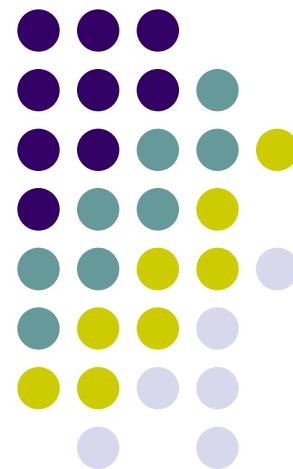


# **The NMR Lab at the School of Chemical Sciences University of Illinois - Spring 2017**

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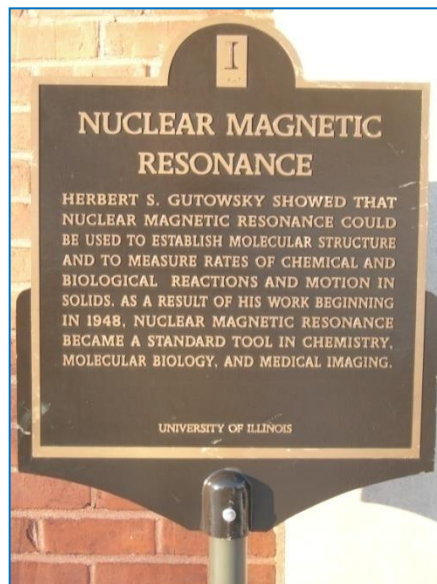
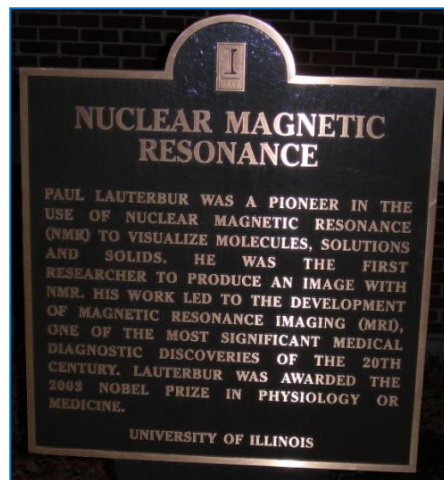
Dr. Dean Olson, Director  
dolson@illinois.edu; 146 RAL  
217-244-0564 (Lab); 722-9432 (Cell)



## Illinois:

- A tradition of NMR
- A community of NMR

**Prof. Anthony Leggett**  
**Nobel Prize, 2003**  
**Superfluidity and**  
**Superconductivity**



A plaque just outside  
the Chemical Life Sciences  
Laboratory  
commemorating  
**Paul Lauterbur**,  
Professor of Chemistry,  
U of Illinois. Nobel Prize,  
2003 for MRI.

Another plaque, outside  
Noyes Lab (SE corner),  
honors **Herb Gutowsky**  
Professor of Chemistry,  
U of Illinois.  
He was the first to “apply the  
nuclear magnetic resonance  
method to chemical  
research. His experimental  
and theoretical work on the  
**chemical shift effect and its  
relation to molecular  
structure.**”

# An easy, fast way to the SCS website



scs nmr

About 225,000 results (0.19 seconds)

Everything

Images

Videos

News

Shopping

More

Champaign, IL  
[Change location](#)

All results

[Related searches](#)

[More search tools](#)

▶ [NMR Laboratory, School of Chemical Sciences, University of Illinois](#) ☆ 🔍

The School of Chemical Sciences **NMR** Lab is the finest academic laboratory in the country in terms of the availability and types of services offered. ...

[www.scs.illinois.edu/nmr/](http://www.scs.illinois.edu/nmr/) - [Cached](#)

[PDF] [A GUIDE TO THE SCS NMR LABORATORY](#) ☆ 🔍

File Format: PDF/Adobe Acrobat - [Quick View](#)

NMR Lab Instrumentation Cost Rate Summary. See the **SCS NMR** Website for the ...

[www.scs.illinois.edu/nmr/handouts/getting\\_started/UGL010-20JAN11.pdf](http://www.scs.illinois.edu/nmr/handouts/getting_started/UGL010-20JAN11.pdf)

[VOICE NMR Lab - School of Chemical Sciences | University of ...](#) ☆ 🔍

This web site has been moved. Please go to <http://www.scs.uiuc.edu/nmr> ...

[www.scs.illinois.edu/~mainzw/VOICE\\_NMR\\_Lab/](http://www.scs.illinois.edu/~mainzw/VOICE_NMR_Lab/) - [Cached](#)

[Show more results from illinois.edu](#)

[SCS NMR Status](#) ☆ 🔍

**SCS NMR** Status. Monday, February 7, 2011. U400 - RAL - OK. U500 - RAL - OK. UI400 - RAL - OK. UI500NB - RAL - OK. VXR500 - RAL - OK. UI300WB - NL - OK ...

[scsnmrstatus.blogspot.com/](http://scsnmrstatus.blogspot.com/) - [Cached](#)

Google: scs nmr <return> (first hit)

[SCS HOME](#)[Spectrometer  
Status Now](#)[Carver B500  
Sample Queue](#)[ChemFOM](#)[Mnova Software](#)[NMR HOME](#)[Staff](#)[Handouts & Tools](#)[NMR Training Puzzle](#)[NMR Rate Table](#)[Instruments](#) ▶[Schedules](#)[Location Maps](#)

## Welcome to the NMR Laboratory

The NMR Lab of the School of Chemical Sciences offers a wide range of spectrometers, probes, and technical capabilities including multi-dimensional, multi-nuclear, and solid-state NMR. Supported by four full-time staff and two student hourlies, ten spectrometers in three locations allow walk-up and long-term NMR experiments 24/7. Spectrometers at 400 MHz, 500 MHz, and 600 MHz are available for short-to-medium length experiments; 750 MHz and 300 MHz wide-bore spectrometers with specialty probes and solids accessories can perform multinuclear and solid state NMR experiments. All are equipped for variable temperature operation. Our ten Varian spectrometers and 1 Bruker spectrometer include (in MHz): Seven liquid-state NMRs: 400 (two), 500 (four), 600; Two solid-state NMRs: 500, 750; Two liquid/solid compatible NMRs: 300 and 750. An automated Bruker CryoProbe was added in the summer of 2016. We also provide automated, on-flow NMR sample analysis (from vials) for undergrad organic chemistry courses offered via the Department of Chemistry. Electronics and IT staff provide additional support.

To make the most of NMR as an analytical tool, all newcomers receive about 4 hours of individual basic training with additional instruction available for variable temperature

# SCS NMR Status Now

Tuesday, January 3, 2017

## SCS NMR Spectrometer Status Now

Updated 3 Jan 2017 (DLO):

Working Status of Spectrometers.

Monday - Friday, 9 a.m. to 5:30 p.m., just walk in.

After business hours, use your i-Card (swipe several times as needed).

Take a quick look  
if you need  
confirmation  
in advance.

### RAL Spectrometers (Check ChemFOM for Availability):

- Carver-Bruker 500 CryoProbe (CB500) - **OK**
  - Ask the staff for account registration, then a trained person in your group for automation instruction.
- U500 - **OK**
- UI400 - **OK** H-1, **C-13**, P-31, F-19; No B-11. Use LN2 bucket for cooling. No spinning.
- UI500NB - **OK**. OK for all 1D and 2D NMR, but calibrate pw90 and T1 for protons using posted modification (very minor).
  - Now optimized for BioPak.
- VXR500 - **OK** for H, C, P, F. VT -60 to +80 C
- SUNDS1 - **OK**
- Printers - Both **OK**


### Noyes Lab Spectrometers

- UI300WB- **OK**; Reservations via Andre Sutrisno.
- UI600 - **OK**; Reservations via Lingyang Zhu.
- chem400 - **OK**; Chem 237 & 205 use only via DLO.

### Chem Life Spectrometer

- VNS750NB - **OK**; Reservations via Lingyang Zhu.  
Currently in Solution-State NMR configuration.

# ChemFOM Website (via SCS NMR)



Time on server  
Tuesday Jan. 3  
11:55:34

- » Admin Home
- » User Home
- » U500 (School of C ▾)
- » Departments
- » Supervisors
- » Resources Admin
- » Maint. Records
- » Users Admin
- » Email List
- » Collaborate & Service
- » Usage Records
- » Purchase Supplies
- » Documents
- » User Report
- » My Profile
- » My Accounts
- » Contact Manager
- » Logout
- » User Forum

**UIUC - FOM - Schedule**

Notes from equipment manager

**Equipment Schedule: U500**

- U500 MHz Spectrometer in 146 RAL
- U500 is now Available
- Your user level on this equipment is: Equipment Manager.

10/17 10/24 10/31 11/07 11/14 11/21 11/28 12/05

Today Jan 3, 2017

Mon 12/12	Tue 12/13	Wed 12/14	Thu 12/15	Fri 12/16
<a href="#">Click to show sessions from midnight to 08:00</a>				
08:00 - 08:10	08:00 - 08:10	08:00 - 08:10	08:00 - 08:10	08:00 - 08:10
08:10 - 08:20	08:10 - 08:20	08:10 - 08:20	08:10 - 08:20	08:10 - 08:20
08:20 - 08:30	08:20 - 08:30	08:20 - 08:30	08:20 - 08:30	08:20 - 08:30
08:30 - 08:40	Samuel Gockel, 08:26-08:32	08:30 - 08:40	08:30 - 08:40	08:30 - 08:40
Raundi Quevedo, 08:45-08:54	08:40 - 08:50	08:40 - 08:50	08:40 - 08:50	Emilio Carlos de Lucca Junior, 08:41-08:51
08:50 - 09:00	08:50 - 09:00	08:50 - 09:00	08:50 - 09:00	
09:00 - 09:10	09:00 - 09:10	09:00 - 09:10	Dean Olson, 09:04-09:08	09:00 - 09:10
09:10 - 09:20	09:10 - 09:20	Anthony Grillo, 09:18-09:23	Menghua Xiong, 09:10-09:28	09:10 - 09:20
Summer Laffoon, 09:22-09:27	09:20 - 09:30	Riley Svec, 09:23-09:36		09:20 - 09:30
Rulin Ma, 09:28-09:40	09:30 - 09:40		Anthony Grillo, 09:31-09:45	09:30 - 09:40
09:40 - 09:50	09:40 - 09:50	Anthony Grillo, 09:40-09:47		09:40 - 09:50
09:50 - 10:00	09:50 - 10:00	Tae Ann Kim, 09:47-09:54	09:50 - 10:00	09:50 - 10:00
10:00 - 10:10	Michelle Richter, 09:56-10:04	Michaela Carlson, 10:09-10:23	Brad Gilbert, 10:01-10:08	10:00 - 10:10
Brad Gilbert, 10:14-10:24	10:10 - 10:20		10:10 - 10:20	Hsuan-Chin Wang, 10:10-10:26
	Ephraim Gabriel Morado, 10:20-10:27		10:20 - 10:30	
10:30 - 10:40	Zhiyuan Han, 10:29-11:01	Yingfeng Yang, 10:25-10:36	Thomas Bearrood, 10:29-10:33	Raundi Quevedo, 10:28-10:33
Cass Richers, 10:35-10:42		Siraj Ali, 10:37-10:47	Courtney Ford, 10:36-10:53	Anasheh Sookezian, 10:38-10:44
Yanhua Xu, 10:49-11:11		Michaela Carlson, 10:50-11:08		10:50 - 11:00
	Bryon Drown, 11:08-11:25	11:10 - 11:20	Bailey Jackson, 10:59-11:19	Lucas Hernandez, 11:07-11:14
Ephraim Gabriel Morado, 11:12-11:21		Michaela Carlson, 11:29-11:42	Wei Liu, 11:19-11:25	Jon Young, 11:19-11:25
Spinner Spinner, 11:31-11:47 //For maintenance	Emma Southgate, 11:30-11:35		Tiara Brown, 11:29-11:36	11:30 - 11:40
	11:40 - 11:50		Nitrogen Nitrogen, 11:37-12:20 //For maintenance	11:40 - 11:50
Sung Hoon Kim, 11:48-11:57	11:50 - 12:00	Yanhua Xu, 11:52-12:10		11:50 - 12:00
	Helium Helium, 12:07-12:22 //For maintenance			12:00 - 12:10
Hsuan-Chin Wang, 12:08-12:30		12:10 - 12:20		12:10 - 12:20
		Melanie Trobe, 12:20-12:34	12:20 - 12:30	Alfredo Garcia, 12:18-12:23
Courtney Ford, 12:30-12:41	Tiara Brown, 12:30-12:39		Liang Ma, 12:30-12:30	12:30 - 12:40
		Brittany Walker, 12:40-12:50		12:40 - 12:50

**Follow the Reservation Protocols  
in Training Booklet and Posted in Lab**

SCS HOME

Spectrometer  
Status Now

Carver B500  
Sample Queue

ChemFOM

Mnova Software

NMR HOME

Staff

Handouts & Tools

NMR Training Puzzle

NMR Rate Table

Instruments ▶

## GETTING STARTED IN THE NMR LAB

---

- NMR Lab Overview ←
- New User Training Booklet - page 1 ←
- NMR Financial Authorization and Responsibility Form ←
- Introduction to Basic NMR
- A Guide to the SCS NMR LAB
- Basic NMR Theory; an Introduction
- UI400 Reservation Protocol
- U500 Reservation Protocol
- UI500NB Reservation Protocol
- VXR500 Reservation Protocol
- NMR Data Access and Backup
- Data Backup and Storage Policies



# General Experiments Handouts

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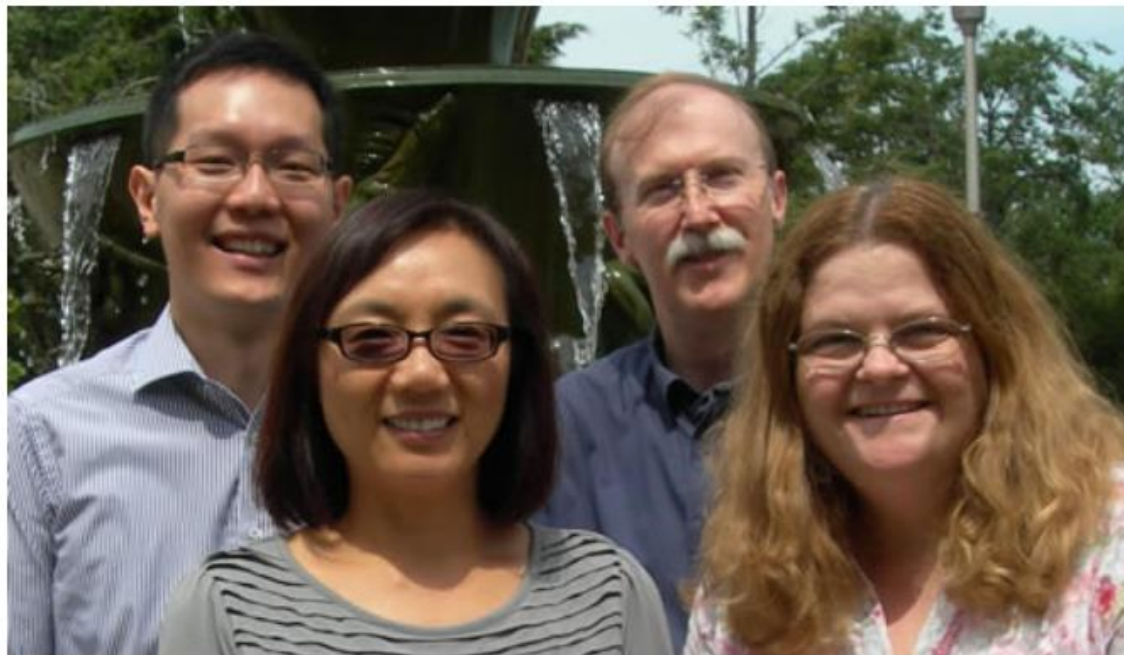
- Abbreviated Command and Parameter List
- Apodization
- APT ←
- $^{13}\text{C}$  Sensitivity for Mass Limited Samples Nano Probe vs 3mm  $^{13}\text{C}\{^1\text{H}\}$
- COSY ←
- DEPT ←
- Deuterated NMR Solvents
- External Referencing of Samples
- HETCOR
- Homodecoupling
- $^1\text{H}\{^{31}\text{P}\}$  — Phosphorus Decoupled Proton NMR on the UI400 or U500
- Locking
- Manipulation of Multiple Spectra
- 90 Degree Pulse Width Determination
- NMR Chemical Shifts
- NOE 1D Difference Experiment-cycloenoe NOE ←
- NOESY1D-(DPFGSE NOE) Experiment for Measurement of Transient NOE's





- Optimizing 1D Array Acquisition Parameters
- Phase Sensitive 2D Data
- Phosphorus 31 Standard QUAD Probe [ $^1\text{H}/^{19}\text{F}$ ] - [ $^{15}\text{N}$ - $^{31}\text{P}$ ] Broadband Probe
- Processing and Phasing Phase-Sensitive 2D Data (includes gHMQC, gHSQC) ←
- Quick GCOSY Experiment on UI500NB ←
- Quick GHMBC Experiment on UI500NB ←
- Quick GHMQC Experiment on UI500NB ←
- Quick Instructions for No-D NMR or How to Take a Spectrum of Your Reaction Mixture ←
- Quick Instructions for the Presat Experiment or How to Suppress your Solvent Peak ←
- Quick Instructions for Using the UI500NB ←
- Quick pw90 (90 Degree Pulse Width) Determination
- Quick T1 Determination
- Sample Preparation, Positioning, and Insertion
- Shimming
- Shimming an NMR Magnet
- T1 Measurement
- User Macros
- Using the Optical Drive on the SUNDS1
- Variable Temperature

## SCS NMR Staff



NMR Lab Staff - (from left to right) Andre Sutrisno, Lingyang Zhu,  
Dean Olson, and Tracie Hubert

**Four full-time staff members**

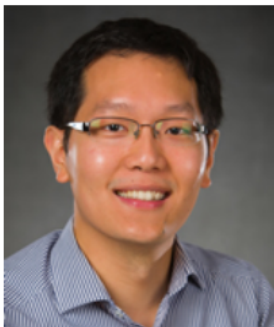


**Tracie Hubert**  
Technical Administrator

146 Roger Adams Lab  
Box 66-5  
(217) 333-2041  
[tlhubert@illinois.edu](mailto:tlhubert@illinois.edu)

**Responsibilities:** Training Intake, ChemFOM and Business Functions

*Tracie is a native of Champaign, Illinois, and has worked in the NMR Lab for over 30 years.*



**Andre Sutrisno, Ph.D.**  
Spectroscopist

55 Noyes Laboratory  
Box 31-1  
(217) 333-4997  
[asutrisn@illinois.edu](mailto:asutrisn@illinois.edu)

Secured Lab

**Responsibilities:** Solid-State NMR, Computers, Software, and System Administration

*Andre grew up in Jakarta, Indonesia, and spent about 10 years in Canada before moving to Illinois.*

**Lingyang Zhu, Ph.D.**  
Spectroscopist

55 Noyes Laboratory  
Box 34-1  
(217) 333-6283  
[lingyang@illinois.edu](mailto:lingyang@illinois.edu)

Secured Lab

**Responsibilities:** Solution NMR, Computers, Software, and System Administration

*Originally from Liaoning province in China, Lingyang comes to us via Colorado where she spent several years in industry before moving to Illinois.*

# SCS NMR Staff



**Dean Olson, Ph.D.**  
Lab Director

146 Roger Adams Lab  
(217) 244-0564  
Box 81-5  
[dolson@illinois.edu](mailto:dolson@illinois.edu)

**Responsibilities:** Overall Lab Operations

*Dean is originally from Saint Paul, Minnesota, USA.*

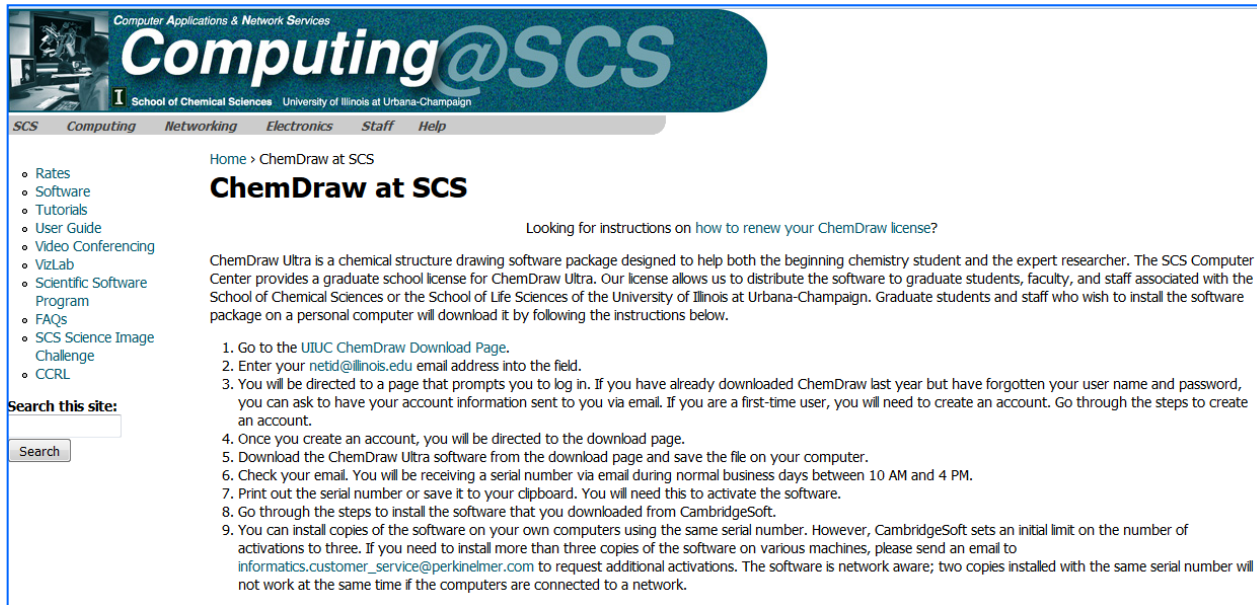
## I. NMR Spectrometers

NMR Instrument	<sup>1</sup> H Freq MHz (Tesla)	Probes	Location
UI300	300 (7.05)	5mm Varian <sup>1</sup> H/X probe, X= <sup>31</sup> P- <sup>15</sup> N (default probe) 10mm GE <sup>15</sup> N- <sup>31</sup> P Broadband probe 20mm GE <sup>17</sup> O- <sup>73</sup> Ge Broadband probe 10mm GE <sup>17</sup> O{X} probe 20mm GE <sup>183</sup> W{X} probe 7mm Chemagnetic <sup>31</sup> P- <sup>29</sup> Si probe 7mm Chemagnetic <sup>29</sup> Si- <sup>15</sup> N probe 4mm Chemagnetic <sup>31</sup> P- <sup>15</sup> N probe 3.2mm Chemagnetic <sup>31</sup> P- <sup>15</sup> N probe Chemagnetic <sup>2</sup> H probe, broadband,	55 NL
Replaced with CB500 Summer 2016			
U500	500 (11.75)	5mm Nalorac QUAD probe ( <sup>1</sup> H, <sup>19</sup> F, <sup>13</sup> C, <sup>31</sup> P)	150 RAL
VXR500	500 (11.75)	5mm Nalorac QUAD probe ( <sup>1</sup> H, <sup>19</sup> F, <sup>13</sup> C, <sup>31</sup> P) PFG Z probe 70 microL Varian <sup>13</sup> C{ <sup>1</sup> H} Nanoprobe	148 RAL
UI500NB	500 (11.75)	5mm Varian <sup>1</sup> H{ <sup>13</sup> C/ <sup>15</sup> N} PFG Z probe 5mm Varian <sup>1</sup> H{ <sup>31</sup> P/X} PFG Z probe 5mm Varian <sup>1</sup> H/X probe, X= <sup>31</sup> P- <sup>15</sup> N 10mm Varian <sup>15</sup> N- <sup>31</sup> P Broadband probe.	146 RAL
VNS500WB	500 (11.75)	3.2mm Triple Resonance HFX MAS Solids Probe, 500 MHz 3.2mm Triple Res HCN MAS Balun Solids Probe 3.2mm Quad Resonance HCDN MAS Solids Probe, VT, 500WB 3.2mm Double Resonance HX MAS Gradient Probe, VT, 500WB 7 mm Doty <sup>15</sup> N- <sup>31</sup> P CPMAS Probe	55 NL
UI600	600 (14.1)	5mm Varian <sup>1</sup> H{ <sup>13</sup> C/ <sup>15</sup> N} PFG X, Y, Z probe 5mm Varian AutoTuneX <sup>1</sup> H/X PFG Z probe, X= <sup>31</sup> P- <sup>15</sup> N 10mm Varian <sup>15</sup> N- <sup>31</sup> P Broadband probe	55 NL
VNS750NB - Magnet Down	750 (17.6)	5mm Varian <sup>1</sup> H{ <sup>13</sup> C/ <sup>15</sup> N} PFG X, Y, Z probe 3mm Varian <sup>13</sup> C{ <sup>1</sup> H}probe 5mm Varian <sup>13</sup> C{ <sup>1</sup> H}probe	A151 CLSL

## NMR Equipment

- 11 Spectrometers
- Over 30 NMR Probes
- 150 Visits/Day to RAL
- Lots of good colleagues
- Vnmr data station
- Ability to get NMR data via your own computer
- CB500 is a 500 MHz automated CryoProbe

# How to get ChemBioDraw



The screenshot shows the 'Computing@SCS' website. The header includes 'Computer Applications & Network Services' and 'School of Chemical Sciences University of Illinois at Urbana-Champaign'. A navigation bar lists 'SCS', 'Computing', 'Networking', 'Electronics', 'Staff', and 'Help'. A left sidebar contains a list of links: Rates, Software, Tutorials, User Guide, Video Conferencing, VizLab, Scientific Software Program, FAQs, SCS Science Image Challenge, and CCRL. The main content area is titled 'ChemDraw at SCS' and includes a link to 'Home > ChemDraw at SCS'. Below the title is a link to 'Looking for instructions on how to renew your ChemDraw license?'. A paragraph describes ChemDraw Ultra as a chemical structure drawing software package. A numbered list of 9 steps provides instructions for downloading and installing the software, including details about account creation, email verification, and activation.

Computer Applications & Network Services  
**Computing@SCS**  
School of Chemical Sciences University of Illinois at Urbana-Champaign

SCS Computing Networking Electronics Staff Help

Home > ChemDraw at SCS

## ChemDraw at SCS

Looking for instructions on how to renew your ChemDraw license?

ChemDraw Ultra is a chemical structure drawing software package designed to help both the beginning chemistry student and the expert researcher. The SCS Computer Center provides a graduate school license for ChemDraw Ultra. Our license allows us to distribute the software to graduate students, faculty, and staff associated with the School of Chemical Sciences or the School of Life Sciences of the University of Illinois at Urbana-Champaign. Graduate students and staff who wish to install the software package on a personal computer will download it by following the instructions below.

1. Go to the UIUC ChemDraw Download Page.
2. Enter your netid@illinois.edu email address into the field.
3. You will be directed to a page that prompts you to log in. If you have already downloaded ChemDraw last year but have forgotten your user name and password, you can ask to have your account information sent to you via email. If you are a first-time user, you will need to create an account. Go through the steps to create an account.
4. Once you create an account, you will be directed to the download page.
5. Download the ChemDraw Ultra software from the download page and save the file on your computer.
6. Check your email. You will be receiving a serial number via email during normal business days between 10 AM and 4 PM.
7. Print out the serial number or save it to your clipboard. You will need this to activate the software.
8. Go through the steps to install the software that you downloaded from CambridgeSoft.
9. You can install copies of the software on your own computers using the same serial number. However, CambridgeSoft sets an initial limit on the number of activations to three. If you need to install more than three copies of the software on various machines, please send an email to [informatics.customer\\_service@perkinelmer.com](mailto:informatics.customer_service@perkinelmer.com) to request additional activations. The software is network aware; two copies installed with the same serial number will not work at the same time if the computers are connected to a network.

**Follow instructions to download ChemBioDraw Ultra 13.0 (Windows or Mac).**

- **E-mail address required**
- **Licensing takes 24 – 48 hr**

<http://www.chem.illinois.edu/clcwebsite/ChemDrawUIUC.html>

**You'll need a UIUC E-mail address.**



# A Few Under-Appreciated NMR Data Processing Shortcuts

ffa	f full aph cdc dc
disp	f full aph cdc dc vsadj dscale
proc	wft f full aph cdc dc ds vsadj dscale
ppmh	wp=10p sp=-0.5p
diff	r1=delta r1? [displays the difference in Hertz between two cursors]
doi	f full intmod='partial' cz cdc dc isadj
ipart	intmod='partial'
plot	pl pscale pap page
plotT	pl pscale pltext page
plotI	vp=12 pl pscale pir pap page
plotA	pl('all') pap page
plotAs	pl('all') pscale pap page
p7	references the chloroform residual signal in $^1\text{H}$ to 7.26 ppm (pick peak first)
p77	references the chloroform residual signal in $^{13}\text{C}$ to 77 ppm (pick peak first)

# Why do NMR? Statics & Dynamics



- Structure confirmation for synthesis
  - Functional groups; counting carbons
- How my compound compares with literature NMR data; multinuclear analysis
- Purity analysis (see next spectrum)
- How much did I make? Quantitative NMR
- Reaction rates or reaction monitoring (VT)
- Rate constants; Equilibrium constants
- Diffusion coefficients: Monomer? Dimer?
- Number-average MW ( $M_n$ ) for polymers



# Can NMR Help Me?



- Investigate chemical questions to see if NMR can provide an answer
  - Don't assume NMR can't do it; it's a rich field
  - NMR has a 2 annual conference (abstracts):
    - Exp. NMR Conf.: <http://www.enc-conference.org>
    - SMASH NMR: <http://www.smashnmr.org/main.asp>
- Take advantage of your colleagues doing NMR; they are a *great* resource
- Stretch your NMR skill set (especially 2D)
  - Better research, publications, thesis
  - People with extra skills get jobs more easily

# Why Visit the NMR Lab?



**“I wish I had done more NMR sooner.”**

**- Quote from a 5<sup>th</sup> year grad student**