



International EXPO/SIR Workshop

c/o Dipartimento di Scienze della Terra
e Geoambientali
University of Bari

Bari, Italy
10-13 JUNE 2014

PROGRAM

10th June 2014

8:00-9:00 Registration

Opening Session

9:15-9:30 **Michele Saviano**
Director of Institute of Crystallography (IC-CNR)
Welcome and opening remarks

9:30-10:30 **Carmelo Giacovazzo**
Main Lecture
**The phase problem and the basic postulate of
the structural crystallography**

Module 1: 10-11 June 2014

Tuesday, 10th June

10:30-11:00 **Coffee break**
Sponsored by RIGAKU

11:00-11:30 **Anna Moliterni**
Unit cell identification

11:30-12:00 **Carmelo Giacovazzo**
Space group determination

12:00-12:30 **Angela Altomare**
Full pattern decomposition

12:30-13:00 **Rosanna Rizzi**
Phasing via Direct Methods

13:00-15:00 **Lunch**

15:00-15:30 **Akihiro Himeda**
RIGAKU communication

15:30-16:30 **Angela Altomare, Corrado Cuocci,
Anna Moliterni, Rosanna Rizzi, Aurelia Falcicchio**
EXPO2014 Computer session

16:30-17:00 **Coffee break**
Sponsored by RIGAKU

17:00-19:00 **Angela Altomare, Corrado Cuocci,
Anna Moliterni, Rosanna Rizzi, Aurelia Falcicchio**
EXPO2014 Computer session

Module 1: 10-11 June 2014

Wednesday, 11th June

9:15-10:00 **Angela Altomare**
Model optimization

10:00-10:30 **Anna Moliterni**
Rietveld refinement

10:30-11:00 **Coffee break**
Sponsored by RIGAKU

11:00-11:40 **Rosanna Rizzi**
Direct space approach

11:40-12:10 **Corrado Cuocci**
Direct space approach in action

12:10-12:25 **Dubravka Sisak**
DECTRIS communication

12:25-13:00
Free time for participant communications

13:00-15:00 **Lunch**

15:00-16:30 **Angela Altomare, Corrado Cuocci,
Anna Moliterni, Rosanna Rizzi, Aurelia Falcicchio**
EXPO2014 Computer session

16:30-17:00 **Coffee break**
Sponsored by RIGAKU

17:00-19:00 **Angela Altomare, Corrado Cuocci,
Anna Moliterni, Rosanna Rizzi, Aurelia Falcicchio**
EXPO2014 Computer session

20:30- **Social dinner**

Module 2: 12-13 June 2014

Thursday, 12th June

8:00-9:00 Registration

(for Participants to Module 2 only)

9:15-10:00 Carmelo Giacovazzo

Theoretical bases of the new phasing approaches in Sir2014

10:00-10:30 Giovanni Luca Cascarano

A program overview

10:30-11:00 Coffee break

11:00-11:45 Maria Cristina Burla and Giampiero Polidori

New phasing approaches: applications

11:45-12:30 Rocco Caliendo

New Patterson algorithms

12:30-13:00 Benedetta Carrozzini

Ab initio structure solution: the Direct Space Refinement process. Part 1 - Small Molecules

13:00-15:00 Lunch

15:00-16:30 Maria Cristina Burla, Rocco Caliendo, Benedetta Carrozzini, Giovanni Luca Cascarano, Annamaria Mazzone, Giampiero Polidori
Sir2014 Computer session

16:30-17:00 Coffee break

17:00-19:00 Maria Cristina Burla, Rocco Caliendo, Benedetta Carrozzini, Giovanni Luca Cascarano, Annamaria Mazzone, Giampiero Polidori
Sir2014 Computer session

Module 2: 12-13 June 2014

Friday, 13th June

9:00-9:45 Giovanni Luca Cascarano

Sir2014 and Electron Diffraction

9:45-10:30 Corrado Cuocci

Solving structures via Simulated Annealing

10:30-11:00 Coffee break

11:00-11:30 Benedetta Carrozzini

Ab initio structure solution: the Direct Space Refinement process. Part 2 - Macromolecules

11:30-12:15 Annamaria Mazzone

Molecular Replacement pipeline

12:15-12:30 Dubravka Sisak

DECTRIS communication

12:30-13:00

Free time for participant communications

13:00-15:00 Lunch

15:00-16:30 Maria Cristina Burla, Rocco Caliendo, Benedetta Carrozzini, Giovanni Luca Cascarano, Annamaria Mazzone, Giampiero Polidori
Sir2014 Computer session

16:30-17:00 Coffee break

17:00-19:00 Maria Cristina Burla, Rocco Caliendo, Benedetta Carrozzini, Giovanni Luca Cascarano, Annamaria Mazzone, Giampiero Polidori
Sir2014 Computer session



Dipartimento di Scienze
della Terra e Geoambientali

Rigaku

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