

*Major technical improvements for
NMR spectroscopy*

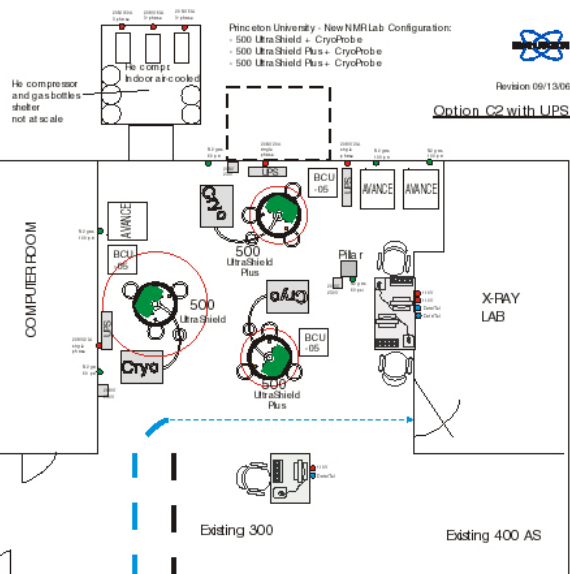
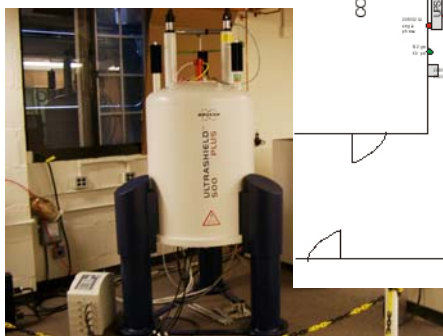
Very high field commercial magnets,
now available up to 950 MHz



Cryoprobes, with 3-5 times higher
sensitivity at the given field strength



*The first of three
new 500 MHz
NMR
instruments at
Princeton*



Cryoprobes:
 TCI ; $^{13}\text{C}/\text{H}$ dual ; QNP (C/P/N,H)

Cryoprobes

A-1: TCI – triple resonance, ^{13}C -enhanced

A-2: DCH – dual $^{13}\text{C}/^1\text{H}$ (^{13}C optimized)

A-3: QNP – four/two nuclei $^{31}\text{P}, ^{13}\text{C}, ^{15}\text{N}/^1\text{H}$

Backup RT probes

X/H (BBO) – X tunable between ^{109}Ag - ^{31}P
(VT: $-180\text{oC}/+150\text{oC}$)

TXI (HCN) – triple resonance
(VT: $-180\text{oC}/+150\text{oC}$)

DCH CryoProbe (Bruker-Biospin)



C = ^{13}C Enhanced 4X

H = ^1H Enhanced 5X

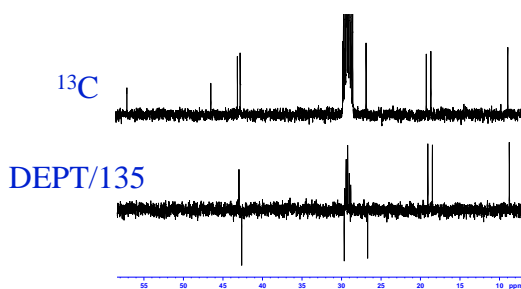
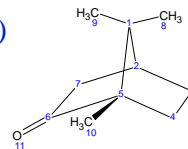
5mm
 ^2H Lock
z-Gradient
Up to 700MHz

(Courtesy of Kim Colson, Bruker-Biospin)

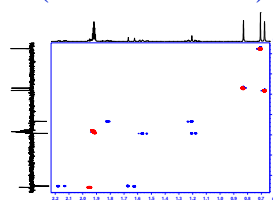
Detection power of the cryoprobe

4.4mg Camphor at 400MHz (DCH cryoprobe)

^1H : 1 scan
 ^{13}C : 1 scan
DEPT : 1 scan
HSQC : 1 scan (3m 40s)



Multiplicity edited
HSQC
(inverse detected)

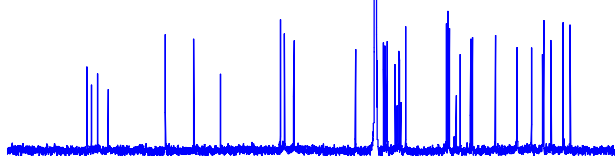


(Courtesy of Kim Colson, Bruker-Biospin)

Azadirachtin – ^{13}C and DEPT

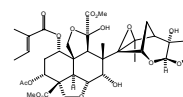
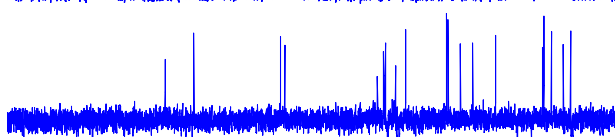
5mm Dual (C,H) z-Grad. CryoProbe

10mM azadirachtin



1 hour
 ^{13}C -NMR

1 minute
DEPT-135



Bruker 5mm 500MHz Dual z-gradient CryoProbe

Azadirachtin was kindly provided by Peter Grice (University of Cambridge UK)

(Courtesy of Kim Colson, Bruker-Biospin)

QNP CryoProbe



^{31}P , ^{13}C , ^{15}N Observe 4X S/N
 ^1H Decouple 4X S/N
 ^2H Lock
z-Gradient
5mm

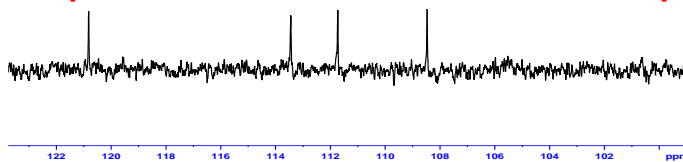
Available at 500MHz

QNP CryoProbe – ^{15}N Observe

^{15}N spectra of 25 mM cyclosporin A
 ^{15}N at natural abundance.

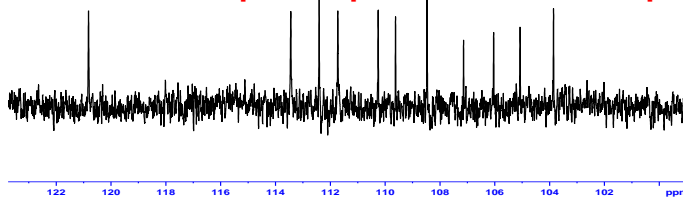
INEPT Expt

13 min expt



Inverse Gated Decoupled experiment

17h expt



500MHz QNP CryoProbe





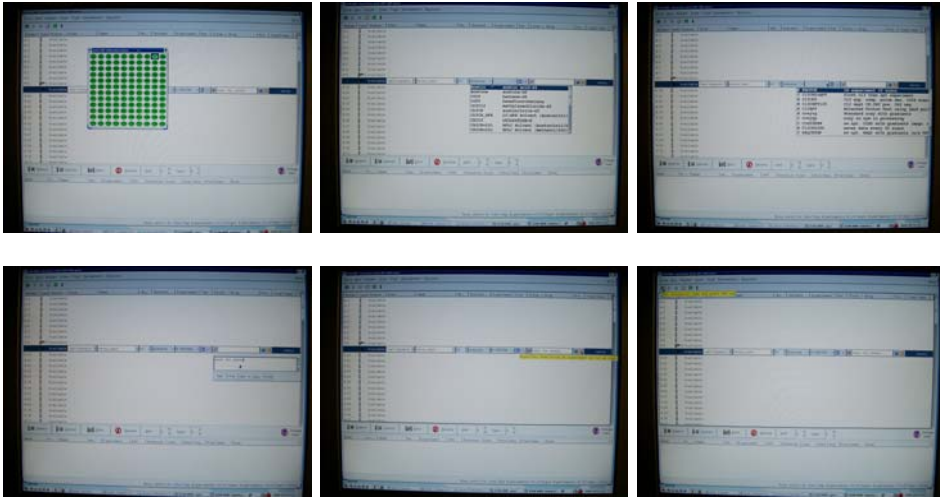


Default use of the Bruker instruments

TopSpin 2.0 (22 for off-line use)^w

Default user operation: automation through IconNMR

IconNMR interface



Important requirements, conditions

7" tubes **only** for the autosamplers !

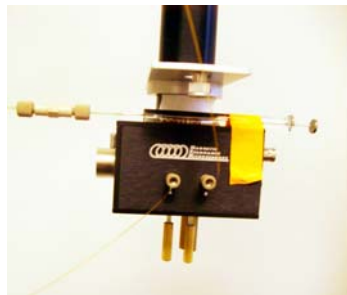
VT between -10oC and +80oC !



Capillary flow probe

(Protasis/MRM)

a competitive device for mass-limited samples



Introducing The One-Minute NMR System

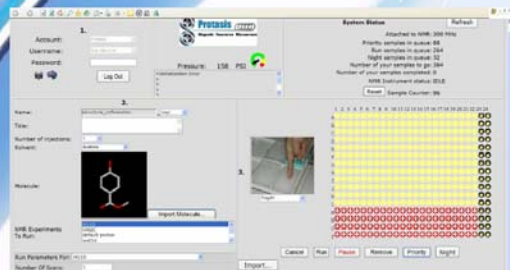
- Optimized Liquid Handling
- Application-Tuned CapNMR Probe
- Exclusive Spectrometer Interfaces
- Robust Software
- Collaboration With Partners and End-Users



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One-Minute NMR Software

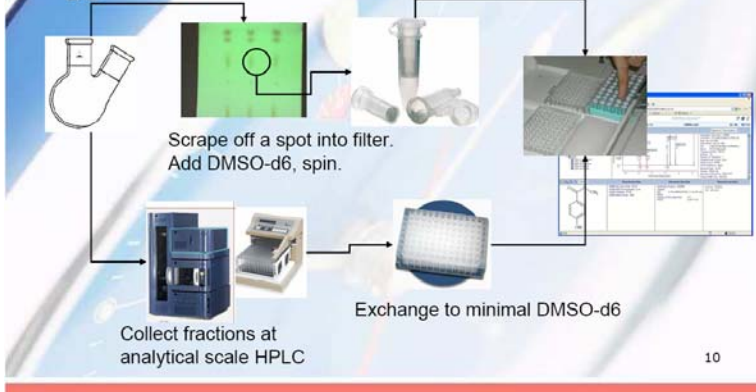
Web-Based Open Access Sample Queue Management



- Secure Log-In
- Individual sample entry and Molecule upload
- .ZIP/.CSV Sample lists and molecule upload
- Bar-code support
- Open SQL Server
- Custom Fields
- LDAP Login

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The Advantages of CapNMR (micro-scale) Scaled-Down Purifications



Robotic capillary NMR system



(as installed at Princeton University in 2005, in collaboration with Protasis/MRM and Novatia)

Additional software

TopSpin 2.0 (22 – floating license)^W

MNova (alpha-2, beta is coming in a month or so)^{WLM}
...in combination with NMRPredict (H, C, F, N)
(Mestrelab, Modgraph – unlimited*)

ACD 1D/2D Processor (v.9.0) (unlimited*)^W
...H and C Predictor (v.8.5, one working copy)

AMIX (1) and AMIX-Viewer (3) (Bruker)^W

NMRPipe, Chenomx, SIMCA-P, XPlor-NIH, etc.

Old instruments?

INOVA-600 – capillary applications

INOVA-500 – other X nuclei (^{11}B , ^{29}Si , etc.) wide VT

INOVA-400 – ^{19}F ?, quick routine use, 8mm probe H/X
wide VT

Mercury-300 – quick routine use, teaching instrument?

What we have?

A-1: Fully operational (except ATM).

A-2: Fully operational with RT (BBO) probe,
cryoprobe to be installed in a few days/a week

A-3: To be installed in few weeks

Cap/R: To be installed in few weeks

What is in the works?

User accounts and settings, selection of suitable
experiments, parameters

Server, networking (old Varian-s later), communication
protocol, archiving, software

*Your comments,
questions,
suggestions...*

Let's talk...