USC College and USC Provost's Nuclear Magnetic Resonance Spectroscopy Center

at the Department of Chemistry

WELCOME TO THE LAB!

We're glad you're here

Your NMR lab is designed and set up to help you address the most common molecular characterization needs that you will encounter. Each instrument is configured to address particular classes of problems, and the management is eager to show you how to use this technology to solve your unique structure determination problems.

NMR FREQUENCY CAPABILITIES

Isotope	Spin	9.39 T Hg 400	9.39 T 400MR	11.74 T 500S	11.74 T AMX-500	14.09 T 600S	Natural Abundance	Relative Sensitivity	Absolute Sensitivity
^{1}H	1/2	399.952	399.952	499.843	499.843	599.944	99.99	62.899	5877.739
^{19}F	1/2	376.331	376.331	470.322	470.322	564.511	100.00	52.400	4897.181
^{31}P	1/2	161.904	161.904	202.340	202.340	242.862	100.00	4.172	389.947
^{7}Li	3/2		155.437	194.258	194.258	233.161	92.41	3.692	318.871
^{119}Sn	-1/2		149.145	186.395	186.395	223.723	8.59	3.262	26.185
^{87}Rb	3/2		130.869	163.555	163.555	196.309	27.83	2.204	57.314
^{11}B	3/2		128.320	160.369	160.369	192.486	80.10	2.077	155.509
^{125}Te	-1/2		126.184	157.699	157.699	189.281	7.07	1.975	13.052
^{71}Ga	3/2		121.972	152.435	152.435	182.962	39.89	1.784	66.512
^{81}Br	3/2		108.015	134.993	134.993	162.027	49.31	1.239	57.099
^{23}Na	3/2		105.795	132.218	132.218	158.697	100.00	1.164	108.801
^{27}Al	5/2		104.215	130.244	130.244	156.327	100.00	1.113	103.999
^{13}C	1/2	100.568	100.568	125.686	125.686	150.856	1.07	1.000	1.000
^{79}Br	3/2		100.206	125.233	125.233	150.313	50.69	0.989	46.864
^{55}Mn	5/2		99.144	123.906	123.906	148.720	100.00	0.958	89.545
^{195}Pt	1/2		85.977	107.450	107.450	128.969	33.832	0.625	19.756
^{29}Si	-1/2		79.459	99.305	99.305	119.192	4.68	0.493	2.159
^{77}Se	1/2		76.277	95.328	95.328	114.418	7.63	0.436	3.111
^{199}Hg	1/2		71.635	89.526	89.526	107.455	16.87	0.361	5.697
^{2}H	1	61.395	61.395	76.729	76.729	92.095	0.02	0.228	0.003
^{15}N	-1/2			50.668	50.668	60.815	0.37	0.066	0.023
^{14}N	1			36.120	36.120		99.632	0.024	2.211
^{95}Mo	5/2			30.775	30.775		15.92	0.017	0.259

RED: Nuclei that are set up on the high-band channel
BLUE: Nuclei that are set up on the broadband channel
GREEN: ^{2}H is available on the lock channel
PURPLE: ^{15}N is has a dedicated channel on the 600 MHz TR probe
BLACK: Nuclei that are available upon request
GREY: Nuclei that are available on the instrument's backup probe

} ^{19}F is dual channel on the AMX-500

This list is not intended to be comprehensive.

NMR SOLVENT DATA

Solvent	B.P. °C	M.P. °C	^{1}H NMR δ (multiplicity) ppm	^{13}C NMR δ (multiplicity) ppm	^{1}H NMR δ (HOD) ppm
Acetic Acid	117.9	16	11.65 (1), 2.04 (5)	178.99 (1), 20.00 (7)	11.5
Acetone	56.2	-94.7	2.05 (5)	206.68 (13), 29.92 (7)	2
Acetonitrile	81.6	-43.8	1.94 (5)	118.69 (1), 1.39 (7)	2.1
Benzene	80.31	5.5	7.16 (1)	128.39 (3)	0.4
Chloroform	67.7	-63.6	7.26 (1)	77.23 (3)	1.56
1,2-Dichloroethane	83.5	-35.7	3.73(1)	43.5 (6)	
Dichloromethane	39.8	-95.1	5.32 (3)	49.15 (7)	1.5
DMF	153	-60.4	8.03 (1), 2.92 (5), 2.75 (5)	163.15 (3), 34.89 (7), 29.76 (7)	3.5
DMSO	189	18.5	2.50 (5)	39.51 (7)	3.3
1,4-Dioxane	101.1	11.8	3.53 (m)	66.66 (5)	2.4
EtOD	78.3		5.29, 3.56, 1.11	56.96 (5), 17.31 (7)	
Diethyl ether	34.6	-117.4	3.48 (4), 1.21(3)	65.91, 15.2	
HMPA	235	7	2.65 (2)	36.87	
MeOH	64.6	-97.7	3.49 (1), 1.09 (1)	49.15 (7)	4.9
Nitromethane	101.2	-29	4.33 (1)	62.5	
Pyridine	115.2	-41.6	8.74 (1), 7.58 (1), 7.22 (1)	150.35 (3), 135.91 (3), 123.87 (5)	5
THF	66	-108.5	3.58 (1), 1.73 (1)	67.57 (5), 25.37 (1)	2.4-2.5
Toluene	110.6	-95	7.09 (m), 7.00 (1), 6.98 (m), 2.09 (5)	137.86 (1), 129.24 (3), 128.33 (3), 125.49 (3), 20.4 (7)	0.4
TEA	89.5	-114.7	2.53 (4), 1.03 (3)	46.25, 11.6	
D_2O	100	0	4.8		4.8

PRICE SCHEDULE

Instrument	Chemistry 8am - 10pm	Chemistry Night	USC College 8am - 10pm	USC College Night	USC 8am - 10pm	USC Night	Commercial 8am - 10pm	Commercial Night
Mercury 400	$0	$0	$0	$0	$0	$0	$90	$45
400MR	$1.50	$1	$5	$2.50	$5	$2.50	$100	$50
AMX-500	$0	$0	$0	$0	$0	$0	$75	$37.50
VNMR 500	$0	$0	$7	$3.50	$10	$5	$125	$62.50
VNMRS 600	$4	$2	$12	$6	$12	$6	$150	$75
MALDI	$0		$30		$40			
IR, UV-vis, fluorimeter, polarimeter	$0		$15		$25			

IN THE EVENT OF AN EMERGENCY

If you break something

Do not worry. Accidents happen.

Follow these instructions to insure that all users and the instrument are safe.

- Try to contact one of the following people (in this order):
  - Allan Kershaw x06376; LJS 159
  - Prof. Travis Williams x05961; H: 323 284-8480; C: 626 262-3961; Wife: 626 376 5130; LHI 104
  - Dr. Ralf Haiges W: x19573; W: x08957
  - Corey Schultz W: x07037; pager: 213 919-0051
- If you are unable to contact one of these persons directly, then email:
  - Allan Kershaw allan@kershaw.usc.edu
  - cc: Prof. Travis Williams travisw@usc.edu
  - cc: Cory Schultz cschultz@usc.edu
- Give the following information to whomever you contact:
  - Where was it broken (in magnet, in spinner. etc)
  - What was in the NMR tube
  - What are the hazards of this sample
  - What are the solvents involved
- Do not attempt to clean the magnet or the spinner yourself.
  - Collect loose broken glass and place in one spot.
  - Do not replace the $CDCl_3$ standard, if this is what was broken.
- Mark the instrument as unusable so no other users will attempt to use it.
  - You are responsible for the instrument until one of the administrators has taken responsibility of the situation from you.
  - Once the problem has been cleared by the administrator, the instrument will be reopened.

Common software bugs and fixes

- VNMRJ often freezes in mid-acquisition. If this happens, press the "stop" and then "setup hardware" buttons in the acquisition window pane. You might also try loading and processing a known-good spectrum. If these do not solve the problem, call one of the administrators above.
- Autolock often fails to find z0. If this happens, try manually locking your solvent, then re-start your automated acquisition.
- Gradient autoshim sometime fails to converge. Try manually locking and shimming, then re-start your automated acquisition.

- Keep the spinners clean! By not leaving fingerprints and oils on the spinners, you help us avoid accumulating residue in the probes and bores.

PENALTIES AND FINES

Accidents are OK. Negligence is not.

Your user fees and the facility budget take care of normal instrument repair and cleaning. If you are using the instrument at the time that an accident happens or an instrument breaks, that's no problem. We'll get it fixed.

Users and research sponsors will be held liable for misuse or abuse of shared research facilities. All users must follow the USC code of ethics. Cheating on a lab, misusing instrumentation, abusing NMR signup rules, damaging or defacing log books, and taking unfair advantage of co-workers are all serious violations that can occur in the NMR lab. None will be tolerated. Ever.

In the event of a property or health threatening

EMERGENCY, DIAL 04321

or, from your cell phone, 213 740 4321

WHAT TO USE AND HOW TO USE IT

How to begin

Sign up for NMR time on the web at http://nmrnet.usc.edu.

What instrument should I use?

- Varian Mercury 400: Small molecule ^{1}H{^{13}C} experiments and kinetics
  - Primary probe: Indirect ^{13}C{^{1}H}, temp: –20° – +80 °C
  - Backup: AutoSwitchable Broadband ^{1}H/^{19}F{^{31}P/^{13}C}, temp: –80° – 130 °C

- Varian 400MR: Small molecule experiments in automation
  - Primary probe: AutoX Broadband ^{1}H-^{19}F{^{31}P-^{15}N}, temp: 25° – 130 °C
  - Backup: AutoSwitchable Broadband ^{1}H/^{19}F{^{31}P/^{13}C}, temp: 25° – 130 °C

  There is no low temperature module on the 400MRs because this feature does not work well with automation features.

- Varian VNMRS 500: Small molecules, materials, kinetics
  - Primary probe: OneNMR ^{1}H-^{19}F{^{31}P-^{15}N}, temp: –80° – 130 °C
  - Backup: AutoX Broadband ^{1}H-^{19}F{^{31}P-^{95}Mo}, temp: –80° – 130 °C

- Bruker AMX-500: Small molecules, low frequency nuclei, ^{1}H{^{19}F}
  - Primary probe: Quad ^{1}H,^{19}F, ^{31}P, ^{13}C, temp: –100° – 100 °C
  - Backup: Broadband ^{31}P-^{15}N{^{1}H}, temp: –100° – 100 °C
  - Backup: Inverse Broadband ^{31}P-^{15}N{^{1}H}, temp: –100° – 100 °C

- Varian VNMRS 600: Macromolecules, difficult small molecules, extended duration VT experiments
  - Primary probe: Triple Resonance ^{1}H{^{13}C}{^{15}N}, temp: –20° – 80 °C
  - Backup: AutoX Broadband ^{1}H-^{19}F{^{31}P-^{15}N}, temp: –80° – 100 °C

How do I retrieve and process my data?

Data can be downloaded from ftp://nmrnet.usc.edu. FIDs can be processed via ssh://vnmrwrk.usc.edu or AcornNMR NUTS under the USC site licenses. Ask for assistance getting started.

FACILITY MANAGER AND DIRECTORS

Allan Kershaw
Manager

Travis Williams
Small Molecule NMR

Mark Thompson
Optical, Mass, and X-ray

Rich Roberts
Macromolecular NMR

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National Center for Research Resources