



1st Brazilian Hands-on Workshop: SIR/EXPO 2014

Tentative Program: November 3 - 7

Monday

- An introduction on the Phase Problem and the Crystal Structure Solution
- An Overview of Structure Solution by SIR2014 program
- An Overview of Structure Solution by EXPO2014 program
- Download and installation of the programs EXPO2014 and SIR2014
- **First Training on SIR2014**
 - Theory and practice: crystal structure solution of small/medium sized molecules; tutorial on selected practical examples.
 - Hands on SIR2014 program. The students are encouraged to work alone on topics discussed in the lectures and on examples provided by teachers or on their own data.

Tuesday

- **First Training on EXPO2014**
 - Theory and practice: indexing and space group determination, crystal structure solution by reciprocal space methods, Rietveld Refinement; tutorial on selected practical examples.
 - Hands on EXPO2014 program. The students are encouraged to work alone on topics discussed in the lectures and on examples provided by teachers or on their own data.
- **Training on EXPO/SIR2014**
 - Hands on SIR2014 and EXPO2014 programs. The students are encouraged to work alone on topics discussed in the lectures

and on examples provided by teachers or on their own data.

Wednesday morning

▪ **Second Training on SIR2014**

- Theory and practice: crystal structure solution *via* electron diffraction data; tutorial on selected practical examples.
- Hands on SIR2014 program. The students are encouraged to work alone on topics discussed in the lectures and on examples provided by teachers or on their own data.

Wednesday afternoon: *free time*

Thursday

▪ **Training on EXPO/SIR2014**

- Theory and practice: crystal structure solution by direct space methods; tutorial on selected practical examples.
- Hands on EXPO/SIR2014 program. The students are encouraged to work alone on topics discussed in the morning and on examples provided by teachers or on their own data.

Friday morning

▪ **Training on SIR2014**

- Theory and practice: introduction to *ab-initio* structure solution of macromolecules; tutorial on selected practical examples.