



In collaboration with



Elettra Sincrotrone Trieste

Wednesday, 2 October

Chair: Nicola Corriero

09:00-10:00 Corrado Cuocci
Direct space methods solution

10:00-10:30 *Coffee break*

10:30-13:00 A. Altomare, N. Corriero, C. Cuocci,
A. Falcicchio, A. Moliterni, R. Rizzi

EXPO Computer Session
Direct space methods solution

13:00-14.30 *Lunch*

Chair: Aurelia Falcicchio

14:30-14:45 Jasper Plaisier
Status of the diffraction beamlines
at Elettra

14:45-15:30 Nicola Corriero
Qualitative phase analysis

15:30-16:15 Giovanni Cavallo
Powder characterization by QUALX

16:45-16:45 *Coffee break*

16:45-18:30 A. Altomare, N. Corriero, C. Cuocci,
A. Falcicchio, A. Moliterni, R. Rizzi

QUALX Computer Session

Thursday, 3 October

Chair: Corrado Cuocci

09:00-09:30 Nicola Corriero
The OChemDb software

09:30-11:00 A. Altomare, N. Corriero, C. Cuocci,
A. Falcicchio, A. Moliterni, R. Rizzi

OChemDb Computer session

11:00-11:30 *Coffee break*

Chair: Benny-Danilo Belviso

11:30-12:15 Rocco Caliandro
RootProf: principles, workflow and new
graphical user interface

12:10-12:40 Pietro Guccione
New algorithms for fast extraction of
information from *in situ* powder
diffraction data

12:40-13:00 Alessandro Zappi
Quantifying API polymorphs in solid
formulations

13:00-14.30 *Lunch*

Chair: Rocco Caliandro

14:30-15:15 Marco Milanesio
Monitoring *in situ* experiments
with RootProf

15:15-15:45 Benny Danilo Belviso
RootProf: from theory to practise

16:45-18:15 *Coffe break*

16:15-18:30 R. Caliandro, B. D. Belviso
RootProf Computer session

18:30-19:00 *Closing session*



Expo&more International Workshop

Organized by the Institute of Crystallography -
CNR, Bari, Italy

30 September - 3 October 2019

Crystallographic Software for Powder Diffraction Data

Videoconference room of
Polytechnic of Bari,
via Amendola 126/b, Bari, Italy



Monday, 30 September

- 08:30-13:00 *Registration*
- 09:30-9:45 *Welcome and opening session*
- Michele Saviano (Director of Institute
of Crystallography IC-CNR)

Chair: Rosanna Rizzi

- 09:45-10:30 Angela Altomare
The structure solution process
in the Expo Software

- 10:30-11:00 Aurelia Falcicchio
Starting with EXPO

- 11:00-11:30 *Coffee break sponsored by Rigaku*

- 11:30-12:30 Anna Moliterni
Indexing

- 12:30-13:00 Akihiro Himeda
EXPO in the Rigaku software

- 13:00-14:30 *Lunch*

Chair: Angela Altomare

- 14:30-15:00 Anna Moliterni
Space group determination

- 15:00-15:30 Rosanna Rizzi
Full pattern decomposition

- 15:30-16:00 *Coffee break sponsored by Rigaku*

- 16:00-18:00 A. Altomare, N. Corriero, C. Cuocci, A.
Falcicchio, A. Moliterni, R. Rizzi
EXPO Computer Session
Indexing and Space group determination

- 18:30-20:00 *Welcome party sponsored by Rigaku*

Tuesday, 1 October

Chair: Anna Moliterni

- 09:00-10:00 Rosanna Rizzi
Reciprocal space methods solution

- 10:00-11:00 Angela Altomare
Structural model optimization

- 11:00-11:30 *Coffee break*

- 11:30-13:00 Corrado Cuocci
Direct Space Solution

- 13:00-14:30 *Lunch*

- 14:30-16:00 A. Altomare, N. Corriero, C. Cuocci,
A. Falcicchio, A. Moliterni, R. Rizzi
EXPO Computer Session
Solution by Direct Methods

- 16:00-16:30 *Coffee break*

- 10:30-13:00 A. Altomare, N. Corriero, C. Cuocci,
A. Falcicchio, A. Moliterni, R. Rizzi
EXPO Computer Session
*Structure model optimization
and Rietveld refinement*

- 20:00- *Social dinner*