

2019 NMR Users Workshop

Steps for Protein NMR Structure Determination

High-Field NMR Center & GRC NMR LAB Academia Sinica

Date: Aug 14-16, 2019

Places: 8F Lecture Room & B2 HFNMRC, IBMS, Academia Sinica

Language: Chinese (Handout in English/Chinese) 中文解說為主

Instructors/ TAs:

Dr. Chi-Fon Chang (GRC, Academia Sinica) 張七鳳

Ms. Pei-Ju Fang (HFNMRC, Academia Sinica) 方珮如

Ms. Yi-Ping Huang (GRC, Academia Sinica) 黃意評

Dr. Yuan-Chao Lou (CHEM, Academia Sinica) 羅元超

Ms. Tsun-Ai Yu (HFNMRC, Academia Sinica) 游春愛

Software Installation TA

Mr. Roland Lee (HFNMRC, Academia Sinica) 李玉順

Topics:

- Useful Experiments for Protein NMR
- Protein Production and Labeling
- NMR Data Collection & Processing using Topspin
- Protein Resonance Assignment using Sparky
- Protein Structure Calculation using CYANA
- Protein Structure Display using MOLMOL

Hands-On:

- NMR Data Collection (in groups, 分組進行)
- NMR Data Processing (請安裝Topspin)
- Protein Backbone Assignment (請安裝Sparky)
- Protein Structure Calculation (請安裝Molmol及 PuTTY)

Registration Webpage: <https://www.nmr.sinica.edu.tw/Workshop/Workshop2019/>

Registration Deadline: **Aug. 08, 2019**

2019 NMR Users Workshop (Tentative Program)

Steps for Protein NMR Structure Determination

High-Field NMR Center & GRC NMR LAB

Academia Sinica

Day 1 : Aug. 14 (Wednesday)

Introduction & Lectures

Place: 8F Lecture Room, IBMS

- 10:00-10:20 Opening & Introductory Overview**
(Dr. Chinpan Chen & Dr. Chi-Fon Chang)
- 10:20-10:50 NMR Approach for Protein Studies (Dr. Chi-Fon Chang)**
- 10:50-11:10 Coffee Break**
- 11:10-12:00 Protein Production and Labeling (Ms. Tsun-Ai Yu)**
- 12:00-13:30 Lunch Break**
- 13:30-14:00 Basic NMR Operation & Topspin Overview (Dr. Chi-Fon Chang)**

Data Collection 14:00~ (in groups)

Place: HFNMR, B2, IBMS or GRC NMR LAB, 1F, GRC

- 90 degree pulse and O1 optimization
- 1D 1H solvent suppression
- 2D 15N-HSQC & 13C-HSQC Experiments
- Set up 3D Experiments for Protein Assignment

For those who need help on Software Installation, please bring your laptop to HFNMR, B2, IBMS during Day1.

*Topspin 安裝步驟: https://www.nmr.sinica.edu.tw/Workshop/Workshop2019/Doc/HowToGet_TopSpinCMC_FreeLicense_SOP.pdf

*Sparky 下載: <https://nmrfam.wisc.edu/nmrfam-sparky-distribution/> 解壓縮即可使用

*MOLMOL 下載: <https://sourceforge.net/projects/molmol/files/Installation%20Files/> 解壓縮即可使用

*PuTTY 下載: <https://www.putty.org/> 下載適當版本即可免費安裝

2019 NMR Users Workshop **(Tentative Program)**

Steps for Protein NMR Structure Determination

High-Field NMR Center & GRC NMR LAB

Academia Sinica

Day 2 : Aug. 15 (Thursday)

Place: 8F Lecture Room, IBMS, Academia Sinica, Taipei

Practical Session I (Topspin)

10:00-10:50 **Data Processing using Topspin (Part I) (Dr. Chi-Fon Chang)**

10:50-11:10 **Coffee Break**

11:10-12:00 **Data Processing using Topspin (Part II) (Dr. Chi-Fon Chang)**

12:00-13:30 **Lunch Break**

Practical Session II (Sparky)

13:30~ **Protein Resonance Assignment using Sparky**
(Ms. Yi-Ping Huang)

Day 3: Aug. 16 (Friday)

Place: 8F Lecture Room, IBMS, Academia Sinica, Taipei

Practical Session III (CYANA & MOLOL)

10:00-10:50 **Structure Calculation using CYANA (Part I) (Ms. Pei-Ju Fang)**

10:50-11:10 **Coffee Break**

11:10-11:30 **Structure Display using MOLMOL (Ms. Tsun-Ai Yu)**

11:30-12:00 **Structure Calculation using CYANA (Part II) (Ms. Pei-Ju Fang)**

12:00-13:30 **Lunch Break**

Group Discussion

13:30~ **Q&A**