              |
| 15:30 - 16:00 | Pre Function Area, Mini Hall                                                                                                                                                                                               |
|               | Poster Session - I                                                                                                                                                                                                         |
| 16:00 - 17:15 | Poster Hall-1                                                                                                                                                                                                              |
| MS1           | Manish Kesherwani, University of Madras, India "Identification of novel natural inhibitor for NorM - A multidrug and toxic compound extrusion transporter-An in silico molecular modeling and simulation studies" #MS1-PS1 |
| MS1           | Jebastin T, Bharathiar University, India "Invitro and insilico studies on integral membrane protein complexes involved in virulence and survival of enteric Gram negative bacterium" #MS1-PS2                              |
| MS1           | Arul Amal Dass, Madurai Kamaraj University, India "Modelling and structural characterization of outer membrane adhesion protein t2544 from s. typhi" #MS1-PS3                                                              |
| MS1           | <b>Prabu Manoharan,</b> Madurai Kamaraj University, India "Computational profiling of channel forming outer membrane proteins (OMPs)" #MS1-PS4                                                                             |

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| MS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Rajabrata Bhuyan, University of Kalyani, India "Conformational dynamics of Shaker-Type Kv1.1 ion channel in open, closed, and two mutated states" #MS1-PS5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| MS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | <b>Takashiro Akitsu,</b> Tokyo University of Science, Japan<br>"Linearly polarized light-induced anisotropic orientation of binuclear Ni(II), Cu(II) and Zn(II) schiff base complexes and methyl orange in PVA" #MS2-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Suresh Kuthuru, University of Hyderabad, India "Pharmaceutical cocrystals of nitazoxanide: solubility, stability and bioavailability studies" #MS2-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| MS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Avishek Dey, Indian Institute of Technology, Kharagpur, India "Cocrystals and salts of pyridine-3,5-bis(1-methyl-benzimidazole-2-yl) with pyromellitic acid: aromatic guest inclusion and separation via benzimidazole-carboxylic acid heterosynthon" #MS2-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
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| MS2 | Subhankar Saha, Indian Institute of Science, Bangalore, India<br>"Graded Ir-filters for supramolecular synthons: distinguishing different geometries of same interaction"<br>#MS2-PS8                                |
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| MS2 | <b>Jian Gong Ma,</b> Nankai University, China "Solvent-free conversion of CO <sub>2</sub> with a Cu cluster under ambient conditions" #MS2-PS9                                                                       |
| MS2 | Jarugu Narasimha Moorthy, Indian Institute of Technology, Kanpur, India "De novo approaches to the development of crystalline porous materials (MOFs) and amorphous organic light emitting diodes (OLEDs)" #MS2-PS10 |
| MS3 | Akifumi Higashiura, Institute for Protein Research, Osaka University, Japan "Approaches for coherent X-ray diffraction imaging of Paramecium bursaria chlorella virus-1" #MS3-PS1                                    |
| MS4 | <b>Dileep Vasudevan,</b> Institute of Life Sciences, Bhubaneswar, India "Structural characterization of caseinolytic protease-associated chaperone proteins" #MS4-PS1                                                |
| MS4 | Carman Tse, Osaka University, Japan "Structural analysis of a newly identified polyamine synthase BpsA from Thermococcus kodakarensis" #MS4-PS2                                                                      |
| MS4 | Junso Fujita, Osaka University, Japan "Structural-change mechanism of bacterial cell division protein FtsZ from Staphylococcus aureus" #MS4-PS3                                                                      |
| MS4 | <b>Abdul Ajees Abdul Salam,</b> Manipal University, India "Structural and modelling studies of human As(III) S-adenosylmethionine methyltransferases" #MS4-PS4                                                       |

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| MS4 | <b>Ajit Kumar Singh</b> , Institute of Life Sciences Bhubaneswar, India "Structural and functional characterization of Arabidopsis thaliana FKBP53 - a multi-domain histone chaperone" #MS4-PS13                                                            |
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| MS4 | Saroj Hazari, BGC Trust University Bangladesh, India "Synthesis, characterization and biomedical activities of a new macocyclic ligand and its copper(II) complexes. Crystal and molecular structure of [CuLal(ClO <sub>4</sub> ) <sub>2</sub> ]" #MS4-PS14 |
| MS4 | Sushil Kumar, Institute of Life Sciences, India "Interaction studies of influenza a virus matrix protein M1, with host nucleosomal elements" #MS4-PS15                                                                                                      |
| MS4 | Sayani Sarkar, Bose Institute, India "Monomeric RING E3 RNF13 activates E2 - ubiquitin independent of interaction with additional moieties" #MS4-PS16                                                                                                       |
| MS4 | Pritam Naskar, Bose Institute, India "Structural insights into symbiosis receptor kinase and its gatekeeper substituents" #MS4-PS17                                                                                                                         |
| MS4 | Ruchi Anand, Indian Institute of Technology Bombay, India<br>"Search for molecular tunnels" #MS4-PS18                                                                                                                                                       |
| MS4 | Vengadesan Krishnan, Regional Centre for Biotechnology, India "Successful structure solution for shaft pilin SpaA from Lactobacillus rhamnosus GG using fragmented approach and distant homolog "structural insights into SpaCBA pilus assembly" #MS4-PS19  |
| MS4 | Adaitya Behera, Bose Institute, India "Structural analysis of RING E3 ligase ZNRF1 in complex with the ubiquitin conjugating enzyme, UBE2N" #MS4-PS20                                                                                                       |

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| MS4 | Mahesh Chand, Indian Institute of Science Education and Research, India "Structural and functional characterization of Type ISP restriction-modification enzymes" #MS4-PS21                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| MS4 | Jyoti Baranwal, Indian Institute of Science Education and Research, Pune, India "Structural studies on MgIA, a small GTPase in spatial positioning of Myxococcus xanthus motility complexes" #MS4-PS22                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| MS5 | <b>Nur Ahamad,</b> Shahjalal University of Science and Technology, Bangladesh "Fabrication of nanocomposite consists of $Fe_3O_4$ and silver nanoparticles to engineer efficient photocatalyst and platform for photovoltaic device" #MSS-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS5 | Yong-il Kim, Research Institute of Standards and Science, Korea "Joint structural refinement of X-ray and neutron powder diffraction data on lead magnesium nio- bate-lead titanate" #MSS-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS5 | <b>Wang hay Kan,</b> University of Texas at Austin, USA "First Fe-based Na <sup>+</sup> -ion-cathode with two distinct types of polyanions: Fe <sub>2</sub> P <sub>2</sub> SiO <sub>10</sub> " #MS5-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS5 | <b>Moon-Gun Choi</b> , Yonsei University, Korea "Mechanochemically induced structural transformation from [Ag(dmotz)( $CF_{s}SO_{s}$ )]n to {[Ag(dmotz)]( $CIO_{s}$ } involving anion-? interactions" #MS5-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| MS5 | Chatphorn Theppitak, Naresuan University, Thailand "New family of cadmium(II) and zinc(II) compounds with N-(2'-pyridylmethylene)aniline derivatives: stoichiometry and solvent-controlled syntheses, structures and luminescent properties" #MS5-PS5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| MS5 | <b>Sajal Chandra Mazumdar</b> , Bangladesh University of Engineering and Technology, Bangladesh "Structural, magnetic and dielectric properties of BLFO-NCZFO multiferroic composites" #MSS-PS6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |

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| MS5 | <b>Bablu Das,</b> Bangladesh University of Engineering and Technology, Bangladesh "Structural and magnetic properties of Gd substituted Ni-Cu-Zn ferrites" #MSS-PS7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| MS5 | <b>Yadagiri Karampuri</b> , Indira Ghandhi Centre for Atomic Research, India "Physical properties of DyMn0 <sub>3</sub> with isotrivalent ion ( $Bi^{3+}$ ) substitution at Dy site" #MS5-PS8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| MS5 | Yun-Liang Soo, National Tsing Hua University, Taiwan "Effects-of thermal-annealing-on Co local structures in (Y, Co)-codoped nanoceria probed by XAFS" #MSS-PS9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| MS5 | <b>Takamitsu Yamanaka,</b> Osaka University, Japan "Different electron-phonon interaction inducing structure transition of SrTiO <sub>3</sub> at low temperature and high pressure" #MS5-PS10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| MS5 | Rajashri Urkude, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur, India "X-ray diffraction study of Bi <sub>2-x</sub> Mn <sub>x</sub> Se <sub>2</sub> topological insulators" #MS5-PS11                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS5 | Karabi Nath, Indian Institute of Technology, Kharagpur, India "Metal organic frameworks and coordination polymers in separation science" #MSS-PS12                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| MS5 | <b>Mohammed Kamrul Haque Bhuiyan,</b> Bangladesh "Characterization of Ba1-xSr $_x$ (Fe $_0$ , $Ta_0$ , $y$ 0, $y$ 0, perovskites as Pb free ferroelectric materials" #MS5-PS13                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS5 | <b>Kartik Maity,</b> Indian Institute of Technology, Kharagpur, India "One-dimensional water cages with repeat unit of $(H_2O)_{24}$ resembling pagodane in 3D-coordination polymer: proton conducting and tunable luminescence emission by adsorption of anionic dyes" #MSS-PS14                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |

| MS5 | Manish Kumar Mishra, Indian Institute of Science, India "Designing mechanical properties of molecular crystals" #MSS-PS15                                                                                  |
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| MS5 | Yosuke Nishikawa, Osaka University, Japan "Updated structure of the dynein stalk region from the Mus musculus cytoplasmic dynein." #MS5-PS16                                                               |
| MS5 | MV Reddy, National University of Singapore, Singapore "Application of X-ray powder diffraction technique in the area of advanced energy storage functional materials" #MSS-PS17                            |
| MS5 | <b>Uma Shankar</b> , Indian Institute of Technology, BHU Varanasi, India "Suppression of charge ordering transition in nanocrystalline $La_{\alpha}$ , $Ca_{\alpha}$ , $MnO_{\gamma}$ -ceramics" #MS5-PS18 |
| MS5 | <b>Guofeng Cheng,</b> Shanghai Institute of Ceramics, Chinese Academy of Sciences, China "Effect of lattice parameters variation on magnetization in BiFeO, with Pr, Ba co-doping" #MS5-PS19               |
| MS5 | Nagarajan Veeraputhiran, Indian Institute of Science, India "Oxalic acid cross-linked poly(4-vinlypyridine) microgel for selective dye adsorption" #MS5-PS20                                               |
| MS5 | Linia Tashmim, University of Dhaka, Bangladesh "Synthesis and characterization of cobalt doped mullite type bismuth aluminate" #MS5-PS21                                                                   |
| MS5 | <b>Pradeep Shanbogh</b> , Poornaprajna Institute of Scientific Research, India "Local and average structure of BiREWO <sub>B</sub> ( $RE = Eu$ and $Tb$ ) nano photocatalyst" #MS5-PS22                    |
| MS5 | Prem Prakash, Indian Institute of Technology Bombay, India "High resolution structures of Aspergillus niger glutamate dehydrogenase, an enzyme with unique features" #MS5-PS23                             |

| MS5 | Mohammad Julhash Miah, Bangladesh University of Engineering & Technology, Bangladesh "Structural, microstructural and magnetoelectric effect studies of multiferroic xBST-(1-x)BFDO solid solution" #MS5-PS24                                           |
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| MS5 | Champika Hettiarachchi, University of Peradeniya, Sri Lanka "Crystalline state thermo and photochromic reactivity of a benzospiropyran in a self-assembled 3D honeycomb network of 1,3,5-benzenetricarboxylic acid" #MS5-PS25                           |
| MS5 | <b>Tapas Debnath Debnath,</b> University of Dhaka, Bangladesh "New series of vanadium doped rubidium hexagonal tungsten bronze, RbxW1-yVy0 <sub>3</sub> " #MS5-PS26                                                                                     |
| MS5 | <b>Takuma Sakata,</b> Yokohama National University, Japan "Solid-state optical properties of 2,5-diamino-3,6-dicyanopyrazine dyes with small alkyl substituents on the amino groups" #MSS-PS27                                                          |
| MS5 | Akhilesh Kumar Singh, School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), India "Investigation of structure-property correlations in multifunctional ceramics and multiferroic composites" #MS5-PS28 |
| MS5 | <b>Duong Huyen</b> , Hanoi University of Science and Technology, Vietnam "Effect of TiO <sub>2</sub> size and polymorph on properties of PPy/TiO <sub>2</sub> nanocomposites" #MSS-PS29                                                                 |
| MS6 | Emil Espes, Excillum, Sweden "Current status of the liquid-metal-jet X-ray source technology" #MS6-PS1                                                                                                                                                  |
| MS6 | Ravindra Singh Solanki, Department of Physics, Tamkang University, Taiwan "Study of the correlations and dynamics of spins in an XY-like spin-glass system (Ni <sub>0.40</sub> Mn <sub>0.60</sub> )TiO <sub>3</sub> " #MS6-PS2                          |

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| MS6 | <b>Ono Shoki,</b> Nagoya Institute of Technology, Japan "Evaluation of crystallite size from synchrotron powder diffraction data collected with a flat two-dimensional X-ray detector" #MS6-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| MS6 | Shih-Lin Chang, National Synchrotron Radiation Research Center, Taiwan "Single-mode hard X-ray monochromator using crystal cavity resonance" #MS6-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| MS6 | <b>Dae-Woong Kim,</b> Pohang University of Science and Technology, Korea "Introduction of the supramolecular crystallography beamline (BL2D-SMC) at the Pohang Light Source II, Korea" #MS6-PS5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| MS6 | <b>Takashi Ida,</b> Nagoya Institute of Technology, Japan "Multiple two-dimensional X-ray detecting system on a powder diffraction beamline BL5S2 at AichiSR" #MS6-PS6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| MS6 | Ashwani Kumar, Bhabha Atomic Research Centre, India "Protein crystallography beamline of indus-2: current status & future plan" #MS6-PS7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS6 | <b>Biplab Ghosh</b> , Bhabha Atomic Research Center, India "Recent development at the PX-BL21 (Indus-2) beamline to facilitate anomalous diffraction experiment" #MS6-PS8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| MS6 | Maurizio Polentarutti, Elettra-Sincrotrone Trieste, Italy "Xpress and XRD2: Indo-Italian scientific partnership for a dedicated high pressure diffraction and macro- molecular crystallography beamlines at Elettra Trieste" #MS6-PS9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| MS6 | Andreas Kleine & Carsten Michaelsen, Incoatec GmbH, Germany "High-brightness-microfocus sources for chemical crystallography" #MS6-PS10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |

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| MS6  | Naohiro Matsugaki, KEK, Japan "Native SAD experiments at the photon factory BL-1A" #MS6-PS11                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| MS13 | <b>Tsutomu Nakamura,</b> National Institute of Advanced Industrial Science and Technology, Japan "Crystal structure and multiple crystal forms of archaeal N,Ndiacetylchitobiose deacetylase" #MS13-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| MS13 | <b>Yasuo Hata,</b> Institute for Chemical Research, Kyoto University, Japan "Structural studies on resorcinol-catabolic enzymes" #MS13-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| MS13 | <b>Subhash Chandra Bihani,</b> Bhabha Atomic Research Centre, India "FrnE is a novel disulfide oxidoreductase system in prokaryotes" #MS13-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS13 | Amit Das, Bhabha Atomic Research Centre, India "Protein kinase A catalytic subunit primed for action through time lapse X-ray crystallography of Michaelis complex formation." #MS13-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS13 | Md. Mahfuzur Rahman, University of Hyogo, Japan "Structural analysis of a periplasmic heme-binding protein in bacterial heme importer system." #MS13-PS5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS13 | Shamayeeta Ray, Indian Institute of Technology Bombay, India "Crystal structure of the phenol binding domain of MopR: a selective aromatic pollutant sensor" #MS13-PS6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| MS13 | Srinivasan Sundararaj, Monash University, Australia "Structural recognition of CD1d-restricted microbial lipid antigen by type II natural killer T cells" #MS13-PS7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

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| MS13 | Manjula R, National Institute of Mental Health and Neurosciences, India "Discovery of novel human SIRT1 inhibitors by in silico screening" #MS13-PS8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| MS13 | Se Won Suh, Seoul National University, Korea, "The cell-shape determining Csd6 from Helicobacter pylori constitutes a new family of L,D-carboxypepti-dase" #MS13-PS9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| MS13 | Vandana Gaded, Indian Institute of Technology Bombay, India "Structure and function determination of an uncharacterized enzyme from Mycobacterium smegmatis of the cytidine deaminase superfamily" #MS13-PS10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| MS13 | Ruchika Bhujbalrao, Indian Institute of Technology Bombay, India "Structural and biochemical studies of ksga methyltransferase from Bacillus subtilis involved in ribosome biogenesis" #MS13-PS11                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| MS13 | Anitha J, Manipal Centre for Virus Research, India "Structural analysis of Influenza A(H1N1)pdm virus with N295T mutation in the catalytic site" #MS13-PS12                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| MS13 | <b>Vitul Jain,</b> International Centre for Genetic Engineering and Biotechnology, India "Structure of prolyl-tRNA synthetase-halofuginone complex provides basis for development of novel drugs against malaria and toxoplasmosis" #MS13-PS13                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS13 | <b>Pavithra G C,</b> Poornaprajna Institute of Scientific Research, India "Functional insights from the structures of purine phosphoribosyltransferases of pathogenic bacteria." #MS13-PS14                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| MS13 | Christopher Squire, University of Auckland, New Zealand "Ripping into racemic crystals; the structure of potato snakin-1" #MS13-PS15                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |

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| MS13 | <b>Hisato Hirano,</b> The University of Tokyo, Japan "Structure-guided engineering of CRISPR-Cas9 PAM specificity" #MS13-PS16                                                                                               |
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| MS13 | Manish Thakur, University of Mysore/Jubilant Biosys Ltd., India<br>"First crystal structure of a novel protein tyrosine kinase6, PTK6 at 2.3Å resolution" #MS13-PS17                                                        |
| MS13 | Jesmita Dhar, Bose Institute, India "Identification of a novel secondary structure, topi" #M513-P518                                                                                                                        |
| MS13 | Yusuke Nakamichi, Laboratory of Supramolecular Crystallography Institute for Protein Research, Osaka University, Japan "The high-resolution X-ray crystal structure of the capping enzyme from rice dwarf virus" #MS13-PS19 |
| MS13 | Faizah AlMalki, Saudi Arabia "Structural studies on Trypanosoma brucei flap endonuclease wilde type (TbFEN-WT)" #MS13-PS20                                                                                                  |
| MS13 | Ishan Rathore, Indian Institute of Technology Bombay, India "Structural and functional studies on activation of histo-aspartic protease (HAP)" #MS13-PS21                                                                   |
| MS13 | Vandana Mishra, Indian Institute of Technology Bombay, India "Understanding the activation mechanism of plasmepsins from Plasmodium falciparum" #MS13-PS22                                                                  |
| MS13 | Shwu-Huey Liaw, National Yang-Ming University, Taiwan "Structural basis of poly(3-hydroxylbutyrate) hydrolysis by PhaZ depolymerase from Bacillas thuringien- sis" #MS13-PS23                                               |

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| MS14 | <b>Shalini Suresh,</b> Chemistry Research Centre, (Affiliated to Kuvempu University) SSMRV Degree College, India "Crystal packing forces steering the assembly of N-salicylidineaniline derivatives into hydrogen bonded supramolecular laces: crystal structures and Hirshfeld surface analysis" #MS14-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| MS14 | <b>Suzanna Ward,</b> Cambridge Crystallographic Data Centre, UK "50 Years of sharing crystal structures" #MS14-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| MS14 | Harjeet Kaur, M. D. University Rohtak, India "Points to ponder in the study of polytypism in MX2 layered compound" #MS14-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| MS14 | Somnath Dey, University of Bayreuth, Germany "Modulation, twinning and crystal structures of Λ-Co(sepulchrate) trinitrate at low temperatures" #MS14-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS14 | <b>Ugin Inbaraj N</b> , National Institute of Technology, Trichy, India "Intermolecular interactions in the solid state of secondary acetaminophen mannich bases" #MS14-PS5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| MS14 | Moshiur Rahman, Jahangirnagar University, Bangladesh "Metal sulfur nitrogen bonded complexes of iron and ruthenium and their X-ray crystal structures" #MS14-PS6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| MS14 | <b>Kunal Jha,</b> Shiv Nadar University, India "Five solvatomorphs of a stilbene derivative: a systematic study of solvent interactions" #MS14-PS7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| MS14 | Hare Ram Yadav, Indian Institute of Science Education and Research Mohali, India "Can weak C-HF hydrogen bond(s) alter the packing features in the presence of strong hydrogen bond: An experimental and computational study on fluorinated amides" #MS14-PS8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |

| MS14 | Debika Datta, Indian Institute of Technology Guwahati, India                                                                                                                                                                  |
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|      | "Nucleated growth of bush-like peptide superstructures" #MS14-PS9                                                                                                                                                             |
| MS14 | <b>Sanjay Tailor,</b> Sardar Patel University, India "Synthesis, Hirshfeld analysis and crystal structure of silver and copper complexes of sulfamethazine" #MS14-PS10                                                        |
| MS14 | Sounak Sarkar, Indian Institute of Science, India "Overcrowded naphthalene: an analysis of the competition between intramolecular CI•••CI peri interactions and intermolecular CI•••CI and CI•••π interactions" #MS14-PS11    |
| MS14 | Rajni Kant, University of Jammu, India "An insight into the crystallography of Ni - xanthate complexes" #MS14-PS12                                                                                                            |
| MS14 | Vaishali Sawant, Shivaji University, India "Synthesis, structure, and photoluminescence of copper(I) complexes of N-(2-{{(2E)-2-(4-nitrobenzylidene) hydrazinyI]carbonyI} phenyI)benzamide and triphenyIphosphine" #MS14-PS13 |
| MS14 | Martin Adam, Bruker AXS GmbH, Germany "New X-ray sources and X-ray detectors for fast and efficient in-house experiments" #MS14-PS14                                                                                          |
| MS14 | Rahul Dubey, Sardar Patel University, India "Novel Silver complexes of 4-amino-N-pyridinylbenzenesulfonamide (sulfapyridine) and 4-Ami- no-N-(2,6-dimethoxypyrimidin-4-yl) benzenesulfonamide (sulfadimethoxine)" #MS14-PS15  |
| MS14 | Urmila H. Patel, Sardar Patel University, India "Synthesis, spectroscopic characterization and crystal structure of cadmium complexes of 1,10 - Phenan throline" #MS14-PS16                                                   |

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| MS14         | Alexandra Griffin, Rigaku Oxford Diffraction, UK                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|              | "Ultra-fast structure determination and structure solution tools in CrysAlisPro v38" #MS14-PS17                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| MS14         | <b>Noor Shahina Begum,</b> Bangalore University, India "Synthesis and crystallographic analysis of fluoro substituted arylidene derivatives of thiazolopyrimidines' #MS14-PS18                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS14         | <b>Raj Gautam</b> , Indian Institute of Science, Bangalore, India "Do carboximide-carboxylic acid combinations form co-crystals: role of hydroxyl substitution on the formation of co-crystals and eutectics" #MS14-PS18                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS14         | <b>Sowmya A</b> , MS Ramaiah Institute of Technology, Bangalore, India "Crystal and molecular structure of biologically active substituted imidazo[2,1-b][1,3,4]thiadiazoles" #MS14-PS19                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS14         | Lavanya Rajarajeswari G, India "Intermolecular interactions in substituted benzene-1,2-dicarboxyl- ates" #MS14-PS20                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| MS14         | <b>Lawrence Wong</b> , Hong Kong University of Science and Technology, Hong Kong "Aryltartramides - a family of chiral diols for resolution" #MS14-PS21                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| MS15         | Roksana Parvin, Bangladesh University of Engineering and Technology, Bangladesh "Structural and magnetic properties of nanocrystalline Li <sub>x</sub> Cu <sub>0.1</sub> Co <sub>0.1</sub> Zn <sub>0.8-2x</sub> Fe <sub>2+2</sub> O <sub>4</sub> prepared by auto combustion technique" #MS15-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| MS15         | Alok Kumar Mukherjee, Jadavpur University, India "Compositional and architectural variation in human kidney stones from nucleus to periphery: an integrated powder X-ray diffraction (PXRD) and scanning electron microscopy (SEM) approach" #MS15-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |

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| MS15   | Martin Schreyer, Institute of Chemical and Engineering Sciences, Singapore                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|        | "Structure solution from a single multiphase powder" #MS15-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS15   | Ganggang Wang, Chengdu Institute of Biology, Chinese Academy of Sciences, China                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|        | "Structural insight into the reaction mechanism of CotA laccase from Bacillus subtilis" #MS15-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| MS15   | Shamila Sarwar, Bose Institute, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| IVISTS | "Optimization of crystal growth using ZnO nanoparticles" #MS15-PS5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|        | Hidehiro Uekusa, Tokyo Institute of Technology, Japan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| GIS    | "Hydration / dehydration mechanism of pharmaceutical crystals by ab initio structure determination from                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|        | powder diffraction data" #GIS-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| GIS    | Sudhir Mittapalli, University of Hyderabad, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| CID    | "Can we exchange water in a hydrate structure: a case study of etoricoxib" #GIS-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| GIS    | Swapna Battini, University of Hyderabad, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| CID    | "Polymorphism of aldose reductase inhibitor epalrestat" #GIS-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| CIC    | Tanaya Chatterjee, Bose Institute, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| GIS    | "Interaction of protein L-isoaspartyl methyltransferase (PIMT) with antiepileptic drugs" #GIS-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| GIS    | Dewei Joel Toh, Institute of Molecular and Cell Biology, Singapore                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|        | "The development of subfamily selective and cell-active FTO inhibitor as anti-obesity drug" #GIS-PS5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|        | Deepak Kumar, National Institute of Immunology, New Delhi, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| GIS    | "Mycobacterium tuberculosis HisB: A potential molecular target for the design of new anti-TB agents"                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|        | #GIS-PS6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|        | ·                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |

|                                                                              | Keynote - I                                                                                                                               |  |  |
|------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| 17:15 - 18:00                                                                | Mini Hall                                                                                                                                 |  |  |
| Chair:                                                                       | Chacko Jobichen, National University of Singapore, Singapore                                                                              |  |  |
| Speaker:                                                                     | Michelle Dunstone, Monash University, Australia "Packing a giant punch: The MACPF/CDC pore forming protein superfamily" #KN-1             |  |  |
|                                                                              | Keynote - II                                                                                                                              |  |  |
| 17:15 - 18:00                                                                | Hall-1                                                                                                                                    |  |  |
| Chair:                                                                       | Alison Edwards, Australian National Science and Technology Organization, Australia                                                        |  |  |
| Speaker:                                                                     | Sue-Lein Wang, National Tsing Hua University, Taiwan "Recent developments and prospects in porous inorganic framework materials" #KN-2    |  |  |
|                                                                              | Keynote - III                                                                                                                             |  |  |
| 17:15 - 18:00                                                                | Hall-2                                                                                                                                    |  |  |
| Chair:                                                                       | Liang Tong, Columbia University, USA                                                                                                      |  |  |
| Speaker:                                                                     | Michi Suga, Okayama University, Japan "Mechanism of photosynthetic water-splitting based on the atomic structure of photosystem II" #KN-3 |  |  |
| Evening Program - Talks by-Roger Durst (Bruker) & Biplab Ghosh (BARC, India) |                                                                                                                                           |  |  |
| 18:15 - 19:15                                                                | Mini Hall                                                                                                                                 |  |  |
| Conference Dinner - Sponsored by Bruker                                      |                                                                                                                                           |  |  |
| 19:15 - 20:30                                                                | Food Court                                                                                                                                |  |  |

| DAY-3: MONDAY, DECEMBER 7, 2015 Plenary Session - III          |                                                                                                                                                                                                                    |               |           |
|----------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------|-----------|
|                                                                |                                                                                                                                                                                                                    | 09:00 - 10:00 | Mini Hall |
| Chair:                                                         | Se Won Suh, Seoul National University, Korea                                                                                                                                                                       |               |           |
| Speaker:                                                       | <b>Kenneth Harris</b> , Cardiff University, UK "New experimental techniques for exploring crystallization pathways and structural properties of solids" #PL-3                                                      |               |           |
|                                                                | Morning Coffee                                                                                                                                                                                                     |               |           |
| 10:00 - 10:30                                                  | Pre Function Area, Mini Hall                                                                                                                                                                                       |               |           |
| Microsymposium 7 — New Tools and Methods in Structural Biology |                                                                                                                                                                                                                    |               |           |
| 10:30 - 12:30                                                  | Mini Hall                                                                                                                                                                                                          |               |           |
| Co-Chairs:                                                     | Eunice EunKyeong Kim, Korea Institute of Science and Technology, Korea<br>Kam Zhang, RIKEN, Japan                                                                                                                  |               |           |
| 30 minutes                                                     | Min YAO, Hokkaido University, Japan "Solution free crystal-mounting method for collecting high quality data using low energy X-ray" #MS7-1                                                                         |               |           |
| 30 minutes                                                     | Yuihui Dong, Institute of High Energy Physics, China "Phase retrieval in protein crystallography" #MS7-2                                                                                                           |               |           |
| 20 minutes                                                     | Krithika Gokulnath, University of Madras, India "Conversion of amino acid sequence in proteins to Indian classical (Carnatic) music: auditory and raga patterns suggest insights about secondary structure" #MS7-3 |               |           |

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| 20 minutes    | Prashantha Karunakar, PES University, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|               | "Towards automated determination of the number of molecules in the asymmetric unit of a protein crystal" #MS7-4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 20 minutes    | Yogavel Manickam, International Centre for Genetic Engineering and Biotechnology , India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|               | "Concurrent incorporation of two or more metals into protein crystals for SAD phasing using in-house copper X-ray source" #MS7-5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Micro         | osymposium 8 — Metal-Organic Frameworks and Organic: Inorganic Hybrid Materials                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 10:30 - 12:30 | Hall-1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Co-Chairs:    | Tong-bu Lu, Sun Yat-Sen University, China                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|               | Christopher Sumby, University of Adelaide, Australia                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| 30 minutes    | Rahul Banerjee, CSIR-National Chemical Laboratory, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|               | "Metamorphosis of metallohydrogels to crystalline metal-organic frameworks" #MS8-1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| 30 minutes    | Peng Cheng, Nankai University, China                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|               | "Lanthanide metal-organic frameworks" #MS8-2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| 20 minutes    | Sumi Ganguly, Indian Association for the Cultivation of Science, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
|               | "Stimuli responsive breathing behavior in Co(II) MOFs accompanied by single-crystal to single-crystal                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|               | transformation and magnetic property changes : Experimental and theoretical study" #MS8-3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| 20 minutes    | David Turner, Monash University, Australia                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|               | "Chiral coordination polymers: interpenetration and enantioselective separations" #MS8-4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |

| 20 minutes    | Mithun Paul, Indian Association for the Cultivation of Science, India                                     |
|---------------|-----------------------------------------------------------------------------------------------------------|
|               | "Coordination Polymers Derived from Non-steroidal-anti-inflammatory drugs for Cell Imaging and Drug       |
|               | Delivery" #MS8-5                                                                                          |
|               | Microsymposium 9 – Electron Microscopy and Diffraction                                                    |
| 10:30 - 12:30 | Hall-2                                                                                                    |
| Co-Chairs:    | Masaki Takata, Spring-8, University of Tokyo, Japan                                                       |
|               | <b>Dominike Elmlund,</b> Monash University, Australia                                                     |
| 30 minutes    | Xiuzhen Yu, RIKEN Advanced Science Institute Japan                                                        |
|               | "Application of Lorentz TEM to crystallographic investigation of magnetic skyrmion" #MS9-1                |
| 30 minutes    | Michael Landsberg, University of Queensland, Australia                                                    |
|               | "The structure of a novel bacterial toxin machinery revealed at near atomic resolution by single particle |
|               | cryo-EM"#MS9-2                                                                                            |
| 20 minutes    | Bostjan Kobe, University of Queensland, Australia                                                         |
|               | "Structural basis of higher-order assembly signaling by TIR domains in Toll-like receptor pathways"       |
|               | #MS9-3                                                                                                    |
| 20 minutes    | Pavel Afonine, Lawrence Berkeley National Laboratory, USA                                                 |
|               | "Phenix tools for validated refinement of atomic models in cryo-EM maps" #MS9-4                           |
| 20 minutes    | Kiran Kulkarni, National Chemical Laboratory, India                                                       |
|               | "A hybrid approach to generate pseudo-atomic model from single-particle electron microscopy and protein   |
|               | crystallography" #MS9-5                                                                                   |
|               |                                                                                                           |

| Lunch          |                                                                                                                   |  |
|----------------|-------------------------------------------------------------------------------------------------------------------|--|
| 12:30 - 13:30  | Food Court                                                                                                        |  |
|                | Lunch Time Meeting - Mitchell Guss:                                                                               |  |
| New initiative | New initiatives of IUCr Commission on Biological Macromolecules (for macromolecular crystallography participants) |  |
| 12:30 - 13:30  | Hall-1                                                                                                            |  |
|                | Microsymposium 10 – Structural Plasticity of Proteins                                                             |  |
| 13:30 - 15:30  | Mini Hall                                                                                                         |  |
| Co-Chairs:     | Catherine Day, University of Otago, NZ                                                                            |  |
|                | Bostjan Kobe, University of Queensland, Australia                                                                 |  |
| 30 minutes     | Rajan Sankaranarayanan, Centre for Cellular and Molecular Biology, Hyderabad, India                               |  |
|                | "Mechanistic plasticity in a chiral proofreading fold and its implications" #MS10-1                               |  |
| 30 minutes     | Brett Collins, University of Queensland, Australia                                                                |  |
|                | "Molecular insights into the assembly of caveola membrane domains by cavin proteins" #MS10-2                      |  |
| 20 minutes     | 20 minutes Ansuman Biswas, Indian Institute of Science, India                                                     |  |
|                | "Structural studies of different steps in the reaction pathway of Aquifex aeolicus thymidylate kinase"            |  |
|                | #MS10-3                                                                                                           |  |
| 20 minutes     | Jason M Brouwer, Walter and Eliza Hall Institute of Medical Research, Australia                                   |  |
|                | "Structural insights into Bak activation and oligomerisation" #MS10-4                                             |  |

| 20 minutes    | Praveena Thirunavukkarasu, Monash University, Australia                                                                                                                                    |
|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Zommutes      | "The structural and molecular insights into natural killer T cell receptor (NKT) and CD1d-glycolipid recognition" #MS10-5                                                                  |
|               | Microsymposium 11 – Reactions and Dynamics in the Solid State                                                                                                                              |
| 13:30 - 15:30 | Hall-1                                                                                                                                                                                     |
| Co-Chairs:    | Hidehiro Uekusa, Tokyo Institute of Technology, Japan Pance Naumov, New York University, Abu Dhabi, United Arab Emirates                                                                   |
| 30 minutes    | Andrew Goodwin, Oxford University, UK "Function from flexibility" #MS11-1                                                                                                                  |
| 30 minutes    | Masako KATO, Department of Chemistry, Hokkaido University, Japan "Luminescent copper (I) complexes exhibiting chromic phenomena" #MS11-2                                                   |
| 20 minutes    | Manas Panda, New York University Abu Dhabi, United Arab Emirates "Dynamic crystalline materials as smart molecular machinery: Insight into the mechanism of actuation" #MS11-3             |
| 20 minutes    | Randika Lakmali, University of Peradeniya, Sri Lanka "Structure-photochromic reactivity correlation of unsubstituted and halo substituted spiropyrans in BaSO <sub>4</sub> matrix" #MS11-4 |
| 20 minutes    | R. Prasada Rao, National University of Singapore, Singapore "Ion transport studies in sodium electrodes for high energy density rechargeable batteries" #MS11-5                            |

| Microsymposium 12 – Recent Developments in Crystal Growth |                                                                                                                 |  |
|-----------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|--|
| 13:30 - 15:30                                             | Hall-2                                                                                                          |  |
| Co-Chairs:                                                | Barnali Chaudhuri, Institute of Microbial Technology, Chandigarh, India                                         |  |
|                                                           | Chris Squire, University of Auckland, New Zealand                                                               |  |
| 30 minutes                                                | Naomi Chayen, Imperial College, UK                                                                              |  |
|                                                           | "Enhancing the success of crystallization by design of unconventional methodologies" #MS12-1                    |  |
| 30 minutes                                                | Fasseli Coulibaly, Monash University, Australia                                                                 |  |
|                                                           | "Microcrystallography of in vivo crystals" #MS12-2                                                              |  |
| 20 minutes                                                | Kwang-Hwa Lii, National Central University, Taiwan                                                              |  |
|                                                           | "High-temperature, high-pressure hydrothermal crystal growth" MS12-3                                            |  |
| 20 minutes                                                | Patrick Shaw Stewart, Douglas Instruments, UK                                                                   |  |
|                                                           | "Understanding random crystal screening with microseeding-"how new strategies can improve productivity" #MS12-4 |  |
| 20 minutes                                                | Shilpa T, Manipal Institute of Technology, India                                                                |  |
|                                                           | "Laser induced crystallization of glycine using multi-walled-carbon-nanotubes" #MS12-5                          |  |
| Afternoon Tea                                             |                                                                                                                 |  |
| 15:30 - 16:00                                             | Pre Function Area, Mini Hall                                                                                    |  |

|               | Poster Session II                                                                                                                                                                                                                              |  |
|---------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| 16:00 - 17:15 | Poster Hall-2                                                                                                                                                                                                                                  |  |
| MS7           | Sreetama Das, Indian Institute of Science, India "Incorporating dynamics information to improve cis-peptide based function annotation of proteins" #MS7-PS1                                                                                    |  |
| MS7           | <b>William Duax,</b> Hauptman Woodward MRI, USA "Archaea, a recent branch on the tree of life" #MS7-PS2                                                                                                                                        |  |
| MS7           | <b>HyeJin Yoon,</b> Seoul National University, Korea "Binding modes of cholesterol bind proteins NPC1L1 and NPC1 with cholesterol: A docking study" #MS7-PS3                                                                                   |  |
| MS7           | Akira Kinjo, Osaka University, Japan "Unified statistical model of protein multiple-sequence alignment integrating long-range correlation and insertions" #MS7-PS4                                                                             |  |
| MS7           | <b>Benazir Alam,</b> Saha Institute of Nuclear Physics, India "SCCA1-mediated regulation of proteolytic activity of lysosomal cysteine proteases" #MS7-PS5                                                                                     |  |
| MS7           | Satya Brata Routh, Centre for Cellular and Molecular Biology, India "Chiral proofreading during translation of the genetic code: mechanistic insights and functional implica- tions" #MS7-PS6                                                  |  |
| MS7           | Md. Abu Zubair, Mawlana Bhashani Science and Technology University, Tangail, Bangladesh "Purification of Nymphaea nouchali tuber lectin by alternative way and inhibition of tumor growth in vivo in mice by GO/G1 cell cycle arrest" #MS7-PS7 |  |

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| MS7 | Md. Nurujjaman, Rajshahi University, Bangladesh "Isolation and characterization of a lectin from the pulp of pomegranate (Punica granatum)" #MS7-PS8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| MS7 | Jimin Park, Korea "A search for antibiotics against Burkholderia pseudomallei using one step sequential assay method" #MS7-PS9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS7 | Yoonhwa Jo, Korea "Oxidative inhibition of GmhB from Burkholderia thailandensis" #MS7-PS10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| MS7 | Monika Antil, Jaypee Institute of Information Technology, India "Cloning, expression and characterization of isocitrate lyases of Mycobacterium tuberculosis" #MS7-PS11                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| MS7 | Syed Rashel Kabir, Bangladesh "Moringa oleifera seed lectin inhibited tumor growth by inducing apoptosis and S cell cycle arrest in Ehrlich ascites carcinoma cells in vivo in mice" #MS7-PS12                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| MS8 | Koushik Sarkar, Indian Association For The Cultivation of Science, India "A structure-property correlation study on rationally designed Mn(II) based coordination polymers in context of observed meta-magnetism and heterogeneous catalysis" #MS8-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| MS8 | Bhavinkumar Chavda, Sardar Patel University, India "Synthesis, crystal structure analysis and Hirshfeld study of cobalt and nickel complexes of sulfamerazine" #MS8-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| MS8 | Partha Pratim Bag, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, China "Outstanding drug loading capacity by water stable microporous 2D MOF: A potential drug carrier" #MS8-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |

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| MS8 | Rujuta Doshi, Indian Institute of Science, India "Measurement of specific heat and magnetocaloric effect in a dense metal organic framework, Tb(HCOO)3" #MS8-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| MS8 | Abin Sebastian, University of Hyderabad, India "Caffeic acid derived iron nanoparticles: Synthesis, characterization, and implication for rice plant growth in calcareous soils" #MS8-PS5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| MS8 | Prakash Kanoo, Indian Institute of Science, Bangalore, India "Porous functions in the nanospaces of flexible and not so flexible, metal-organic frameworks" #MS8-PS6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| MS8 | Savitha Govardhan, Indian Institute of Technology Kanpur, India "Rational design and synthesis of sterically-rigidified novel organic building blocks: Diverse metal-organic materials" #MS8-PS7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| MS8 | Pujari Chandrasekhar, Indian Institute of Technology Kanpur, India<br>"Functional metal-organic frameworks (MOFs) based on rationally designed organic linkers" #MS8-PS8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS8 | Arindam Mukhopadhyay, Indian Institute of Technology Kanpur, India "Towards photoresponsive porous metal-organic materials based on photochromism of 2,2-diarylbenzo- pyrans (chromenes)" #MS8-PS9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| MS8 | G M Golzar Hossain, University of Dhaka, Bangladesh "Metal complexes of sulfamethazine" #MS8-PS10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| MS9 | Samiran Pramanik, Jadavpur University, India "Composition and morphological characterization of human gallstones using IR spectroscopy, SEM and X-ray Rietveld analysis" #MS9-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |

The 13th Conference of the Asian Crystallographic Association 2015

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| MS9          | Kimi Azad, Indian Institute of Technology Delhi, India "Dissecting non-enveloped capsid disassembly using flock house virus as a model system" #MS9-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|              | Saumya Bajaj, Indian Institute of Technology Delhi, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| MS9          | "Structural determinants of the membrane penetrating ability of the Flock House Virus gamma peptide through cryoelectron microscopy and single particle reconstruction" #MS9-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| MS10         | Mahalakshmi Ramachandran, Advanced Centre for Treatment Research and Education in Cancer, India "Fine-specificity of domain-motif interaction and the role of structure: a case study with proteasomal chaperones" #MS10-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| MS10         | Henry Tang, Lawrence Berkeley National Laboratory, USA "Pushing the limits in enzyme engineering with the model enzyme phosphoenolpyruvate carboxykinase" #MS10-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| MS10         | Prasenjit Bhaumik, Indian Institute of Technology Bombay, India "Structural studies on Aspergillus niger glutamate dehydrogenase, an enzyme with unique functional properties" #MS10-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS10         | Suman Pandey, Indian Institute of Technology Bombay, India "High resolution structures of periplasmic glucose binding protein of Pseudomonas putida CSV86 reveals structural insights into its substrate specificity" #MS10-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| MS11         | Akira Yoshiasa, Graduate School of Science and Technology, Japan "Crystal structure and isosymmetric phase transition of high temperature C2/c clinoenstatite." #MS11-PS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| MS11         | Ryosuke Kusu, Kumamoto University, Japan<br>"Raman spectroscopy of metastable MgSiO3 high temperature C2/c clinoenstatite." #MS11-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |

| MS11 | Poria Kishorkumar. C., Veer Narmad South Gujarat University, India "Dissolution kinetics and reactivity at dislocation studies on naturally grown and surgically removed kidney stones." #MS11-PS3                                    |
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| MS11 | <b>Takashi Ohhara,</b> J-PARC Center, Japan Atomic Energy Agency, Japan "Single crystal neutron diffraction study of a crystalline-state photoisomerization by using a new TOF-Laue neutron diffractometer SENJU at J-PARC" #MS11-PS4 |
| MS11 | Naba Kamal Nath, National Institute of Technology, Meghalaya, India "Photomechanical bending of organic molecular crystals" #MS11-PS5                                                                                                 |
| MS12 | Sunil Chaudhary, Maharshi Dayanand University, India "Effect of phase transitions in lead iodide crystals as radiation detectors" #MS12-PS1                                                                                           |
| MS12 | Ramesh Ganduri, Indian Institute of Science, India "Multi-component adducts of pyridoxine: an evaluation of the formation of eutectics and molecular salts" #MS12-PS2                                                                 |
| MS12 | <b>Deepali Verma</b> , Jaypee Institute of Information Technology, India "Recombinant production, biochemical characterization and crystallization of cyse from Klebsiella pneumoniae" #MS12-PS3                                      |
| MS12 | <b>Richa Bhardwaj,</b> Panjab University, Chandigarh, India "Structural properties investigation in zno nano-flower synthesized via hydrothermal route" #MS12-PS4                                                                     |
| MS12 | <b>Venkataramanan Mahalingam,</b> IISER Kolkata, India "Lanthanide-doped nanocrystals: Growth, luminescent properties and applications" #MS12-PS5                                                                                     |

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| MS16 | Mintu Chandra, Indian Institute of Science Education and Research, Bhopal, India "Insights into molecular switch: crystal structure analysis of wild-type and fast hydrolyzing mutant of EhRabX3, a tandem ras superfamily GTPase from Entamoeba histolytica" #MS16-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| MS16 | <b>Debasish Chattopadhyay</b> , University of Alabama at Birmingham, USA "High resolution crystal structures of protein phosphatase5- inhibitor complex provide insight for selectivity" #MS16-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| MS16 | Shabnam Tarahi Tabrizi, Macquarie University, Australia "Crystal structure of GUN4 protein and its function in singlet oxygen production and chloroplast to nucleus signalling" #MS16-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| MS16 | Ashok Varma, Advanced Centre for Treatment Research and Education in Cancer, India "Structural characterization of extended N-terminal of BRCA1 BRCTs" #MS16-PS4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| MS17 | Ramakrishna Gowda, Govt College for Women Kolar, India "Crystal structure of 4-[5-Chloro-3-(4-chloro-phenyl) benzofuran -2-yl]-6 methyl-chromen -2-one" #MS17-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| MS17 | Udaya Bhaskara Rao Khandavilli, University College Cork, Ireland, "Crystal engineering, a solution to solid problems of chemistry" #MS16-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| MS17 | Mohan Bhadbhade, University of New South Wales, Australia "Synchrotron studies on inclusion behaviour of herbicides: simazine, atrazine and terbuthylazine" #MS16-PS3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| MS18 | Md. Amran Hossain, Kyoto Institute of Technology, Japan "Melt-isothermal crystallization behavior and melt viscosity of poly(3-hydroxybutyrate-co-3hydroxyhexa noate) thin films" #MS18-PS1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |

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| MS18          | Andreas Kleine, Incoatec GmbH, Germany "Upgrading SAXS setups with Incoateca's microfocus source and/or scatterless pinholes SCATEX" #MS18-PS2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |  |
|               | Conference Dinner - Sponsored by Rigaku                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |  |
| 19:00 - 22:00 | Swabhumi, Kolkata                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |  |
|               | DAY-4: TUESDAY, DECEMBER 8, 2015                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |  |
|               | Keynote Session - IV                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |  |
| 09:15 - 10:00 | Mini Hall                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |  |
| Chair:        | Peter Czabotar, Walter and Eliza Hall Institute of Medical Research, Australia                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |  |
| Speakers:     | Haitao Li, Tsinghua University, China                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |  |
|               | "Mark the "readership" for transcription control" #KN-4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |  |
|               | Keynote Session - V                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |  |
| 09:15 - 10:00 | Hall-1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |  |
| Chair:        | Masaki Kawano, Tokyo Institute of Technology, Japan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |  |
| Speakers:     | Parimal Bharadwaj, Indian Institute of Technology Kharagpur, India                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |  |
|               | "Studies on metal organic frameworks through chemical crystallography" #KN-5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |  |
|               | Morning Coffee                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |  |

| 10:00 - 10:30 | Pre Function Area, Mini Hall                                                                                                                                                                                          |  |
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|               | Microsymposium 13 — Hot Structures in Biology                                                                                                                                                                         |  |
| 10:30 - 12:30 | Mini Hall                                                                                                                                                                                                             |  |
| Co-Chairs:    | Rajan Sankaranarayanan, Centre for Cellular and Molecular Biology, Hyderabad, India<br>Ruchi Anand, Indian Institute of Technology, Mumbai, India                                                                     |  |
| 30 minutes    | Yanli Wang, Institute of Biophysics, China "Crystal structure of the RNA-guided immune surveillance cascade complex" #MS13-1                                                                                          |  |
| 30 minutes    | Ryuichiro Ishitani, The University of Tokyo, Japan "Molecular mechanisms of membrane transporter" #MS13-2                                                                                                             |  |
| 20 minutes    | Saikrishnan Kayarat, Indian Institute of Science Education and Research, Pune, India "Structure based mechanism of translocation coupled nucleolytic cleavage by Type ISP restriction-modifi- cation enzymes" #MS13-3 |  |
| 20 minutes    | <b>Julian Vivian,</b> Monash University, Australia "Immune surveillance: Viral escape and drug hypersensitivity" #MS13-4                                                                                              |  |
| 20 minutes    | Jayaraman Sivaraman, National University of Singapore, Singapore "Neutralization mechanism of hepatitis E virus by monoclonal antibodies" #MS13-5                                                                     |  |
|               | Microsymposium 14 – Chemical Crystallography: Hot Structures                                                                                                                                                          |  |
| 10:30 - 12:30 | Hall-1                                                                                                                                                                                                                |  |
| Co-Chairs:    | Jan Wikaira, University of Canterbury, NZ<br>Mohan Bhadbhade, University of New South Wales, Australia                                                                                                                |  |

| 30 minutes    | Manabu Hoshino, The University of Tokyo, Japan                                                                      |
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|               | "Chemical crystallography using the crystalline sponge method" #MS14-1                                              |
| 20 minutes    | Mingwen Shi, University of Western Australia, Australia                                                             |
|               | "How does the electrostatic nature of 18-crown-6 affect guest molecules upon complexation in the solid              |
|               | state?"#MS14-3                                                                                                      |
| 20 minutes    | <b>Gwilherm Nenert,</b> PANalytical, The Netherlands                                                                |
|               | "Crystal structure of hydrated fluorides $MF_2$ .4 $H_2$ 0 ( $M = Zn$ , $Ni$ , $Co$ ): a combined approach" #MS14-4 |
| 20 minutes    | Tanusri Dey, Jadavpur University, India                                                                             |
|               | "Three nimesulide derivatives: ab-initio structure determination from X-ray powder diffraction and                  |
|               | molecular electrostatic potential analysis" #MS14-5                                                                 |
|               | Microsymposium 15 — Nanocrystallography and Powder Diffraction                                                      |
| 10:30 - 12:30 | Hall-2                                                                                                              |
| Co-Chairs:    | Arunachalm Ramanan, Indian Institute of Technology, Delhi, India                                                    |
|               | Parthasarathi Dastidar, Indian Association for the Cultivation of Science, Kolkata, India                           |
| 30 minutes    | Masaki Kawano, Pohang University of Science and Technology, Korea                                                   |
|               | "X-ray snapshots of labile species in interactive pores" #MS15-1                                                    |
| 30 minutes    | Venkataramanan Mahalingam, Indian Institute of Science Education and Research, India                                |
|               | "Lanthanide-doped nanocrystals: Growth, luminescent properties and applications" #MS15-2                            |
| 20 minutes    | <b>Bob He,</b> Bruker AXS, USA                                                                                      |
|               |                                                                                                                     |
|               | "Recent advances in two-dimensional powder XRD" #MS15-3                                                             |

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| 20 minutes    | Martin Schreyer, Institute of Chemical and Engineering Sciences, Singapore                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|               | "Structure solution from a single multiphase powder" #MS15-4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| 20 minutes    | Brendan Kennedy, University of Sydney, Australia                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|               | "Understanding the interplay between the magnetic and crystal structure in Sr <sub>2</sub> YRuO <sub>6</sub> " #MS15-5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
|               | Lunch                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| 12:30 - 13:30 | Food Court                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| Lun           | ch Time Meeting - Meeting of the International Program Committee for AsCA 2016                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| 12:30 - 13:30 | Board Room                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|               | Microsymposium 16 – Structural Biology of Signalling Pathways                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 13:30 - 15:30 | Mini Hall                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Co-Chairs:    | Shwu-Huey Liaw, National Yang-Ming University, Taiwan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|               | <b>Hanna Yuan,</b> Academia Sinica, Taiwan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| 30 minutes    | Liang Tong, Columbia University, USA                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|               | "Structure and function of cyclic-di-AMP signaling" #MS16-1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| 30 minutes    | Shin-ichi Terawaki, Gunma University, Japan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|               | "Structural basis for regulation of cell differentiation signaling" #MS16-2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |

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| 20 minutes        | Mohammad Obayed Ullah, North South University, Bangladesh                                                                                                                                                                   |  |
|                   | "The TLR signaling adaptor TRIF/TICAM-1 has an N-terminal helical domain with structural similarity to                                                                                                                      |  |
|                   | IFIT proteins" #MS16-3                                                                                                                                                                                                      |  |
| 20 minutes        | Catherine Day, University of Otago, New Zealand                                                                                                                                                                             |  |
|                   | "A new twist in the regulation of ubiquitin transfer by RING E3 ligases" #MS16-4                                                                                                                                            |  |
| 20 minutes        | Angus Cowan, Walter and Eliza Hall Institute of Medical Research, Australia                                                                                                                                                 |  |
|                   | "Structural investigation of Bax oligomerisation" #MS16-5                                                                                                                                                                   |  |
|                   | Microsymposium 17 – Chemical Crystallography: General Interest                                                                                                                                                              |  |
| 13:30 - 15:30     | Hall-1                                                                                                                                                                                                                      |  |
| Co-Chairs:        | lan Williams, Hong Kong University of Science and Technology, Hong Kong                                                                                                                                                     |  |
|                   | <b>Srinivasan Natarajan,</b> SSCU, Indian Institute of Science, Bangalore, India                                                                                                                                            |  |
| 30 minutes        | Ashwini Nangia, University of Hyderabad, India                                                                                                                                                                              |  |
|                   | "Chemical crystallography and human medicine" #MS17-1                                                                                                                                                                       |  |
| 30 minutes        | Alison Edwards, Australian Nuclear Science and Technology Organisation, Australia                                                                                                                                           |  |
|                   | "Crystal structure determination - beyond least-squares refinement" #MS17-2                                                                                                                                                 |  |
| 20 minutes        | Fraser White, Rigaku Corporation, UK                                                                                                                                                                                        |  |
|                   | "Getting more from data processing with CrysAlisPro" #MS17-3                                                                                                                                                                |  |
| 20 minutes        | Swastik Mondal, Max-Planck-Institut fur Kohlenforschung, Germany                                                                                                                                                            |  |
|                   | "Unravelling the mysteries of boron carbide" #MS17-4                                                                                                                                                                        |  |
|                   |                                                                                                                                                                                                                             |  |

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| 20 minutes    | <b>Srinivasulu Aitipamula</b> , Institute of Chemical and Engineering Sciences, Singapore "Insights into cocrystal-excipient compatibility: griseofulvin-acesulfame cocrystal hydrate as a model system" #MS17-5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|               | Microsymposium 18 – Small Angle Scattering                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| 13:30 - 15:30 | Hall-2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Co-Chairs:    | Sono Sasaki, Kyoto Institute of Technology, Japan<br>Yoshiyuki Amemiya, University of Tokyo, Japan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| 30 minutes    | Yuya Shinohara, Department of Advanced Materials Science, The University of Tokyo "Anomalous small-angle X-ray scattering of rubber at sulfur K-edge" #MS18-1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 30 minutes    | <b>Chun-Jen Su,</b> National Synchrotron Radiation Research Centre, Taiwan "Competition between entropy and enthalpy in the binding of melittin with ULV vesicles of different phosphate lipid chain lengths" #MS18-2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| 20 minutes    | Angela Criswell, Rigaku Oxford Diffraction, USA "Biological solution scattering studies using a HyPix-3000 hybrid pixel array detector" #MS18-3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 20 minutes    | Jitendra Mata, Australian Nuclear Science and Technology Organisation, Australia "Quokka - The 40 M pinhole SANS instrument at the opal reactor", #MS18-4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| 20 minutes    | <b>Bhoje Gowd,</b> CSIR-National Institute for Interdisciplinary Science and Technology, India "Pathways of cylindrical orientations in PS-b-P4VP diblock copolymer thin films upon solvent vapor annealing" #MS18-5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|               | Afternoon Tea                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 15:30 - 16:00 | Pre Function Area, Mini Hall                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
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| Rising Star Session |                                                                                                                                                                                                                                                   |
|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 16:00 – 17:30       | Mini Hall                                                                                                                                                                                                                                         |
| Chair:              | Jenny Martin, University of Queensland, Australia                                                                                                                                                                                                 |
| 15 minutes          | Sajesh Thomas, University of Western Australia, Australia "Insights into mechanical properties of molecular crystals from energy frameworks and quantum crystallography" #RS-1                                                                    |
| 15 minutes          | Rajesh Ghai, University of New South Wales, Australia "Molecular mechanism of ER-plasma membrane junction maintenance by integral ER membrane proteins, ORPS/ORP8" #RS-2                                                                          |
| 15 minutes          | Vidya Mangala Prasad, Purdue University, USA "Structural studies on the rubella virus capsid protein and its implications on the virion structure", #RS-3                                                                                         |
| 15 minutes          | Michelle Christie, University of Queensland, Australia "Opening up to vesicle fusion: The effect of Munc18c and membrane anchoring on Syntaxin-4 function" #RS-4                                                                                  |
| 15 minutes          | Rahul Shukla, Indian Institute of Science Education and Research, India "Crystallographic and computational investigation of intermolecular interactions involving organic fluorine with relevance to the hybridization of the carbon atom" #RS-5 |
| 15 minutes          | Suman Bhattacharya, Indian Association for the Cultivation of Science, India "Thermal expansion and hydrogen bonds: a case study on polymorphic systems with different hydrogen bond dimensionalities" #RS-6                                      |
|                     | Plenary Session - IV                                                                                                                                                                                                                              |

## The 13th Conference of the Asian Crystallographic Association 2015

| 17:30 – 18:30             | Mini Hall                                                                                   |
|---------------------------|---------------------------------------------------------------------------------------------|
| Chair:                    | Mitchell Guss, University of Sydney, Australia                                              |
| Speaker:                  | Mamannamana Vijayan, Indian Institute of Science, Bangalore, India                          |
|                           | "Structural diversity and ligand specificity in lectins. From plants to Mycobacteria" #PL-4 |
| Closing Ceremony          |                                                                                             |
| 18:30 – 18:45   Mini Hall |                                                                                             |



## **Conference Organiser**

Prof. Pinak Chakrabarti

Chair LOC, Department of Biochemistry,

and Bioinformatics Centre P1/12 CIT Scheme VIIM , Kolkata 700 054, India T: +91-33-2569-3253, M: +91-9830751009, Fax: +91-33-2355-3886 E: pinak.chak@qmail.com, pinak@jcbose.ac.in

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