NMR structure calculation with ARIA

Practical course 2016

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http://aria.pasteur.fr

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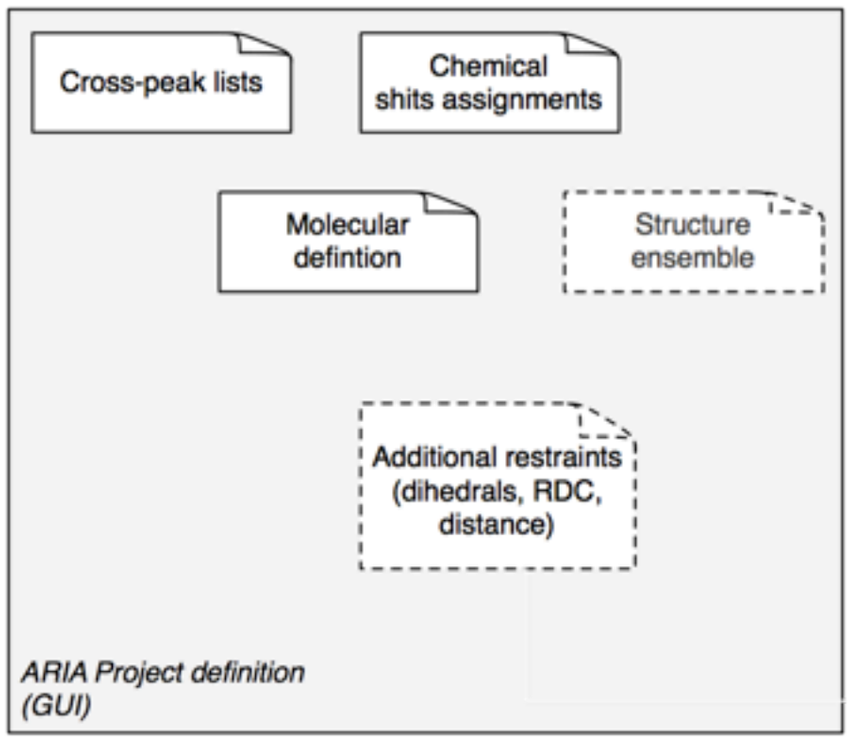
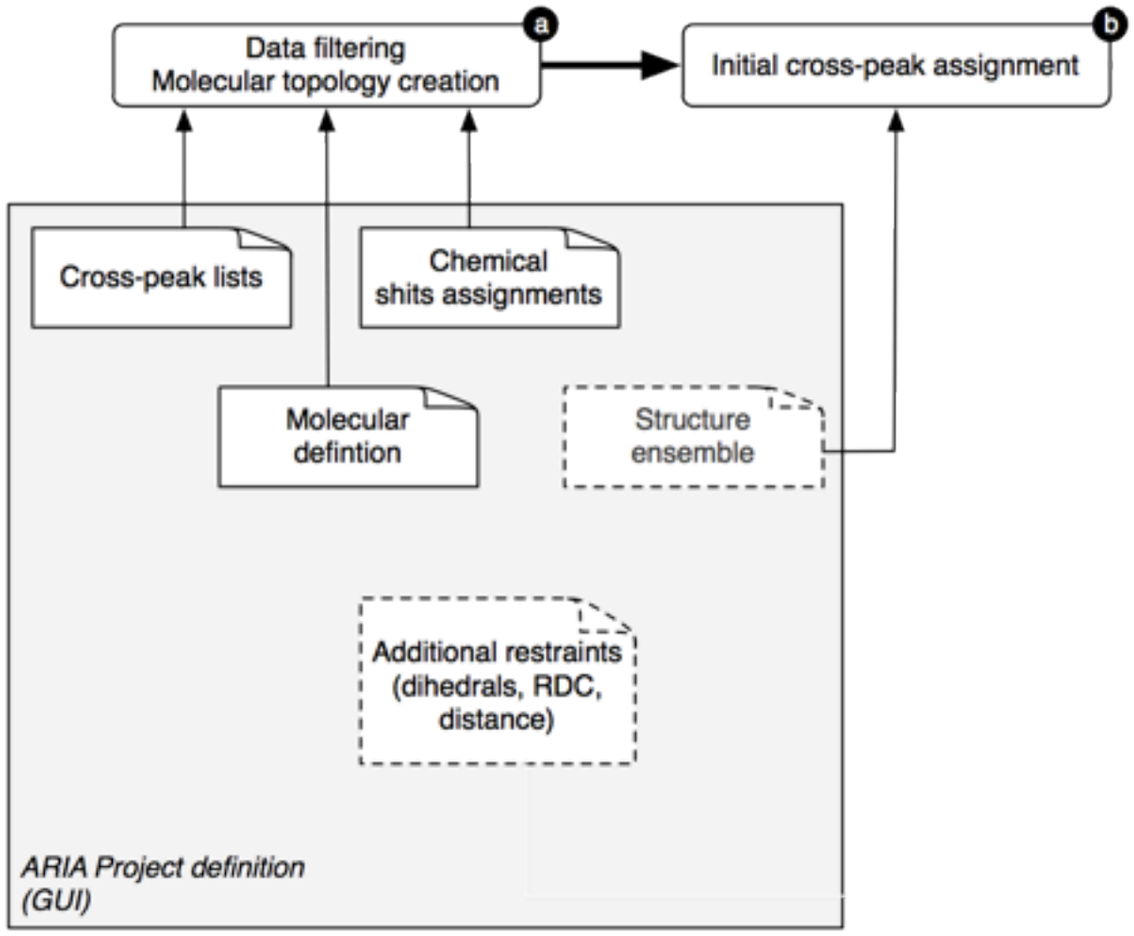
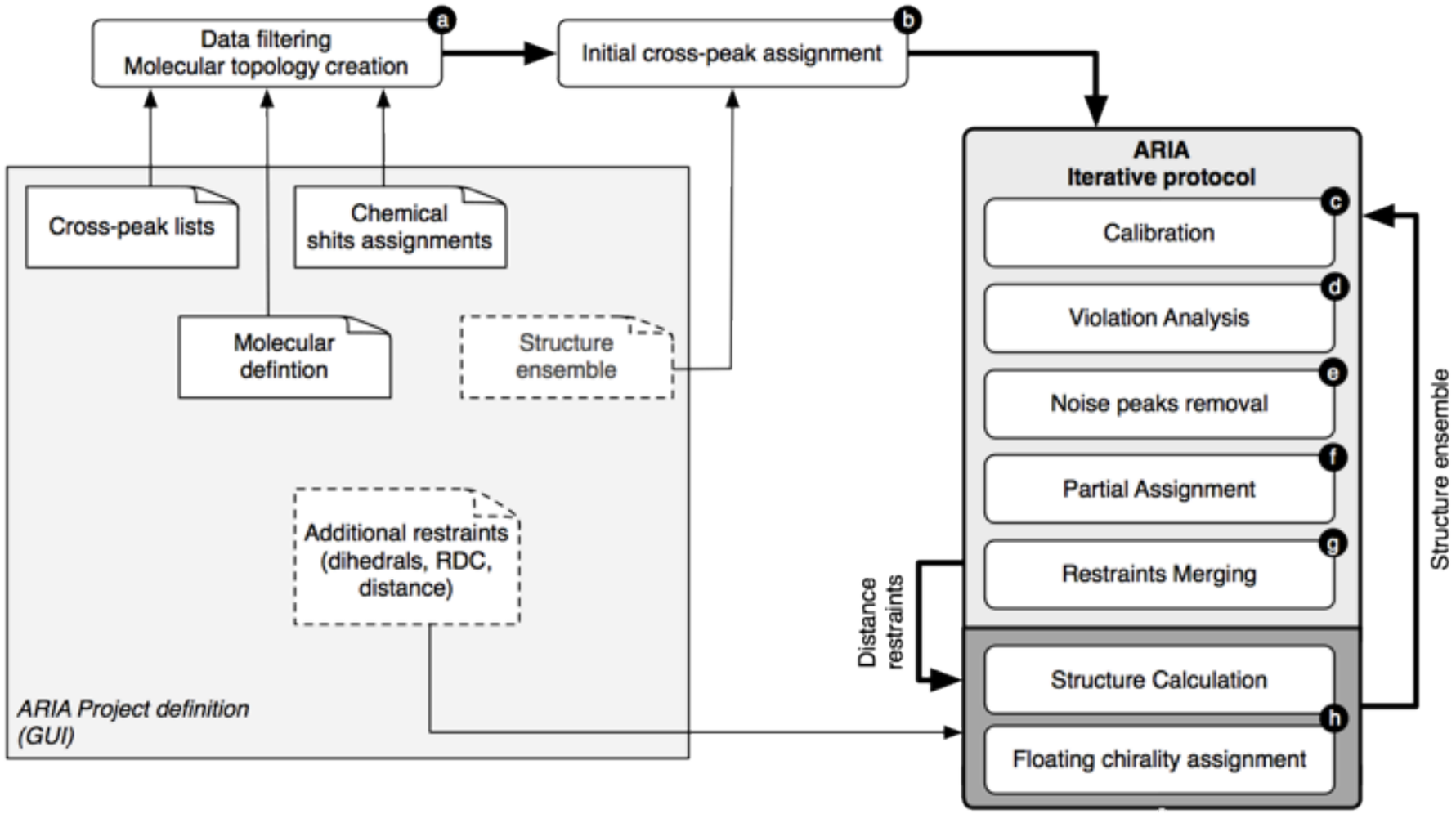
ARIA protocol: step 1



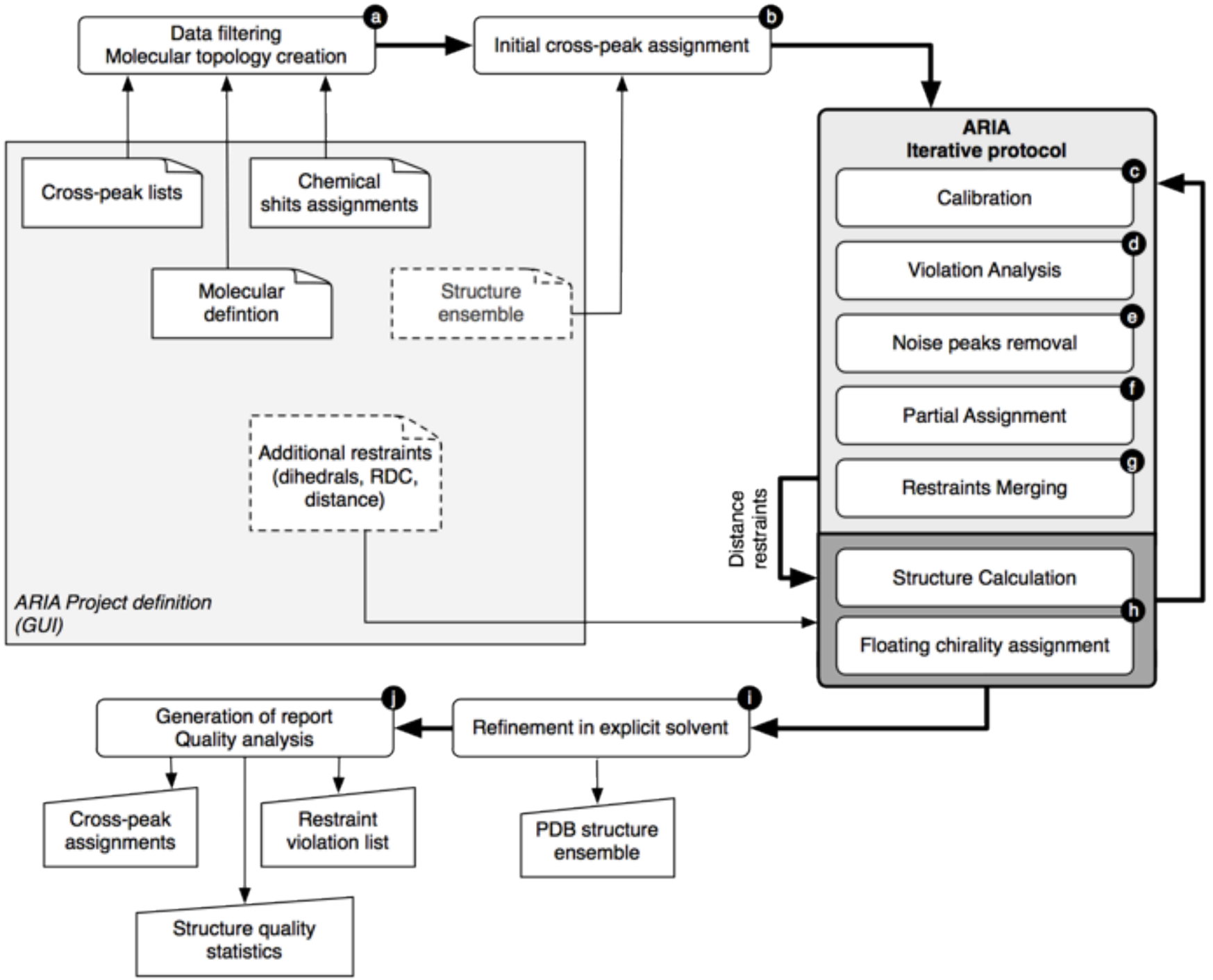
ARIA protocol: step 2



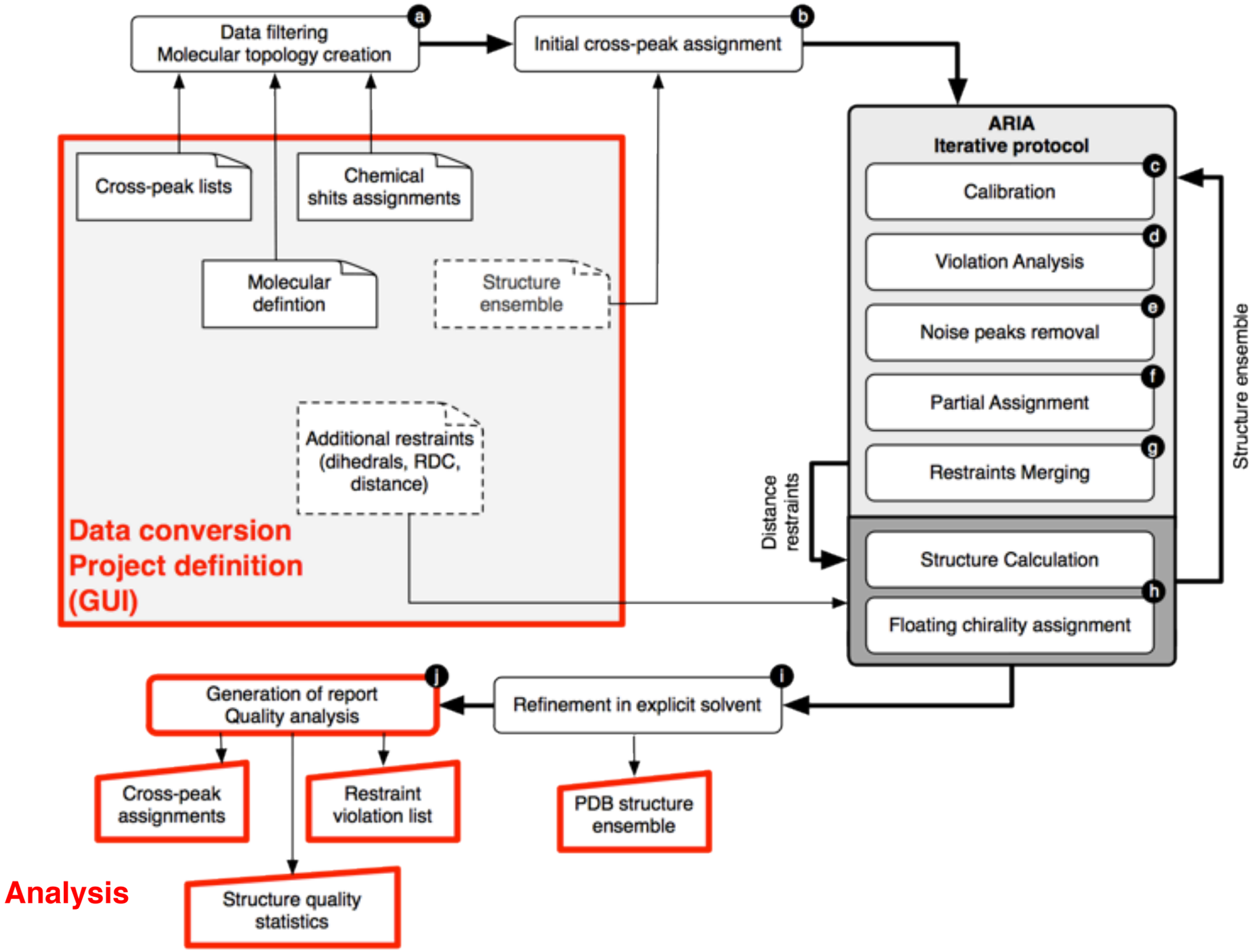
ARIA protocol: step 3

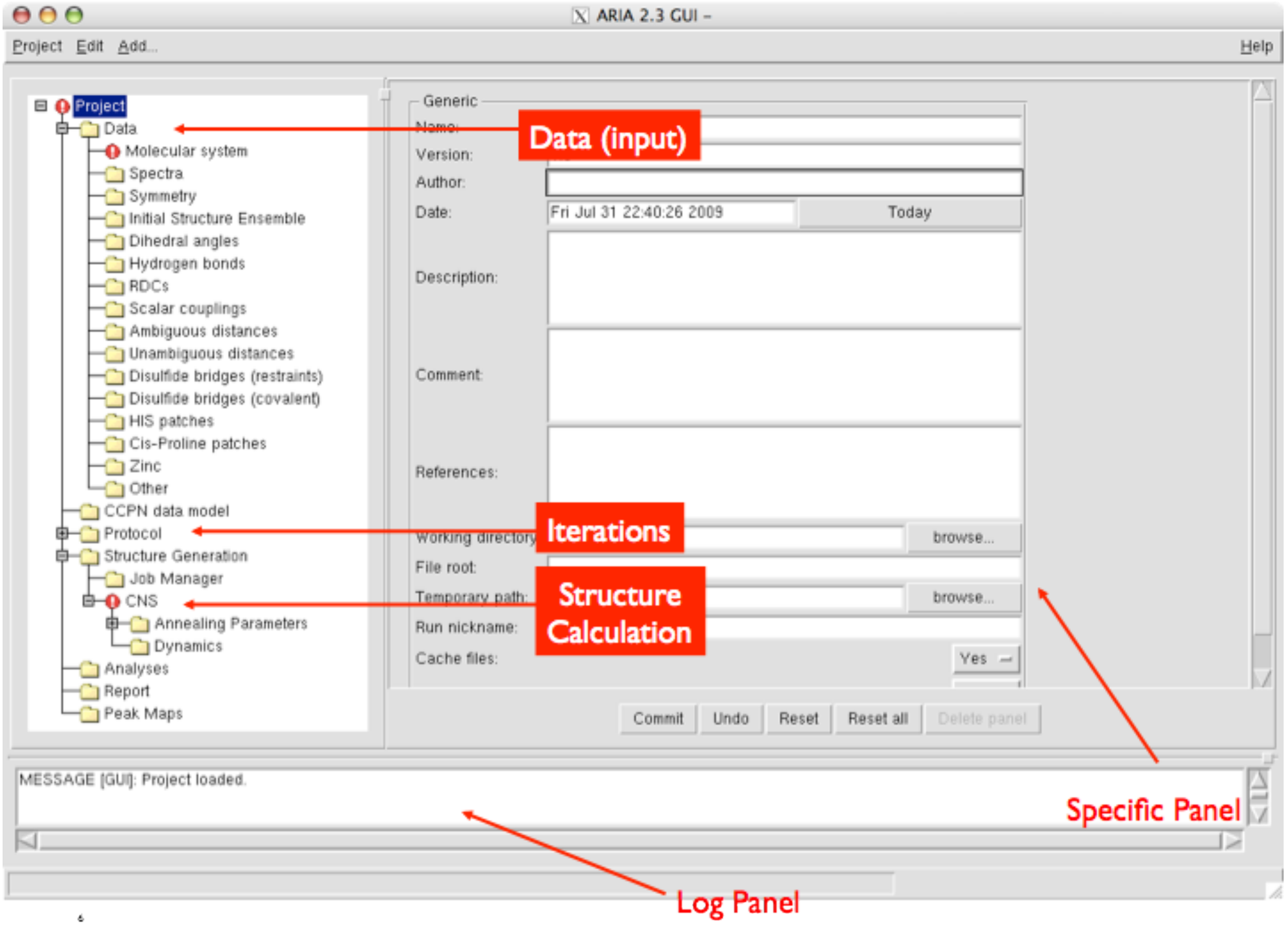


ARIA protocol: step 4



ARIA protocol: today




ARIA 2.3 GUI –
Project Edit Add... Help
Project
Data
Molecular system
Spectra
Symmetry
Initial Structure Ensemble
Dihedral angles
Hydrogen bonds
RDCs
Scalar couplings
Ambiguous distances
Unambiguous distances
Disulfide bridges (restraints)
Disulfide bridges (covalent)
HIS patches
Cis-Proline patches
Zinc
Other
CCPN data model
Protocol
Structure Generation
Job Manager
CNS
Annealing Parameters
Dynamics
Analyses
Report
Peak Maps
Generic
Name:
Version:
Author:
Date:
Fri Jul 31 22:40:26 2009
Today
Description:
Comment:
References:
Working directory:
browse...
File root:
Temporary path:
browse...
Run nickname:
Cache files:
Yes
Commit
Undo
Reset
Reset all
Delete panel
Data (input)
Iterations
Structure Calculation
Specific Panel
MESSAGE [GUI]: Project loaded.
Log Panel

ARIA commands

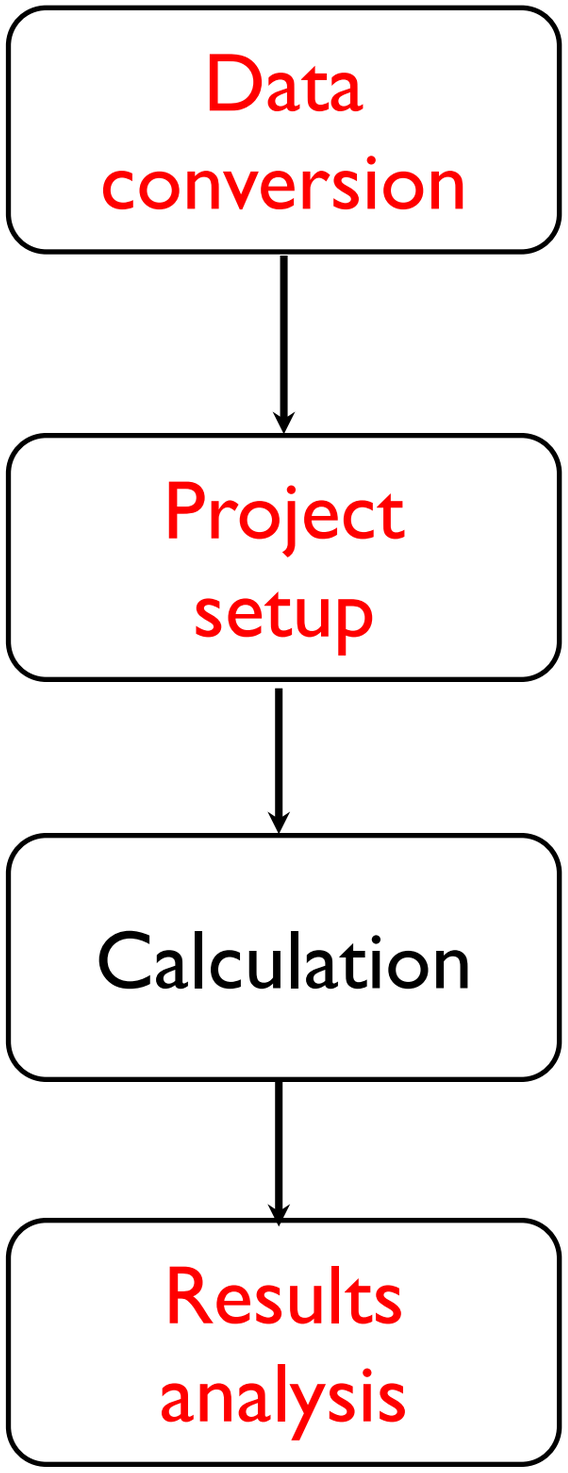
```
(aria2 --convert conversion.xml)
```

```
aria2 -g run1.xml
```

```
aria2 -s run1.xml
```

```
aria2 run1.xml
```

```
....
```



Practical

- Calculation of *tudor* domain (56 res.)
- ARIA 2.3 / CNS 1.2 (installed)
- Available data (**flat files** or **CCPN project**):
  - Sequence
  - 13C and 15N NOESY peak-lists
  - Chemical shifts assignments
  - Restraints (hydrogen bonds, torsion angles from coupling constants, RDC)

A. Conversion of data from *Xeasy* format to ARIA XML format

OR

B. *CCPN* Project

Practical

1. Setup environment *(repeat for new terminals)*
2. Step-by-step protocol
3. mostly pre-calculated to give more time for analysis

4. advanced analysis (if time allows it)