

# 2023 NMR Users Training (II)

## Basic NMR SOP for Small Molecules & Metabolomics Analysis

此次訓練課程除簡單介紹核磁共振的應用原理外，將介紹核磁共振實驗進行小分子及代謝體訊號分析的基本步驟。其中代謝體分析將由生醫轉譯研究中心羅元超博士介紹~

In this basic training course, we will briefly introduce how to apply NMR on small molecules and metabolomics analysis. Dr. Yuan-Chao Lou from BioTReC will introduce how to make use of Bruker IVDr.

# Day 1 : 10/24 Tuesday

## Part I: Lectures (1F, GRC, Academia Sinica)

Instructor: Dr. Chi-Fon Chang, GRC & HFNMRC

10:00-10:10      Opening & Introductory Overview

10:10-11:00      Basic NMR Concept & Applications

11:00-11:20      Short Break

11:20-12:00      Useful Experiments for Small Molecule

12:00-13:30      Lunch Break

13:30-14:30      NMR Data Collection & Processing using Topspin

## Part II: Practical Hands-On (HFNMRC & GRC NMR Labs )

14:30-17:00      Hands on in Groups

## Day 2 : 10/25 Wednesday

### Part I: Lectures (1F, GRC, Academia Sinica)

Instructor: Dr. Yuan-Chao Lou, NBRP (BioTReC)

10:00-10:50 Metabolomics NMR using IVDR (I)

10:50-11:10 Short Break

11:10-12:00 Metabolomics NMR using IVDR (I)

12:00-13:30 Lunch Break

13:30-14:30 NMR Data Collection using Icon-NMR

### Part II: Practical Hands-On (HFNMRC & GRC NMR Labs)

14:30-17:00 Hands on in Groups

# 2023 NMR Users Training (II)

Basic NMR SOP for  
Small Molecules & Metabolomics Analysis

## Opening & Introductory Overview

Chi-Fon Chang  
Manager, HFNMRC  
Senior Research Specialist/Scientist, GRC  
Academia Sinica  
2023.10.24

# 高磁場核磁共振中心 High-Field NMR Center

www.nmr.sinica.edu.tw

中央研究院

Login

English



High Field 高磁場核磁共振中心  
Nuclear Magnetic Resonance Center

首頁 簡介 + 規劃與成果 + 最新消息 + 服務 + 實驗室資源 +

## HFNMRC

簡介

規劃與成果

最新消息

服務

實驗室資源

Welcome to 高磁場核磁共振中心

- [高磁場核磁共振中心 - 設施推廣影片](#) [2021 Nov.] (影片) \*
- [高磁場核磁共振中心 - 簡介](#) [2021 Jan.] (影片) \*
- [Acknowledgement Template - 使用核心致謝範例](#) \*\*
- [Protein NMR Machine Learning](#)
- [Mnova NMR Academia Sinica Campus License](#) (限院內同仁)

## News and Events

[2023 NMR Training Course II - Basic NMR SOP for Small Molecules & Metabolomics Analysis](#)

[ October 24-25th, 2023 ]

[2023 NMR Training Course I - Fragment-based Screening using NMR](#)

[ March 10th, 2023 ]

[HFNMRC Announcement : NEO500 Open for service.\(20230106\)](#)

[ Jan. 9, 2023 ]

[2022 NMR Training Course I - NMR as a tool for Nature Product Studies](#)

[ April 27th, 2022 ]

[HFNMRC Announcement : NEO600 Open for service.\(20211226\)](#)

[ Jan. 1, 2022 ]

[HFNMRC Announcement : AV600 Console Upgrade.\(20211026\)](#)

[ Nov. 1 - Dec. 15, 2021 ]

## Quick Link

[光譜儀使用時間表  
Time Reservation Table](#)

[儀器設備  
NMR Spectrometers](#)

[使用及管理辦法](#)

[服務流程](#)

[Calibration Data](#)

• [Simple Operation Guide](#)

• [Pulse Calibration Table](#)

• [Temperature Calibration Curve](#)

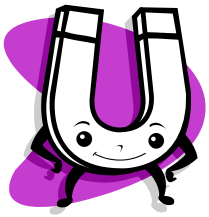
• [SR Calibration Table](#)

[中華民國生物物理學會](#)

[台灣磁共振學會 \(TMRS\)](#)

[Contact Us](#)

[User Login](#)



## High-Field NMR Center Mission

- Provide a state-of-the-art NMR facility to support NMR users
- 提供便捷穩定的高磁場液態核磁共振設施，開放院內同仁及全國使用。
- Provide competent technical support to assist NMR researchers
- 提供高水準技術支援，服務院內及全國核磁共振相關研究。
- Implement new techniques/methodologies for NMR researches
- 適時引進或開發液態核磁共振相關軟硬體技術。
- Train scientists in the field to carry out NMR related researches
- 協助液態核磁共振領域人才培訓，以支援核磁共振相關領域發展。

# High Field NMR Center ( [www.nmr.sinica.edu.tw](http://www.nmr.sinica.edu.tw) )

## AVIII850\_IBMS



19.9T



## AV800\_IBMS With SampleJet



18.8T



## NEO500\_IBMS With SampleXpress



11.8T



## AVIII600\_IBMS With SampleCase



14.1T



## NEO600\_IBMS With SampleCase



## AV600\_CHEM B1, Institute of Chemistry



# NMRs in HFNMRC

NMRs	installed	location	Probes	Notes
AVIII850	2010	IBMS B2	TXI_regular	1H/13C/15N
			TCI_Cryo	
AV800	2004	IBMS B2	TXI_regular	1H/13C/15N; with SampleJet -3 position for regular -96 positions for spinner-free -5 positons for rack (96 well-plate)
			TXI_Cryo	
AVIII600	2008 2007 (1991)*	IBMS B2	TCI_Cryo	1H/13C/15N With SampleCase (60 samples)
NEO600 (2021)	2003	IBMS B2	TCI_Cryo	1H/13C/15N With SampleCase (24 samples)
AV600_CHEM	2002	CHEM B1	TXI_regular	1H/13C/15N
			QXI_regular	1H/13C/15N/31P
			BBO_regular	BB(ex: 13C/15N/31P...)/1H
	2021		TBO regular	1H/19F/BB (ex: 13C/15N/31P...)
NEO500 (2023)	2009 2002 (1996)*	IBMS B2	TXI_Cryo	1H/13C/31P/19F with SampleXpress (60samples)
			QNP_Cryo	



# NMR Probes in HFNMRC

Regular Probe*	Detection	1H (EB) (S/N)	Others (S/N)
500MHz_TXI	1H/13C/15N	450	
600MHz_TXI	1H/31C/15N	1,218	
600MHz_BBO	Broadband	465	465 (13C)
600MHz_QXI	1H/13C/15N/31P	1,193	85(31P)
600MHz_TBO**	Broadband	945 1189(19F)	413 (13C) 404(31P)
800MHz_TXI	1H/13C/15N	2,077	

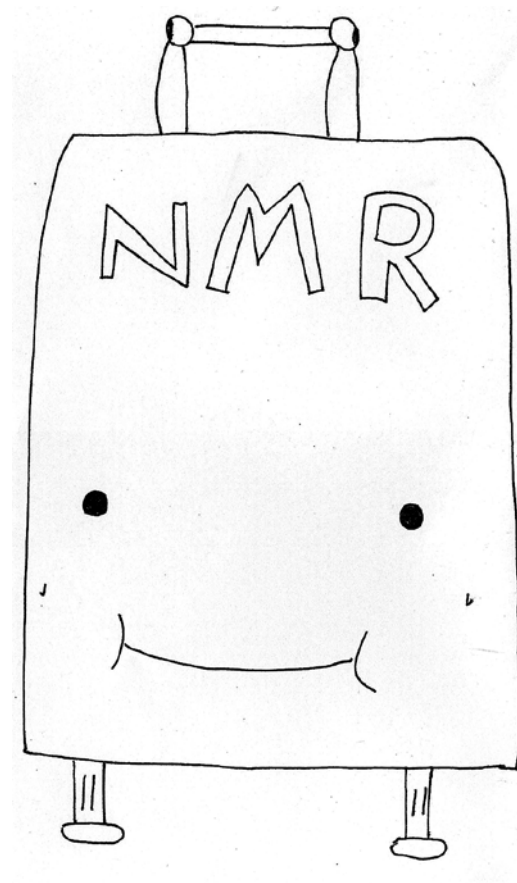
CRYO Probe*	Detection	1H (EB) (S/N)	Others (S/N)
500MHz_TXI	1H/13C/15N	4,196	
500MHz_QNP**	1H/13C/19F/31P	2,000 1197(19F)	1,000 (13C) 988 (31P)
600MHz_TCI(a)**	1H/13C/15N	5,700	710(13C)
600MHz_TCI(b)**	1H/13C/15N	6,530	950(13C)
800MHz_TXI**	1H/13C/15N	6,200	
850MHz_TCI**	1H/13C/15N	8,500	1,600(13C)

\*\*Signal to Noise (S/N )value @ installed date

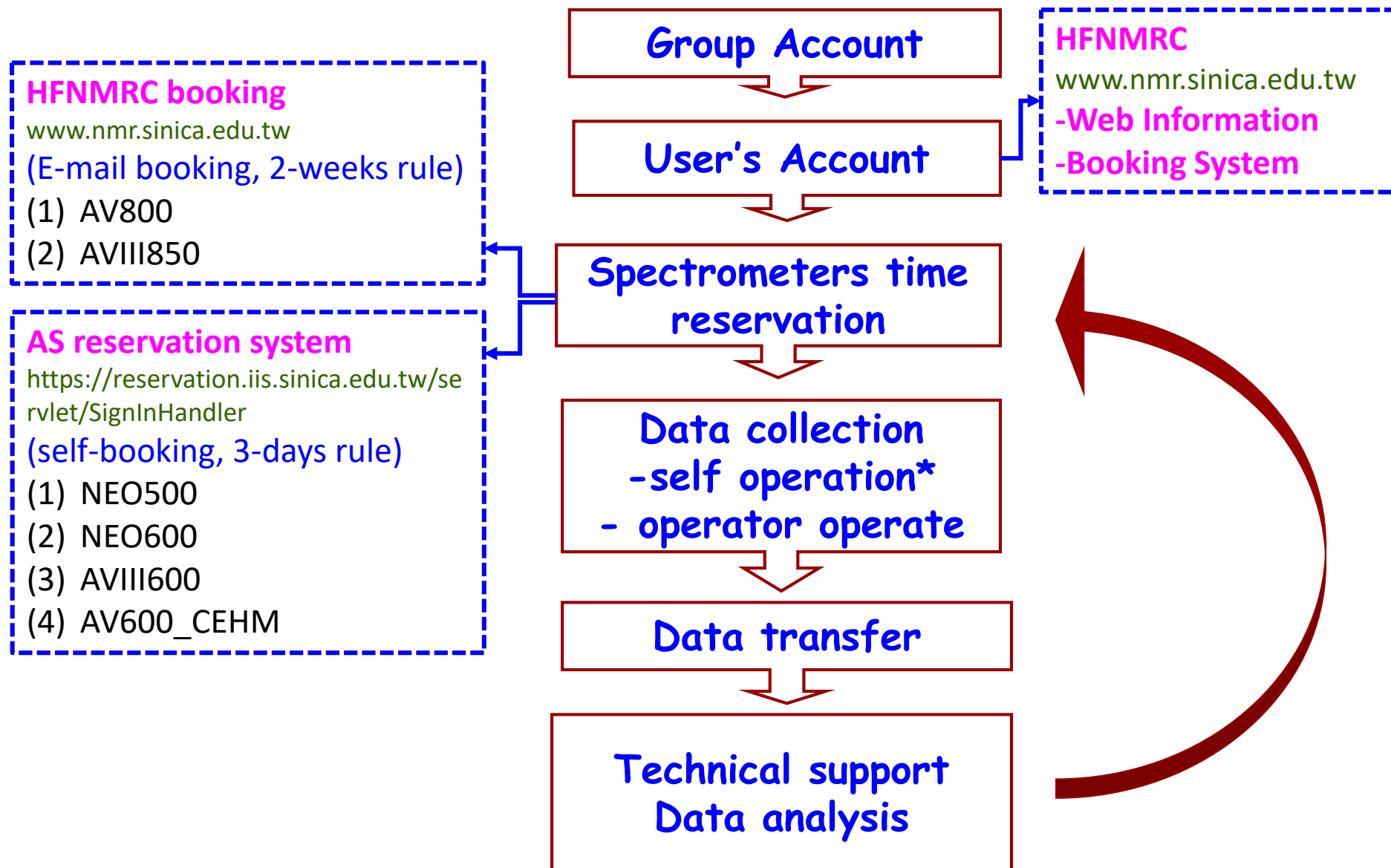
\*\*Currently installed

# How

How to apply HFNMRC service?  
使用高磁場核磁共振中心的各項服務



# HFNMRC Service Flow

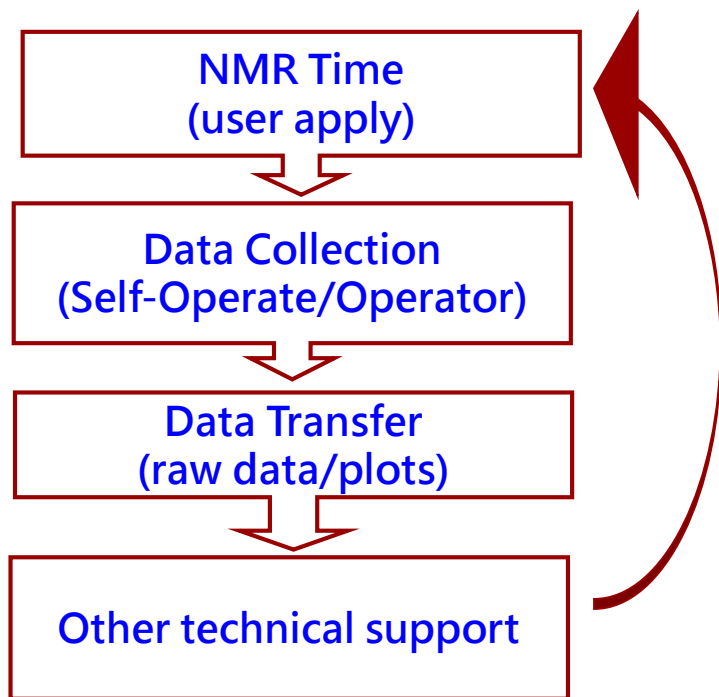


\* Self-Operation License Needed (individual training is available upon Email request)

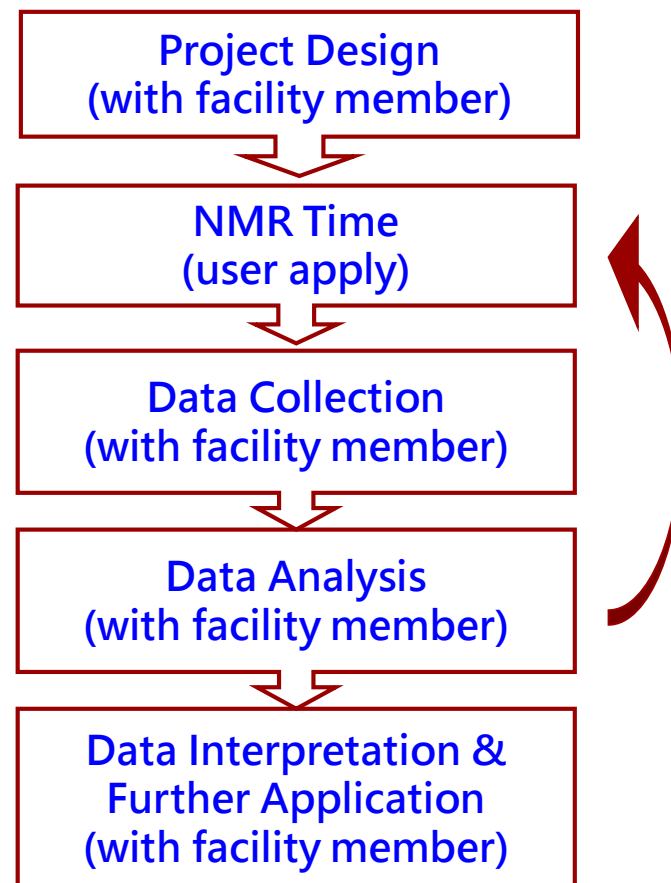
# HFNMRC Service Mode

Service Mode	Description
Routine Service (Basic Mode)	Data acquisition, experimental set up , technical consultation etc. <b>but no data analysis</b>
Advanced Service (Collaborative Mode)	<b>facility members will work with you</b> on project design, planning, data analysis, structure determination and interpretation

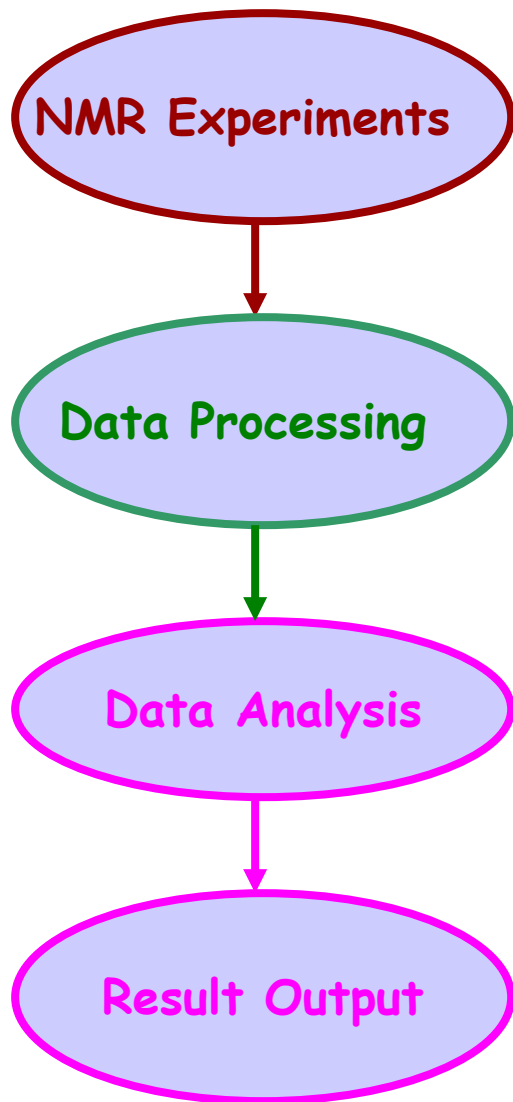
## Routine Service



## Advanced Service



## User-friendly Platform



### 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, homo-, hetero- nuclear

### Parameters setting

expt/proc. parameter setting

### NMR related Software

update and short instruction

# HFNMRC Service Charge (check webpage for most updated information)

## HFNMRC Service Charge

(Starting 2021.01.01)

	Item	Academia Sinica (NT\$)	Academia (NT\$)	Non-academia (NT\$)
1	500MHz <sup>1</sup>	100/hr	110/hr	150/hr
2	600MHz <sup>1</sup>	120/hr	130/hr	180/hr
3	800MHz <sup>1</sup>	180/hr	190/hr	270/hr
4	850MHz <sup>1</sup>	200/hr	210/hr	300/hr
5	Small Molecule Data Collection <sup>2</sup>	1,000/expt	1,000/expt	1,500/expt
6	Experiment Setup Fee for Macromolecule <sup>2</sup>	1,500/expt	1,500/expt	2,000/expt
7	Fragment Based Screening <sup>3</sup> (data collection)	70,000/case	70,000/case	100,000/case
8	Fragment Based Screening <sup>3</sup> (data collection/processing)	100,000/case	100,000/case	150,000/case

\* This fee might be adjusted according to the operational status.

1. In case of regular Room Temperature Probe, reduce N.T.80 per hr.


2. Data collection only, no data analysis nor interpretation is included.

3. Follow existing Fragment Library SOP in HFNMRC. Please find "[Data collection Service](#)" application form for details. Should you need other services, please contact us.

# GRC NMR Facility (Open to Academia Sinica Users)

## AV600R


With SampleExpress Lite

 14.1T



## AV600L

With SampleExpress Lite

 14.1T



## AV400

In HFNMR

 9.4T



Probe		1H (EB)	Others
<b>Cryo Dual (1H/13C)</b>	TP2.x	3,200	<b>2,600 (13C)</b>

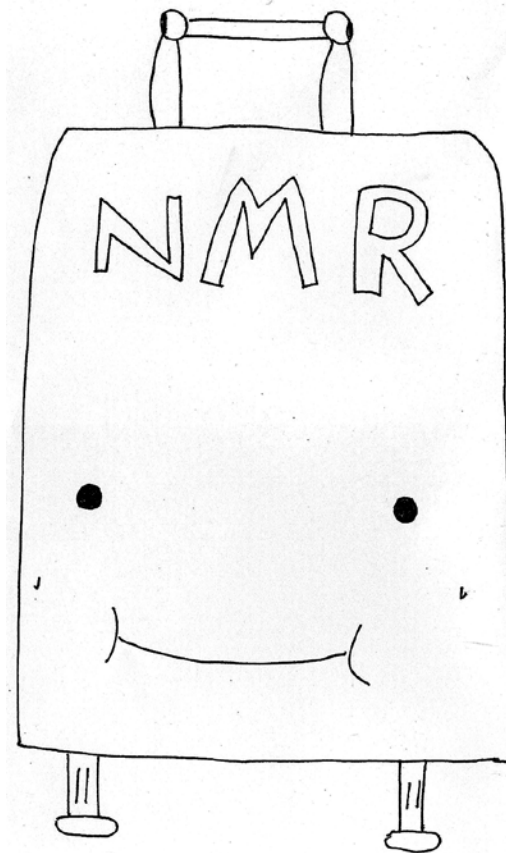
Probe		1H (EB)	Others
<b>Cryo_TCI (1H/13C/15N)</b>	TP3.x	<b>3,800</b>	935 (13C)

Probe		1H (EB)	Others
<b>Dual (1H/13C)</b>	TP2.x	214	176 (13C)

# Who

Looking for Facility Members ?

核心人員







NMR LAB would be happy to work with you,  
and learn from your research !!



**Tsun-Ai Yu**  
HFNMRC



**Pei-Ju Fang**  
HFNMRC



**Geok-Soon Lee**  
HFNMRC/ Hardware



**Yi-Ping Huang**  
GRC





GRC, Academia Sinica  
基因體中心  
&

High-Field NMR Center is supported by  
Dept. of Academic Affairs and Instrument Service  
中研院學術處



**ALL USERS  
(GRC & HFNMC)**