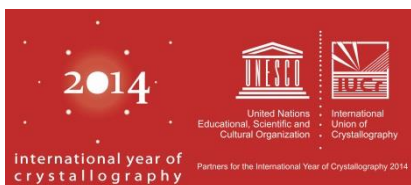


# IYCr2014 South Asia Summit Meeting on *Vistas in structural chemistry* Karachi (Pakistan), International Center for Chemical and Biological Sciences, 28-30 April 2014



Jointly Organized by:

- Ministry of Science and Technology (MoST), Government of Pakistan
- Pakistan Academy of Sciences (PAS)
- Chinese Academy of Sciences (CAS)
- Indian National Science Academy (INSA)
- Commission on Science and Technology for Sustainable Development in the South (COMSATS)



Under the auspices of the International Union of Crystallography (IUCr) and United Nations Educational, Scientific and Cultural Organization (UNESCO)

## Programme

(last update: 14 April 2014)

### Monday, April 28, 2014

#### 9.15-10.40: Session I - Inauguration Ceremony

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: Mr. Aziz Latif Jamal, Husein Ebrahim Jamal Foundation

9.15 Guests seated

9.20 **Mr. Aziz Latif Jamal**, Husein Ebrahim Jamal Foundation - *Welcome Remarks*

9.25 **Prof. Dr. Iqbal Choudhary**, Director, ICCBS - *Remarks*

9.30 **Prof. Dr. Samar S. Hasnain**, Editor-in-Chief of IUCr Journals - *Introduction to the Event*

9.40 **Ms. Kozue Kay Nagata**, Director, UNESCO Islamabad - *Remarks*

9.45 **Ms. Amina Imran Khan**, Secretary General, PNC, UNESCO Islamabad - *Remarks*

9.50 **Dr. Imtinan Elahi Qureshi**, Executive Director, COMSATS - *Remarks*

9.55 **Prof. Dr. Gautam R. Desiraju**, President, International Union of Crystallography - *Address*

10.05 **Prof. Dr. Atta-ur-Rahman**, President, Pakistan Academy of Sciences and Chairman, Organizing Committee - *Address*

10.15 **Chief Guest**, *Inaugural Address*

10.30 **Dr. Sammer Yousuf**, *Vote of Thanks*

#### 10.40-11.00 Group Photo and Reception at the Multipurpose Hall

#### 11.00-12.00: Session II - Metal-Organic Framework Compounds (MOF)

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: Nawaz Tahir

11.00 **Chen Xiao-Ming**, *X-ray crystallographic studies on dynamic and functional coordination polymers*

11.20 **P. K. Bharadwaj**, *Single crystal to single crystal transformations in metal-organic frameworks*

11.40 **Shilun Qiu**, *MOF membrane: Synthesis, Adsorption for Green Application*

#### 12.00-13.00 PANEL DISCUSSION

Panel Chair: S. Natarajan

Panelists: K. Biradha, Bu Xian-He, Cheng-Yong Su, R. Brakaspathy, C.G. Groom, A.A. Attari, Arif Kazmi

Core questions:

1. What is the difference between MOFs and coordination polymers?
2. Can the CSD handle MOFs properly?
3. What should funding policies be for this area? In countries other than China, what should be done?
4. What is the future? What are the directions?
5. How can regional cooperation be fostered in the MOFs and related area?

#### 13.00-14.00 Lunch (Multipurpose Hall, ICCBS)

### 14.00-15.20: Session III - Crystal Engineering and Generic Pharmaceuticals

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: G.R. Desiraju

14.00 **Ashwini Nangia**, *Overview of Pharma Patent Landscape in India*

14.20 **K.J. Roberts**, *Synthonic Engineering: Molecular Scale Tools for the Rational Design of High Quality Crystals for Pharmaceutical Formulation*

14.40 **Eric Hovestreydt**, *Double Dose: combining Single-Crystal and Powder XRD for Analysis of Pharmaceutical Materials*

15.00 **Ghazala Sadiq**, *Informatic approaches to solid form analysis and design*

### 15.20-16.20 PANEL DISCUSSION

Panel Chairs: A. Nangia, K.J. Roberts

Panelists: Abdul-Haseeb Khan, Miao Du, Humaira Mufti, A. Ramanan, K. Biradha

Core questions:

1. Salts and co-crystals. Is it still a problem?
2. Regulatory definition of "co-crystal"
3. Polymorphs and pseudo-polymorphs. Are they the same?
4. Legal questions in generic pharmaceuticals

**16.20-17.00 Tea/Coffee Break (Multipurpose Hall, ICCBS)**

**17.00-18.30 City Tour & Shopping Visits**

**20.00 Dinner (Port Grand, established in 1927 by the Royal British Navy)**

**Tuesday, April 29, 2014**

### 9.00-11.00: Session IV - Chemistry-Biology Interface and Drug Discovery and Designing

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: S.S. Hasnain

9.00 **Zihe Rao**, *A powerful virus inhibitor from structure-based analysis of HV71*

9.15 **R. Vishwakarma**, *Challenges in new drug discovery in South Asia: Can they be overcome?*

9.30 **Abdul Rauf Siddiqi**, *Structural studies of proteins involved in nitric oxide signaling pathways*

9.45 **Zhie-Jie Liu**, *Inhibition of MTHFS in human MCF-7 breast cancer cells and rational drug design*

10.00 **Sammer Yousuf**, *Discovery of anti-leishmanial leads from natural leads*

### 10.15-11.00 PANEL DISCUSSION

Panel Chair: S. Sivaram

Panelists: P. Chakrabarti, R. Viswakarma, D. Yogeswara Rao, Aslam Baig, M. Iqbal Choudhary, Maqsood Ahmed

Core questions:

1. Can we afford drug design of new molecules in the SE Asian region?
2. Role of Natural products in drug discovery and development
3. The status of the field in the region in the international context
4. Are there lessons to be learnt from the best practice in the region?
5. Relevance of this discipline for economic growth and welfare of the region
6. Challenges of informing funding policymakers for the benefits of the field
7. Regional symposia, workshops, exchange of staff & students and shared facilities
8. Role of national academies and IUCr for improving regional collaboration

**11.00-11.15 Tea/Coffee Break (Multipurpose Hall, ICCBS)**

### 11.15-13.00: Session V - Crystallography and complementary methods

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: Moaz ur Rahman

11.15 **E. Arunan**, *Structure of molecular complexes in the gas phase: Are they relevant to solid state?*

11.35 **Bohari Yamin**, *Structural and biological studies of some calix[4]resorcinarene*

11.55 **S.P. Sarma**, *NMR structural characterization of Novel Conotoxins from Marine Snails*

12.15 **Atia-tul-Wahab**, *NMR Spectroscopy in structural biology*

12.35 **Maqsood Ahmed**, *Crystallography at high resolution: X-Rays charge density analysis of small molecules and proteins*

**13.00-14.00 Lunch (Multipurpose Hall, ICCBS)**

### 14.00-15.00: Session VI - Summit Lecture

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: M. Nalecz

**Atta-ur-Rahman**, *Promotion of higher education, science and technology and international cooperation in Pakistan*

**15.00-17.00: Session VII - IUCr: Union & Journals**

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: S.S. Hasnain

15.00 **M.H. Dacombe**, *IUCr membership & what it offers*

15.20 **S.S. Hasnain**, *IUCr journals: Heritage & Future*

15.40 **G.R. Desiraju**, *Chemistry journals of IUCr. Acta B/C/E and IUCrJ. A comprehensive coverage for Chemists*

16.00 **Cheng-Yong Su**, *IUCrJ Chemistry*

16.15 **Zhie-jie Liu**, *IUCrJ Biology*

16.30 **G.R. Desiraju & S.S. Hasnain**, *Discussion from the floor & Summing up of session*

**17.00-17.15 Tea/Coffee Break (Multipurpose Hall, ICCBS)**

**17.15-18.15: Session VIII - Mini-Talks Session**

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: Vijaya Kumar

17.15 **Vinitha M. Thadhani**, *Methods of developing new secondary metabolites*

17.25 **Siti Fairus M. Yusoff**, *Structural Study of Protonated 5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-7,14-dienium Complexes with Copper Salts*

17.35 **Moazur Rahman**, *Functional and structural characterization of a MDR pump of Salmonella typhi*

17.45 **Sadaf Iqbal**, *Characterization and the crystal structure determination of a papain-like cysteine protease from the bulbs of Crocus sativus*

17.55 **Hamizah Mohd Zaki**, *Reaction of ethylenediamine and 2,4-diamino-6-methyl-1,3,5-triazine with oxalic acid in the presence of ammonium thiocyanate*

18.05 **Ahmed Akrem Attari**, *Crystallographic structure analysis of Chitinase enzyme from corms of Crocus vernus*

**18.30-19.15 Visit of the ICCBS Institutions**

**20.30 Dinner (ICCBS Lawns)**

**Wednesday, April 30, 2014**

**9.00-11.00: Session IX - Summit Concluding Session**

Prof. Salimuzzaman Siddiqui Auditorium, ICCBS

Chair: Atta-ur-Rahman

Speakers (15 min each): **Zihe Rao, Shilun Qiu, S. Sivaram, Suresh Das, Aslam Baig, M. Iqbal Choudhary**

**11.00 Tea/Coffee Break (Multipurpose Hall, ICCBS)**

**11.00-12.30 PANEL DISCUSSION**

Panel Chairs: G.R. Desiraju, M. Nalecz

Panelists: Chen Xiao-Ming, Zihe Rao, S. Sivaram, S. Das, Aslam Baig, M. Iqbal Choudhary, R. Brakaspathy, D. Yogeswara Rao, S.S. Hasnain, K. Byrappa, Zhie-Jie Liu, K. Lal, Jved Iqbal Akhter

Core questions:

1. Modalities for setting up schemes for Regional Cooperation
2. Setting up of a regional fund for increasing human mobility
3. Regional training centre of crystallography
4. Role of synchrotron in crystallography
5. Can UNESCO and IUCr help?

**12.30-14.00 Lunch**

**14.00-15.00 Closing Ceremony (including Summit Declaration)**

**15.00-15.30 Closing Reception**

**15.30-17.00 Shopping Visit / Visits to Art Galleries**

**20.30 Dinner at Do Darya (Beach Resort at the Arabian Sea)**

<http://www.iycr2014.org/summits>