Overview of Facility Software for Biomolecular NMR

by

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09/30/2003

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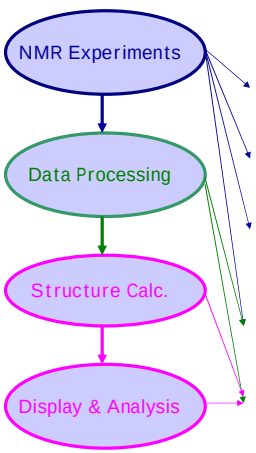
NMR Core Facility Service



Information on web

homepage for user's information

Schedule on the web

spectrometer reservation

Simple Operation Manual

step by step instruction

Useful Experiments

1D, 2D, 3D, 4D homo-, hetero- nuclear

Parameters setting

expt/proc. parameter setting with pp

NMR related Software

update and short instruction

Facility software for biomolecular NMR

NMR data processing software

- **XWINNMR** ***(process NMR data on IRIX 6.X & Linux)***

  License required

- **nmrPipe** ***(process NMR data on IRIX6.X & Linux)***

NMR data analysis software

- **AURELIA** ***(analyze NMR data on IRIX 6.X & Linux)***

  License required

- **nmrDraw** ***(analyze NMR data on IRIX 6.X & Linux)***
- **nmrView** ***(analyze NMR data on IRIX 6.X & Linux)***
- **Sparky** ***(analyze NMR data on Linux)***

NMR auto assignment

- **TATAPRO (on IRIX)**

Structure Calculation related software

- **CSI Chemical Shift Index** ***(making consensus plot on IRIX)***
- **TALOS** ***(dihedral angles prediction on*** **IRIX 6.X & Linux** ***)***
- **XPLOR** ***(structure calculation on IRIX)***
- **CNS** ***(structure calculation on IRIX6.X & Linux)***
- **ARIA** ***(auto NOE assign and structure calculation on IRIX6.X & Linux)***
- **CYANA** ***(auto NOE assign and structure calculation on IRIX6.X & Linux)***

  License required

Structure display & analysis software

- **PROCHECK** ***(structure analysis on IRIX)***
- **INSIGHT II** **(on IRIX , license from computer center)**
- **MOLMOL (on IRIX & Linux)**
- **GRASP** ***(on IRIX) License required***

NMR dynamics

- **MODELFREE (on IRIX, Linux & Euler)**

Tips for using facility software

XWINNMR ***(process NMR data)***

- **Input data : data acquired from xwinnmr**
- **How to run:**

  > xwinnmr (or , for PC, click on xwinnmr icon)

AURELIA ***(analyze NMR data)***

- **Input data: data processed by xwinnmr (2rr, 3rrr, …)**
- **How to run:**

  > aurelia filename

nmrView ***(analyze NMR data)*** http://www.nmrview.com/

- **Input data: data processed by nmrpipe or felix**
- **How to run:**

  > nmrview

TATAPRO ***(auto-assignment)***

- **Input data:**
  1. **peak picking for HNCBCA, CBCA(CO)NH, HNCO, HNCACO**
  2. **sequence in one letter code**
  3. **pml.inp**
  4. **assign.inp**
- **How to run: (the same directory as input data)**

  > pml (to create "master_list"

  > assign (start assignment)
- **Output data:**
  1. **master_list (from pml)**
  2. **assignment.final (final assignment list)**

CSI ***(making consensus plot)*** http://www.pence.ualberta.ca/ftp/csi/csi.html/

- **Input data:**
  1. **chemical shift table for HA, CA, CB, CO**

```
# AA   HA    CA    CB     CO
1   A  4.15  51.8  18.8  174.0
```

  2. **average value for Gly HA, "0" for unassigned, "C" for oxidized cysteine , "B" for reduced cysteine**
- **How to run: (the same directory as input data)**

  > csi (the following the instruction)
- **Output data:**
  1. **text output**
  2. **graphical output**

TALOS ***(dihedral angles prediction)*** http://spin.niddk.nih.gov/bax/software/TALOS/

- **Input data: chemical shift table for N, HA, CA, CB, CO**

```
1   M  HA    4.15
1   M  C   170.54
1   M  CA   54.82
1   M  CB   33.27
2   Q  N   123.01
```

- **How to run: (the same directory as input data)**

  > source nmrpipe

  > talos.tcl –in myshift.tab (to perform the database searches)

  > vina.tcl –in myshift.tab –auto (to summarized the results)

  > vina.tcl –in myshift.tab –ref mystruct.pdb –auto

  > rama.tcl –in myshift.tab (to inspect and adjust the predictions)
- **Output data:**

  pred.tab with predicted phi, psi value

ARIA ***(auto NOE assign and structure calculation)***

http://www.pasteur.fr/recherche/unites/Binfs/aria/

- **Input data:**
  1. **complete chemical shift table and 3 letter sequence file**
  2. **peak picking table for NOESY type experiment**
  3. **additional H-bond, CSI, RDC, or dihedral angles constraint**
- **How to run:**

  > source aria

  > netscape aria.html (to generate new.html file)

  > aria (to generate a "working directory" , and run.cns)

  > netscape aria.html (to edit parameter for structure cal.)

  > aria (start structure calculation based on run.cns)
- **Output data:**

  Structures in pdb

  NOE assignment table

  Structures analysis using procheckNMR

CYANA ***(auto NOE assign and structure calculation)***

- **Input data :**
  1. **complete chemical shift table and 3 letter sequence file**
  2. **peak picking table for NOESY type experiment**
  3. **additional H-bond, CSI, RDC, or dihedral angles constraint**
  4. **init.cya**
  5. **CANDID.cya**
- **How to run:**

  > cyana

  > cyana> CANDID
- **Output data: (ex: Ramachandran plot)**

PROCHECK ***(structure analysis)***

http://www.biochem.ucl.ac.uk/~roman/procheck_nmr/procheck_nmr.html

- **Input data : summary of all structures in pdb**
- **How to run:**

  > procheck

  > procheck_nmr inputname
- **Output data: (ex: Ramachandran plot)**

INSIGHT II **(structure display, license from computer center)**

- **Input data : pdb**
- **How to run:**

  > source insightII

  > insightII

MOLMOL **(structure display)** http://www.mol.biol.ethz.ch/wuthrich/software/molmol/

- **Input data : pdb**
- **How to run:**

  > molmol

GRASP ***(structure display)*** http://honiglab.cpmc.columbia.edu/grasp/

- **Input data : pdb**
- **How to run:**

  > grasp

MODELFREE ***(NMR Dynamic Data Analysis)***

http://cpmcnet.columbia.edu/dept/gsas/biochem/labs/palmer/software/modelfree.html

- **Input data:**
  1. **pdb file**
  2. **R1, R2, NOE data**
  3. **R2/R1 and d(R2/R1) data**
- **Analysis steps:**

  step1: PDBINERTIA (input original pdb to obtain int.pdb)

  step2: R2R1_TM (input R2/R1 data to obtain local tm for each spin)

  step3: QUADRIC_DIFFUSIOM

  (input step1&2 result to obtain Diso, Dration, Theta, Phi)

  step4: ModelFree analysis

  (using data from above to do modelfree analysis)