

2022 NMR Users Training (I)

NMR as a tool for Nature Product Studies

Opening & Introductory Overview

NMR是分析天然物的重要工具之一, 然而如何克服天然物濃度及純度問題是一大考驗. 此次特別邀請化學所吳英彥博士介紹各種有利於天然物分析的NMR實驗方法, 生化所林曉青博士則將分享天然物NMR 圖譜分析的技巧. 歡迎大家踴躍參與此次訓練課程!!

In this training course, we are happy to invite Dr. Ying-Yen Wu (Institute of Chemistry) and Dr. Hsiao-Ching Lin (Institute of Biological Chemistry) to share their experience on Nature Products studies and Data analysis SOP.

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Senior Research Specialist/Scientist, GRC
Academia Sinica
2022.04.27

Part I: Lectures (B1C, IBMS, Academia Sinica)

09:40-	Registration
10:00-10:10	Opening & Introductory Overview Dr. Chi-Fon Chang, GRC & HFNMRC
10:10-11:00	Useful NMR Experiments for Nature Products Dr. Ying-Yen Wu, Chemistry
11:00-11:10	Short Break
11:10-12:00	Tasks in NMR data analysis for Nature Products Dr. Hsiao-Ching Lin, IBC
12:00-13:30	Lunch Break

Part II: Practical Hands-On (B1C & NMR Labs)

13:30-14:20	Setting up NMR Experiment in HFNMRC Dr. Chi-Fon Chang
14:20-14:30	Short Break
14:30-17:00	Hands-on in groups

2022 NMR Users Training (I)

**New Hardware/Software in
High-Field NMR Center**

AV600_IBMS 控制台升級成 AVANCE NEO (AV600 console upgrade to NEO)

The screenshot shows the website of the High Field Nuclear Magnetic Resonance Center (HFNMR Center) at the Academia Sinica. The page features a navigation menu, a main content area with a welcome message and news, and a sidebar with quick links. The announcement regarding the AV600 console upgrade is highlighted with a pink box.

高磁場核磁共振中心 High Field | × +

← → ↻ 不安全 | 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 +

HFNMR

- 簡介
- 規劃與成果
- 最新消息
- 服務
- 實驗室資源

Welcome to HFNMR

- Attention: 高磁場核磁共振中心防疫須知 (HFNMR Safety Precautions)**
- 高磁場核磁共振中心 - 設施推廣影片 [2021 Nov.] (影片) * new !!
- 高磁場核磁共振中心 - 簡介 [2021 Jan.] (影片) * new !!
- Acknowledgement Template - 使用核心致謝範例 new !!**
- Protein NMR Machine Learning new !!**
- Mnova NMR Academia Sinica Campus License (限院內同仁)**

News and Events

HFNMR Announcement : AV600 Console Upgrade (20211026)
[Nov. 1 - Dec. 15, 2021]

[第二十五屆生物物理研討會 | The 25th Biophysics Conference](#)
[May. 20-23, 2021]

[2021 NMR Users Workshop - Steps for Protein NMR Structure Determination \(配合「COVID-19公眾集會因應指引」, 延期舉辦\)](#)
[Jan. 27-29, 2021]

[2020 NMR Training Course II - NMR as a tool for Metabolomics](#)
[Nov. 30th, 2020]

[Symposium : 9th \(biennial\) Western Sydney University & Inaugural Asian Symposium on NMR, MRI & Diffusion 2020](#)
[Dec. 2-3, 2020]

[2020生物醫學核磁共振新知研討會 / 2020 Meeting on the Frontiers of Biological and Medicinal Magnetic Resonance](#)
[Dec. 18, 2020]

>> [more News ...](#)

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

NEO 600
(SampleCase-24 samples)
With TCI Cryoprobe
($^1\text{H}/^{13}\text{C}/^{15}\text{N}$)



AVANCE NEO console
with multi-receiver



What's new for AVANCE_NEO 600 ?

- A SampleCase (24 samples) is available (Please see video)
安裝自動送樣機 (影片介紹)

The image shows two overlapping browser windows from the HFNMRC website. The top window displays the main navigation menu with a link for 'BRUKER NEO 600' highlighted in a pink box. The bottom window shows the content of this page, with a list of resources under the 'Others' section highlighted in a pink box.

BRUKER NEO 600
[[Introduction Page](#)]

- **Calibration Data** [Login](#)
 - Pulse Calibration Table
 - Temperature Calibration Curve
 - SR Calibration Table
- **Others** [Login](#)
 - Tips Using Sample Case (.pdf) [Last updated : 20211230]
 - How to user NEO600 with SampleCase (Chinese) (YouTube video) [Last updated : 20211226]
 - How to user NEO600 with SampleCase (English) (YouTube video) [Last updated : 20211226]

Attention:

(1) Pay attention on the length of your sample tube !!

From the top of spinner to the top of tube <9.5cm

注意樣品管高度!! 樣品管不可突出spinner 9.5cm以上!!



(2) Manually switch sample command : **sx #**

→ your sample position , or empty position

手動變更樣品指令: **sx #** (取出時可轉到沒有樣品的空號即可!!)

(3) To learn icon-NMR for automation, please contact us!

如欲學習設定icon-NMR, 請洽核心人員

What's new for AVANCE_NEO 600 ?

- A SampleCase (24 samples) is available (Please see video)
安裝自動送樣機 (影片介紹)
- NEO must use Topspin4.x or higher version (SOP Video)
NEO 必需使用Topspin4.x 以上版本操作 (影片介紹)
- ◆ Routinely used commends are the same as Topspin2.x or Topspin3.x
指令與Topspin2.x or Topspin3.x 相通
- ◆ Interface is different but not too difficult to follow
介面稍有不同, 熟悉即可
- ◆ HFNMR Standard Experiments and SOP are the same
實驗設定方式與本核心其它NMR相同
- ◆ Please see video for brief introduction, and you can read manual for more details
請看影片簡單介紹, 如需更多細節請參考使用者手冊

◆ Topspin4.x Interface

The screenshot displays the Topspin4.x software interface. The main window is titled 'user_manual_topsp...'. The interface includes a menu bar (1) with options like 'Acquire', 'Process', 'Analyse', 'Applications', and 'Manage'. Below the menu bar is a workflow button bar (2) with icons for 'Create Dataset', 'Sample', 'Lock', 'Tune', 'Spin', 'Shim', 'Pzsol', 'Gain', 'Run', and 'More'. A tool bar (3) is located below the workflow buttons. On the left side, there is a browser and search window (4) showing a search for 'exam1d_13C' and a list of results. Below the search window is a structure window (5) displaying a chemical structure. At the bottom left, there is a command line (6) and a current dataset bar (7) showing '1d_13C 1 1 C:\Bruker\examdata'. The main area is a dataset window (9) displaying a spectrum plot with peaks. Above the spectrum plot are dataset window tabs (10) for 'SPECTRUM', 'PROCPARS', 'ACQPARS', 'TITLE', 'PULSEPROG', 'PEAKS', 'INTEGRALS', 'SAMPLE', 'STRUCTURE', 'PLOT', 'FID', and 'ACQU'. Below the spectrum plot is a status display bar (8) showing '1d_13C 1 1 C:\Bruker\examdata'. On the right side, there is a vertical toolbar (11) with icons for 'Print', 'Export', 'Copy', and 'Publish'. Below the toolbar are viewing options (12) and window switcher/login/setup preferences/help options (13).

1	Menu Bar	8	Status Display Bar
2	Workflow Button Bar	9	Dataset Window
3	Tool Bar	10	Dataset Window Tabs
4	Browser and Search Window	11	Print, Export, Copy and Publish
5	Structure Window, Command Line History, Status Line History	12	Viewing Options
6	Command Line	13	Window Switcher, Login, Setup Preferences and Help
7	Current Dataset Bar		

High Field NMR Center (www.nmr.sinica.edu.tw)

AVIII850_IBMS

 19.9T



AV800_IBMS

With SampleJet

 18.8T



AV500_IBMS

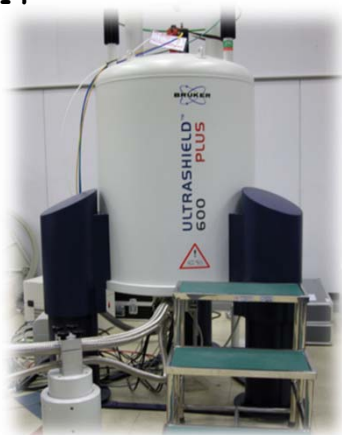
With SampleXpress

 11.8T



AVIII600_IBMS

 14.1T



NEO600_IBMS

With SampleCase

 14.1T



AV600_CHEM

 14.1T



NMRs in HFNMRC

NMRs	Installed	Location	Probes	Note *Current installed probe
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	IBMS B2	TCI_Cryo*	1H/13C/15N
NEO600	2022	IBMS B2	TCI_Cryo*	1H/13C/15N with SampleCase (24 samples)
AV600_CHEM	2002	CHEM B1	TXI/QXI_regular	1H/19F/BB (ex: 13C/15N/31P)
			TBO_regular*	
			BBO_regular	
AV500	2009	IBMS B2	TXI_Cryo	1H/13C/31P/19F with SampleXpress (60samples)
			QNP_Cryo*	



NMR Probes S/N ratio in HFNMRC

Regular Probe*	1H (EB)	Others
500MHz_TXI	450	
600MHz_TXI	1,218	
600MHz_BBO	465	465 (13C)
600MHz_QXI	1,193	85(31P)
600MHz_TBO		
800MHz_TXI	2,077	

CRYO Probe*	1H (EB)	Others
500MHz_TXI	4,196	
500MHz_QNP	2,000	1,000 (13C) 988 (31P)
600MHz_TCI_005	5,700	710(13C)
600MHz_TCI_121	6,530	950(13C)
800MHz_TXI	6,200	
850MHz_TCI	8,500	1,600(13C)

NMR & Probe	Topspin	1H (EB)	Others
AV500_IBMS (Cryo QNP)	TP2.x	2,000	1,000 (13C) 988 (31P) 1,000 (19F)
AVIII600_IBMS (Cryo TCI_005)	TP2.x TP3.x	5,700	710(13C)
NEO600_IBMS (Cryo TCI_121)	TP4.x	6,530	950(13C)
AV600_CHEM (regular TBO)	TP2.x	406	377(13C) 241(31P) 342(19F)
AV800_IBMS (Cryo TXI)	TP2.x	6,200	N/A
AVIII850_IBMS (Cryo TCI)	TP2.x TP3.x	8,500	1,600(13C)

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