TEXAS A&M UNIVERSITY

NMR NEWSLETTER

No. 409

October 1992

TABLE 1 DEUTERATED SOLVENTS

Cat. No.	Description	Formula	Min. Isotopic Purity (%D)	Density (g/mL)	MP (°C)	BP (°C)	$-\chi_v \times 10^6$ @ (°C)
D-11	Acetone-d_6	CD_3COCD_3	99.9%	1.17	-77	56	0.551 (32)
D-120	Acetone-d_6 + 0.1% TMS	CD_3COCD_3	99.9%				
D-13	Acetone-d_6	CD_3COCD_3	99.8%	0.87	-94	57	0.460 (20)
D-121	Aceonte-d_6 + 1% TMS		99.8%				
D-129							
D-14							543 (20)
D-21							0.611
D-122							
D-130							
D-28	Chloroform-d	$CDCl_3$	99.8%	1.50	-64	62	0.740 (20)
D-31	Chloroform-d + 1% TMS		99.8%				

VARIAN

BOX/500 SHEETS

Cat. No.	Paper Size	Instrument Model	Type
WCV-100 (S-100A)	11" X 26"	HA-100, HA-100D	Gridded-Two Color
WCV-60 (A-60C)	11" X 26"	A-60, A-60A, A-60D	Gridded-Two Color
WCV-XL (XL-100)	11" X 26"	XL-100	Gridded-Two Color
WCV-XLFT-100	11" X 26"	XL-100 (FT)	Gridded-Two Color
WCV-XL-200	11" X 26"	XL-200, XL-300, XL-400	Gridded-Two Color
WCV-20 (CFT-20)	11" X 16 3/4" X 17"	CFT-20, FT-80, FT-80A All Model 16 1/2" or 16	Gridded-Two Color Blank

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FORTHCOMING NMR MEETINGS

MRI in the Applied Sciences, Duke University, Durham, North Carolina, **October 25-28, 1992**; Contact: Society of Magnetic Resonance in Medicine, 1918 University Ave., Suite 3C, Berkeley, CA 94704; (510) 841-1899; FAX: (510) 841-2340.

1993 Keystone Symposia on Molecular & Cellular Biology, Taos, New Mexico: **March 8-14, 1993,** *Frontiers of NMR in Molecular Biology - III*; Organizers: T. L. James, S. W. Fesik, and P. E. Wright; Information: Keystone Symposia, Drawer 1630, Silverthorne, CO 80498; Telephone: (303) 262-1230.

34th ENC (Experimental NMR Conference), St. Louis, Missouri, **March 14-18, 1993**; Contact: ENC, 815 Don Gaspar, Santa Fe, New Mexico 87501; Phone: (505) 989-4573; Fax: (505) 989-5073. See TAMU NMR Newsletter 408, 45.

High Resolution NMR Spectroscopy (a residential school), University of Sheffield, England, **April 1993**; Organizer: Dr. B. E. Mann (Sheffield); For information, contact Ms. L. Hart, The Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN, England; Tel.: 071-437-8656.

Additional listings of meetings, etc., are invited.

IK+E M INSTITUTE FOR CLINICAL AND EXPERIMENTAL MEDICINE

MR Unit, Vídeňská 800, 140 00 Praha 4, Czechoslovakia

(received 9/11/92)

Dr. B. L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, California, 94303

Dear Prof. Shapiro:

Pi Signal Splitting in Cadaveric Kidneys Preserved with Collins Solution

The relative ratio PMe/Pi of the intensities of signals of phosphomonoesters (PMe) and intracellular (Pi), obtained from the ^{31}P NMR spectrum, could serve as a marker of the suitability of a kidney for transplantation, or as a measure allowing to assess the success of a transplantation procedure (1). As kidneys intended for transplantation are commonly preserved in Collins solution containing inorganic phosphate, determination of the relative concentration of intracellular phosphate is possible only by deconvolution of the inorganic phosphate signal measured. The problem is that the difference of chemical shifts of both signals is about 0.4 ppm (2,3) see (Figure 1a). In our experience, splitting of the signal of inorganic phosphate into the signals of intracellular and extracellular phosphates was found only in four cadaveric kidneys. No splitting was observed in other 11 cases (see Fig.1b). In these particular cases, determination of the contents of the intracellular Pi concentration is controversial. Since the shimming of our 1.5T whole-body imager is believed to have been identical in all cases, the question arises as to the cause of the failure to differentiate the signal. It can be speculated that, besides imperfect shimming, a low pH gradient between the intracellular and extracellular spaces might be the reason making both signals overlap.

Sincerely,

Milan Hájek
Dana Kurkova

1)Bretan,P.N. et al.: Transpl. 48, 45(1989).
2) Dhasmana,J.P. et al.: J.Cardiovasc.Pharmacol. 5, 1040(1983).
3) Kallerhoff, M. et al.: Urol.Res. 16, 57(1988).

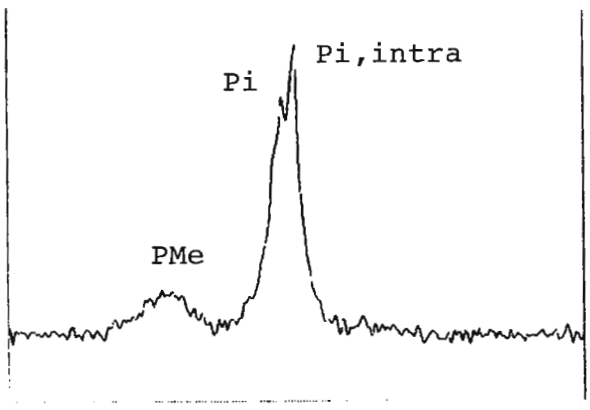

Figure 1a

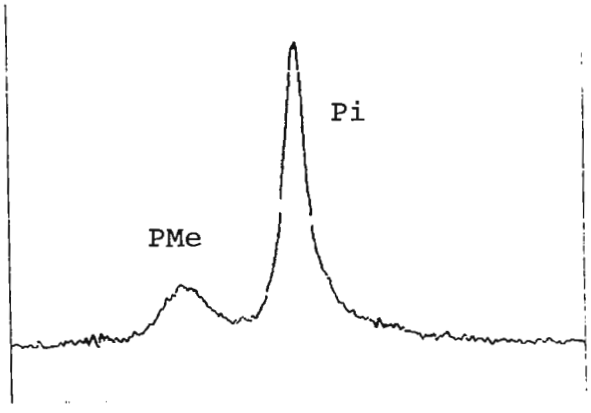

Figure 1b

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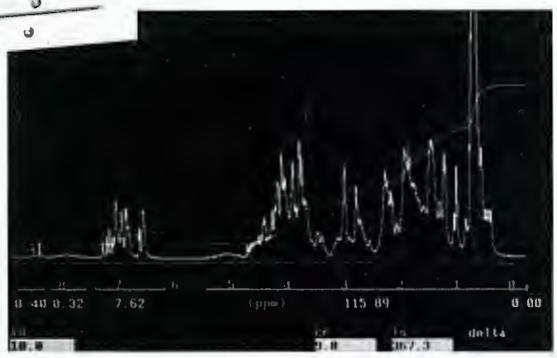

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3304	30–310 MHz	400 W
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Linearity (± 1 dB)	0–900 W
Gain (typ.)	65 dB
Gain flatness	± 2 dB
Input/Output impedance	50 ohms
Input VSWR	< 2:1
Pulse width	20 ms
Duty cycle	Up to 10%
Amplitude rise/fall time	250 ns typ.
Amplitude droop	5% to 20 ms typ.
Phase change/output power	10° to rated power, typ.
Phase error overpulse	4° to 20 ms duration, typ.
Noise figure	11 dB typ.
Output noise (blanked)	< 20 dB over thermal
Blanking delay	< 2 μs on/off, TTL signal
Protection	1. VSWR: infinite VSWR 2. Input overdrive: up to 10 dB 3. Over duty cycle/pulse width 4. Over temperature

Supplemental characteristics:

Connectors, rear panel	1. RF input: BNC (F) 2. RF output: Type N (F) 3. Noise blanking: BNC (F) 4. Interface: 25 pin D(F), EMI filtered
Indicators, front panel	1. AC power on 2. Peak power meter 3. Over pulse width 4. Over duty cycle 5. Over temperature 6. Over drive 7. CW mode
System monitors	1. Forward/Reflected RF power 2. Over pulse width/duty cycle 3. DC power supply fault 4. Thermal fault
Front panel controls	1. AC power 2. Pulse width 3. Duty cycle
Cooling	Internal forced air
Operating temperature	+10 to 40°C
AC line voltage	208/230 VAC, ± 10%, 50–60 Hz
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UNIVERSITY OF THE PACIFIC

College of the Pacific

Department of Chemistry

Bernard L. Shapiro, Editor
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

(received 9/17/92)

Spin-lattice Relaxation of N-Alkylnicotinamides in Cationic Micelles

Dear Barry:

We have applied the method of Gau and Kwak (1) to the binding of an homologous series of N-alkylnicotinamides to cationic micelles of either cetyltrimethylammonium bromide (CTAB) or cetylpyridinium bromide (CPC). This is an interesting test case for this method since the solubilized nicotinamides and the surfactant molecules are both cations so that the binding must necessarily be weak.

The method involves measuring the spin-lattice relaxation rates of the nicotinamide protons in pure D_2O ($R1_{(aq)}$) and in micelle forming surfactant solutions ($R1_{(mic)}$) both in the presence and absence of a low concentration of paramagnetic Mn^{+2} ion. Four relaxation rate measurements are required. The micelle to water distribution, 1-p, can be determined by the expression:

$$1\text{-}p = \frac{R1_{(aq,\,Mn++)} - R1_{(aq)}}{R1_{(mic,Mn++)} - R1_{(mic)}}$$

Typical experimental conditions are 0.044 M N-octyl nicotinamide in 0.103 M cetylpyridinium bromide in D_2O containing 0.0002 M $MnCl_2$. T1 relaxation times were determined at 300 MHz by the inversion recovery $(\pi-\tau-\pi/2-\delta)_N$ pulse sequence with 8 to 12 τ values and a delay δ five times the longest T1. The method works well at 30° and has the advantage that one also gets chemical shift changes and relaxation information for both solubilizate and surfactant which may be interpreted in terms of the intramicellar environment of the solubilized molecule and its effect on molecular motion. For example we find that the binding to CTAB increases with alkyl chain length but that the progressive change in binding energy is small ($\Delta\Delta G$= 1 $KJmol^{-1}$) upon going from N-methyl to N-butylnicotinamide and only when the chainlength is octyl ($\Delta\Delta G$= 3.5 $KJmol^{-1}$) or longer does the hydrophobic interaction between micelle and solubilizate overcome their electrostatic repulsion. Similarly CTAB causes about the same downfield shift on the a-CH_2 chemical shift of the N-methyl and N-butylnicotinamides ($\Delta\delta$=0.023, 0.021 ppm respectively) while longer more hydrophobic compounds are shifted much more (eg. for N-octyl $\Delta\delta$ = 0.054 ppm) indicating a more hydrophobic environment and deeper micelle penetration. Relaxation times mirror the same effect; for this series of cationic solubilizates there is a chainlength threshold before hydrophobic interactions lead to substantial binding to a cationic micelle.

Sincerely

Mike

Michael J. Minch Sharon Wang

(1) Z. Gao, P. E. Waylishen and J. C. T. Kwak, J. Phys. Chem., **95**, 462-467 (1991).

409-6

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25 August 1992 (received 9/14/92)

Dr B L Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, California 94303
USA

Dear Barry

IMAGE DIRECTED SPECTROSCOPY AT 300MHz

We have been spending the last two or three months getting image-directed spectroscopy (^{1}H) started on a Bruker AMX300 89mm system acquired in a collaboration with the Centre for Magnetic Resonance of the University of Queensland in Brisbane. Initial results have been most gratifying, as exemplified by Figure 1, which shows a "typical" ^{1}H spectrum from a 90µl voxel at the centre of the brain of a pentobarbitone anaesthetised rat. We are currently using the technique to characterise differences in metabolite profiles between normal animals and those which have been subjected to various focal ischaemic insults.

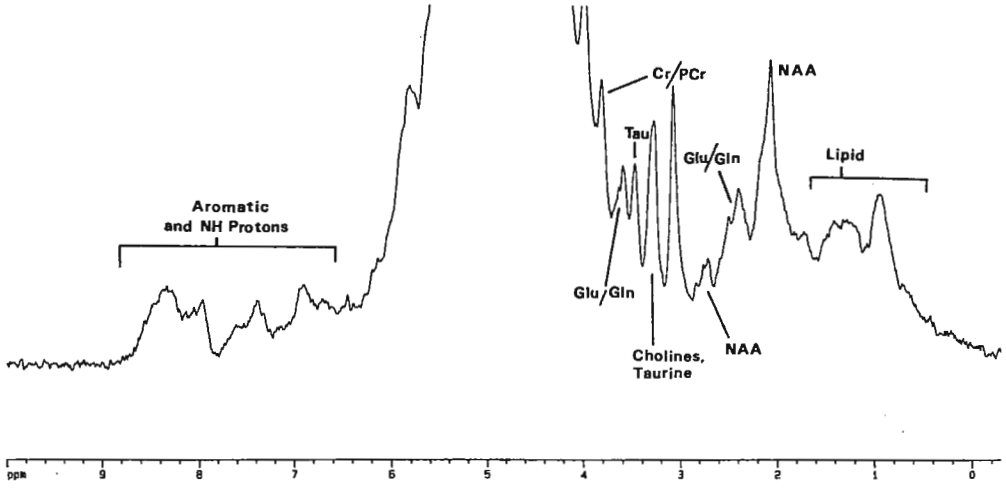


Figure 300MHz ^{1}H NMR spectrum (non-water suppressed) acquired using SPACE [1] from a 90µl cube at the centre of an anaesthetised rat brain. The probe used was constructed in Brisbane and consists of a resonator for optimal B_1 homogeneity as transmitter, and a surface coil receiver.

1. Doddrell D M et al, (1986) J Magn Reson, 68, 367-372.

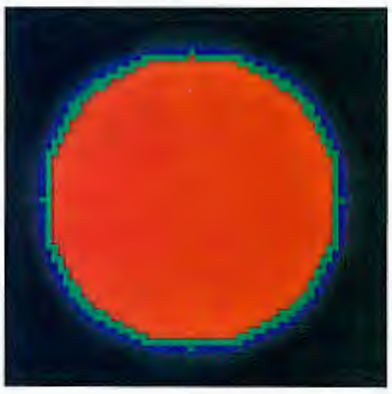
David Reid Liz Moore Charlie Brown

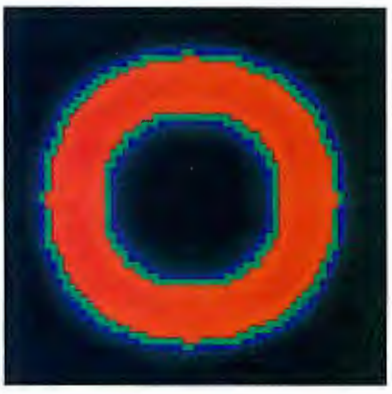
SOLIDSCOPE™

HIGH RESOLUTION SOLID STATE IMAGING

The dual goals in line-narrowing approaches to solid state imaging are (1) to reduce the NMR line width of the sample in order to obtain a high S/N ratio, and (2) to have the line width be uniform across the sample to obtain a distortion free image. Multiple-pulse time-suspension cycles accomplish both of these tasks by averaging all time-independent internal Hamiltonians to zero and thereby reducing the observed NMR signal to a single sharp resonance. To keep the line width narrow over the entire image, the gradient must be applied as short pulses in windows selected such that the gradient evolution is decoupled from the line-narrowing. Finally, "second averaging" is employed in a time-sequenced fashion to reduce error terms while not reintroducing spatial heterogeneity.

The results shown at right are 4 slices from a 64 x 64 x 16 voxel image of a Delrin® phantom, the shape of which is shown schematically below. The voxel size is 92 μm x 92 μm x 625 μm, and the image was acquired on an AMX-400 widebore with a SOLIDSCOPE™ accessory.





A wide range of synthetic organic polymers have been studied with time-suspension cycles and a substantial line-narrowing (on the order of 1000-fold) has always been observed. The SOLIDSCOPE™ is the method of choice for exploring the spatial properties of small (< 10 mm o.d.), rigid polymer samples. Questions such as polymer processing properties, the degree of mixing and blending, the extent of inter-diffusion (as in polymer welds) and the spatial variations in polymer morphology can be addressed.

In other areas, these techniques have already found applications in following solid state chemical reactions, reaction bed dynamics and in observing the spatial variation of coal morphology.

The SOLIDSCOPE™ opens up a new avenue of imaging studies that are only just starting to be exploited.

BRUKER

Bruker Instruments, Inc.
Manning Park, Billerica, MA 01821
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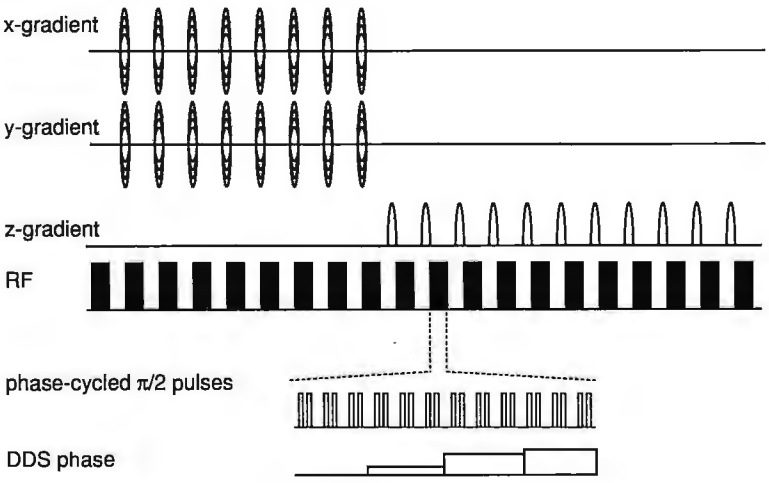
The full three-dimensional imaging pulse sequence is shown below including two phase encoded pulsed gradients (x and y) and the z read gradient. The radio-frequency multiple-pulse cycle is shown schematically where each black box corresponds to one half of a 48-pulse time-suspension cycle. For further line-narrowing, a time-sequenced offset is introduced parallel to the axis of gradient evolution by incrementing the phases of the RF pulses via a direct digital synthesizer (DDS).

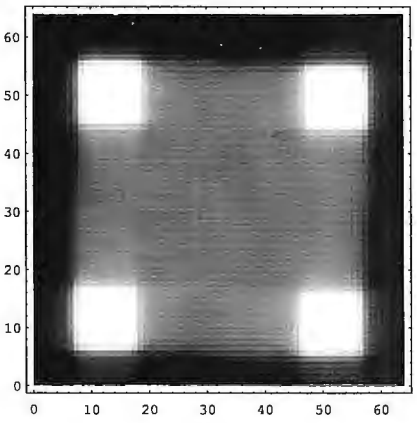
The time-suspension cycle is a multiple-pulse coherent averaging sequence that causes all time-independent linear and bi-linear operators to go to zero. Most notably these include the homonuclear dipolar broadening, and both the anisotropic and isotropic portions of the chemical and susceptibility shifts. Great care is taken to make the pulse-cycle very forgiving of common experimental imperfections, resulting in an easy-to-use method.

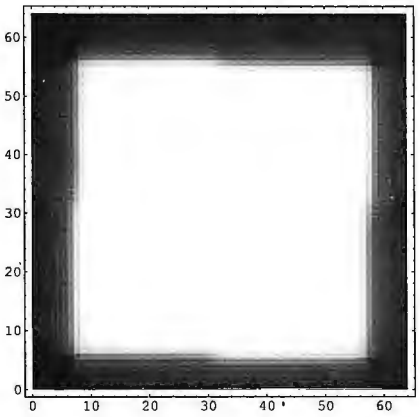
To make the method even more user friendly and to avoid "spin-locking" artifacts, an additional evolution is introduced along the gradient axis by the actions of phase toggles from a direct digital synthesizer. This effectively adds a spatially uniform modulation that coherently but not synchronously averages residual errors.

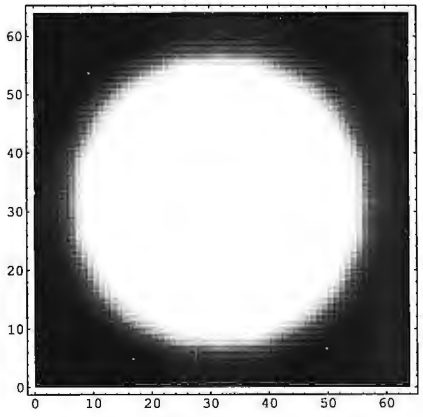
The gradient is applied as a very short (5 μs) sinusoidal pulse during the windows between the RF pulses of the time-suspension cycle. By choosing the gradient windows such that the interaction frame Hamiltonian commutes with the gradient Hamiltonian, the two interactions are separated and the gradient evolution does not interfere with the line-narrowing efficiency of the multiple-pulse cycle. In this fashion a distortion free, high-resolution image of extremely rigid solids is obtained.

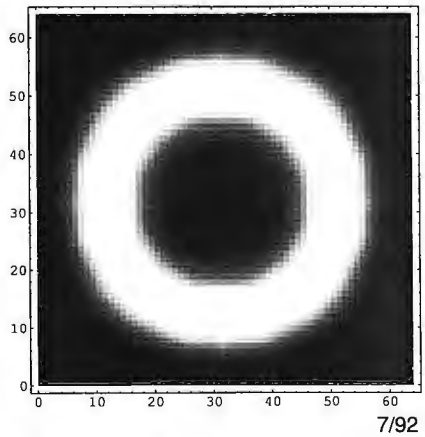
These short gradient pulses are created with novel switcher technology by the pulsed gradient rack that is an integral part of the SOLIDSCOPE™ accessory.











Recent Reviews of Solid State NMR Imaging

J. B. Miller, Trends in Analytical Chemistry, 10, 59 (1991).
P. Jezzard, J. J. Attard, T. A. Carpenter, and L. D. Hall, Progress in NMR Spectroscopy, 23, 1 (1991).
D. G. Cory, Annual Reports on NMR Spectroscopy, 24, 88 (1992).

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7/92

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September 8, 1992
(received 9/10/92)

Dr B.L. Shapiro
966 Elsinore Court
Palo Alto, CA 94303

Dear Dr Shapiro,

From UNIX to Mac

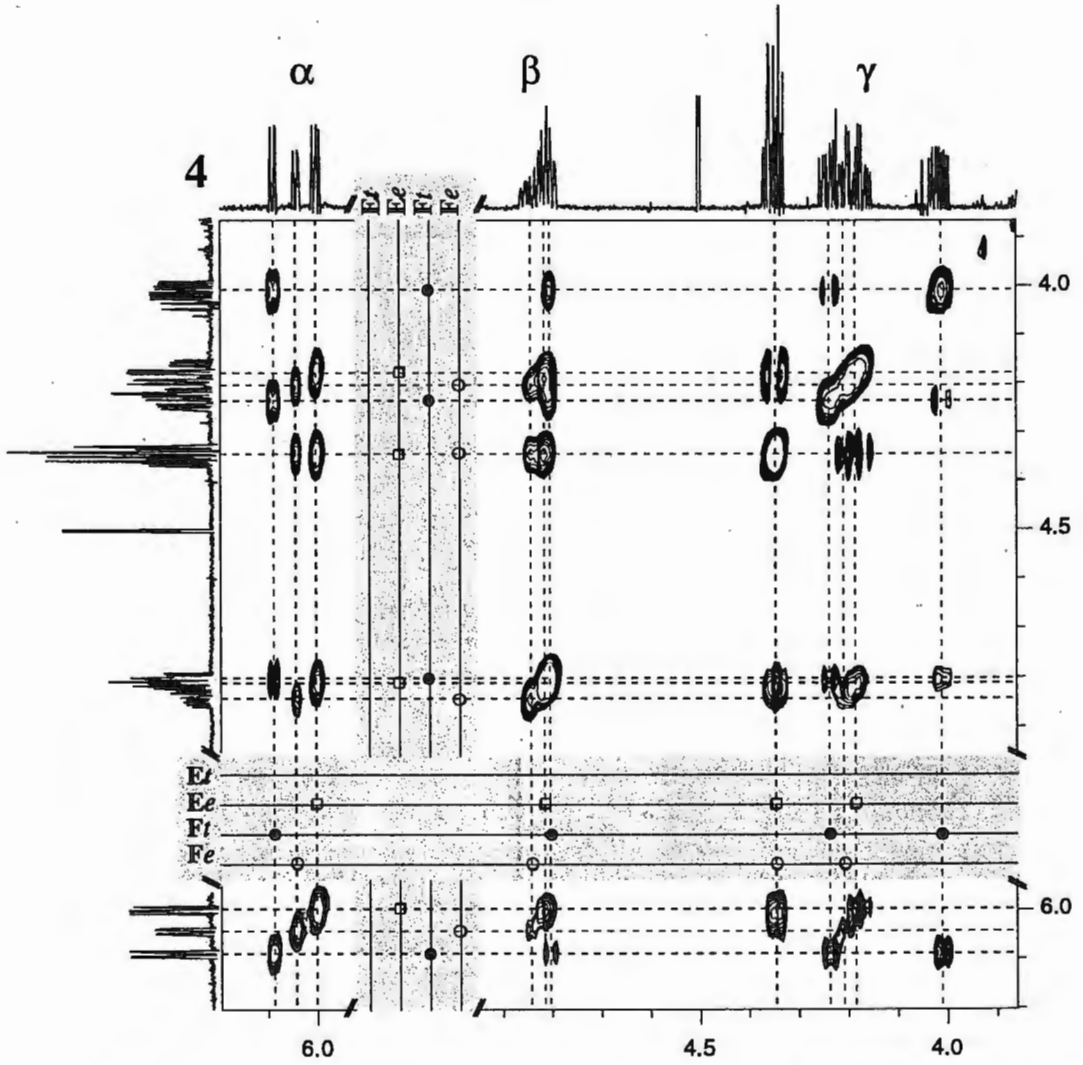
A recent article in your Newsletter by a distinguished team wrote on transferring files from Felix to a MacIntosh (TAMU 407-33). Unfortunately they are not aware of some very nice Mac Utilities or products and have chosen an unbelievably complex path via, heaven forbid, one of those Neanderthal DOS machines that are feebly trying to mimic a real GUI. There is indeed an HPGL conversion program for the Mac and it is written by one, Steve Patt, among the NMR community! I have been using Plotview (formerly MacHP, from Stevens Creek Software) for many years now and it does a fine job.

Additionally, I think users would be interested in simple methods for transferring files between UNIX and Mac machines, whether they are SGI or Sun workstations running FELIX or NMR instruments themselves.

Fetch by Jim Matthews of Dartmouth is Free to educational and non-profit organizations (in /pub/mac on dartvax.dartmouth.edu), and allows simple connection to any UNIX computer and two-way file transfer. It gives the UNIX machine a familiar looking dialog box so you can just double-click your way through the directories and grab any files or directories of interest. This is a great program to facilitate, for example, downloading everything in Rudi Nunlist's XAU directory of useful Macros for the Bruker AMX on the Berkeley NMR bulletin board (bloch.cchem.berkeley.edu, /pub/nmr). A commercial version, called MacFTP, by NRC Resources, has now reverted back to Dartmouth Software. Directory transfer is critical for NMR files on UNIX machines which seem to be an endless conglomeration of directories within directories with a few files scattered about. The FTP protocol itself, and all implementations I have seen on IBM and Mac platforms, allow only pure files to be sent. Fetch 2.1 deals very nicely with the creation and copying of whole directories on practically any UNIX or VMS machine and, of course, the Mac.

NFS is another nice way to go, with products like NFS/Share from Intercon. Even better are UNIX environments on the Mac, all of which support NFS. Tenon Intersystems' MachTen UNIX is a double-clickable desktop application that co-exists with other Mac applications and does not require separate disk partitions. It is a seamless integration of UNIX and the Mac OS on the desktop. For a truly spectacular UNIX, Apple's A/UX 3.0 is brilliant. It is a full-featured UNIX, and Apple's System 7 operating system simply runs as a task under it. Consequently you have access to all of UNIX in a beautiful environment, but all your normal Mac applications run in the normal fashion so that at times it is hard to believe you are really in UNIX. Their NFS is very fast and simple. Simply mount, for example, your silicon graphics drive into a folder/directory with a command like "mount sg:/disk3 /users/jr/disk3" and, bingo, there is the silicon graphics disk on your desktop. You can copy files or whole directories out of it onto any Mac disks by simply dragging as usual, and it is a terrific way to back up masses of data onto optical disks or DAT tape. On the Mac you can compress the files more easily too so that your backups become quite compact. And you can re-organize your UNIX files on the remote machine in a simple and familiar environment.

We would not be without the ability to edit plots for publications and presentations. The example on the following page is a TOCSY which has been 'white-space-compacted', annotated, and had assignment lines added, all in Claris' MacDraw Pro™. Colorizing is also trivial and makes for very nice slides for meetings - the days of photographing the screen (and hoping the audience as far back as the second row will be able to make it out) are over.



A sample figure: the original TOCSY spectrum was 'plotted to disk' (HPGL file) on a Bruker AMX, the HPGL file transferred to the Mac using Fetch and converted to a PICT file with Plotview. The editing and annotation of the figure were then done in MacDraw Pro.

Products Mentioned (List prices are quoted - some companies offer academic discounts etc):
Plotview 3.3, $99.95, Stevens Creek Software, (408) 725-0424.
Fetch 2.1, $25 licence, Free to Educational and non-profit Institutes, Dartmouth College Software Sales, E-Mail: Fetch@dartmouth.edu.
NFS Share, $295, Intercon Systems Corp, (703) 709-9890.
MachTen UNIX, $595, Tenon Intersystems, (805) 962-8202
A/UX 3.0, $709, Apple Computer.
MacDraw Pro, Claris Corp.

Sincerely,

John Ralph

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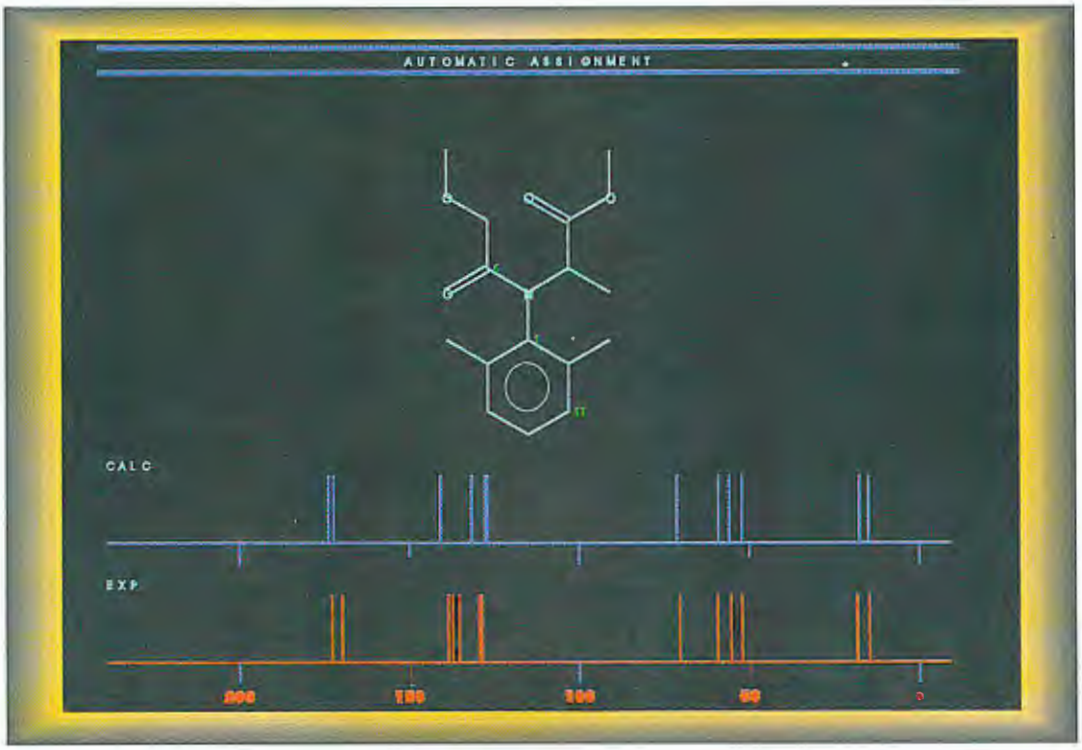
Comparison of the calculated spectrum of a proposed structure with its measured spectrum. The intelligence of CSEARCH is demonstrated by favorable comparison for a structure not contained within the database of 52,000 spectra.



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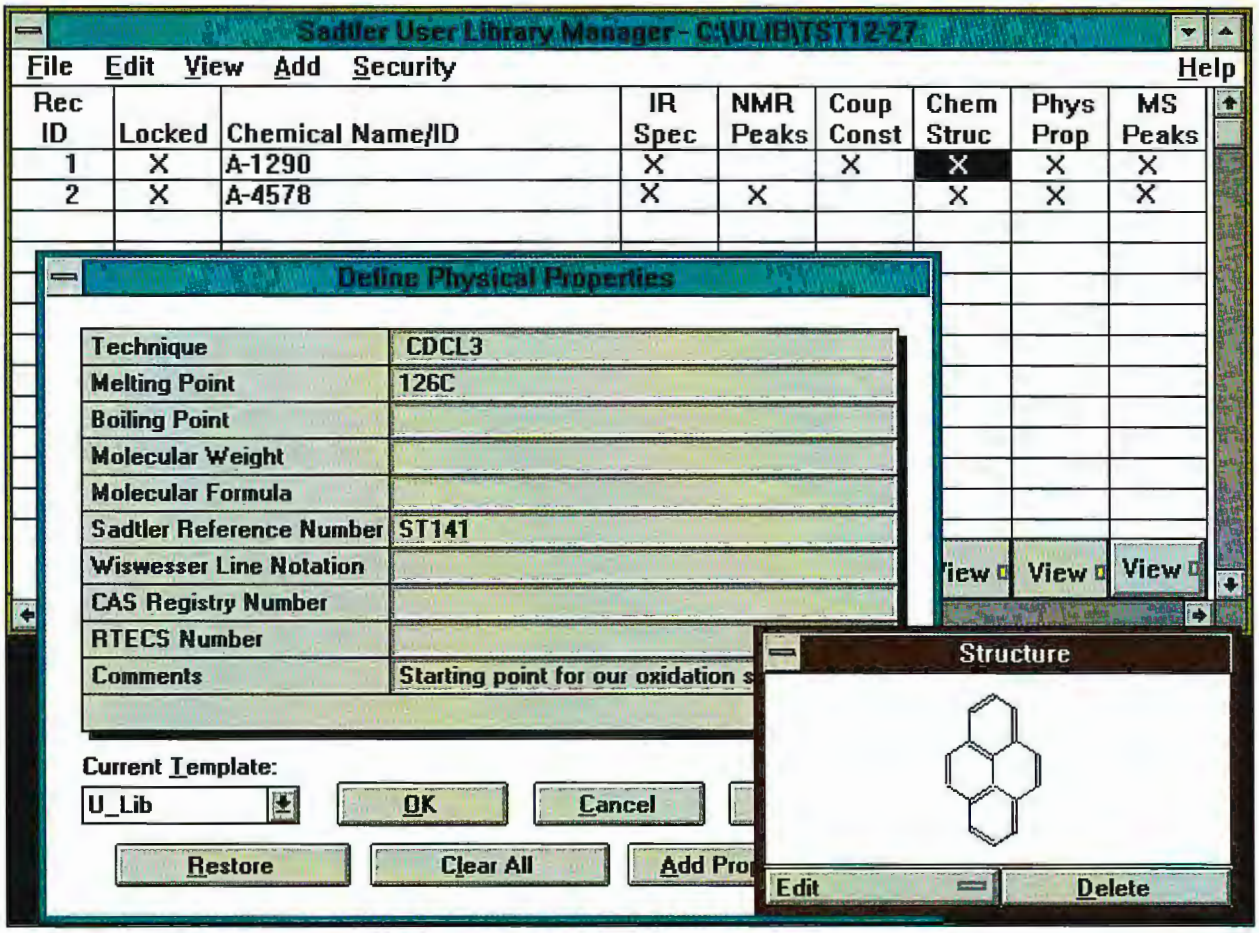

Software and Databases for Personal Computers

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Dr. Bernard L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

August 24, 1992
(received 8/29/92)

Dear Dr. Shapiro

Selective Labelled ^{15}N Spectra of Glutathione S-Transferase

The α-type human B_1B_1 Glutathione S-Transferase (GST) is a 53kD homodimer which belongs to the GST family of proteins which catalyzes the nucleophilic attack of the sulphur atom of glutathione on electrophilic groups in a second substrate. The enzymes are generally considered to serve in the intracellular detoxification of mutagens, carcinogens, and other noxious chemicals. Hence, structural and mechanistic understanding of GST is essential for the elucidation of its detoxification function.

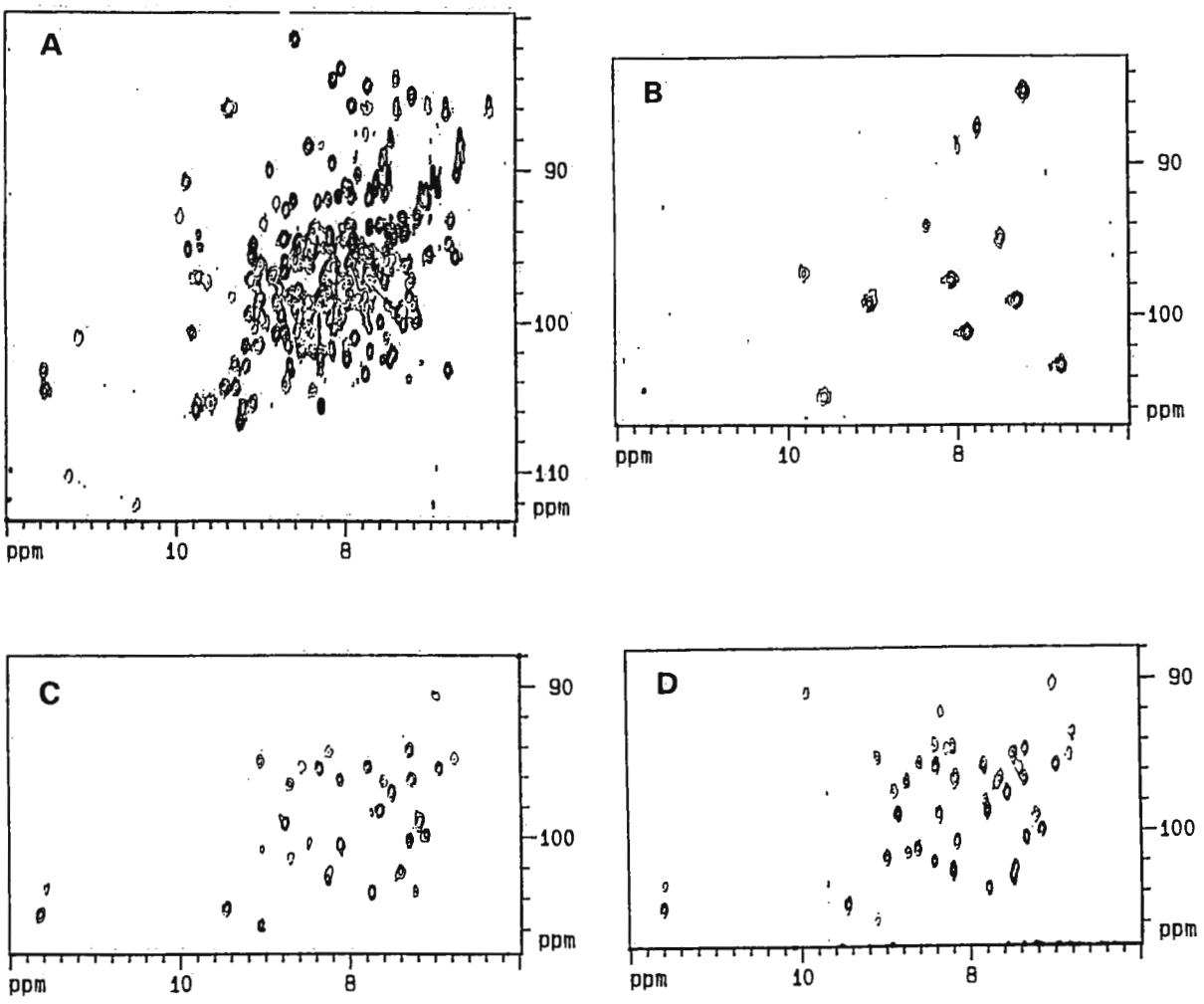
Due to its large molecular weight and its high helical content, the NMR signals overlap severely in conventional 2D and 3D experiments. The short transverse relaxation times prevent good quality TOCSY spectra from being obtained and consequently spin system assignment cannot be obtained from coupling connectivities. Instead, selective ^{15}N and ^{13}C labelling methods are explored for the amino acid assignment.

The inverse HMQC spectrum of ^{15}N uniform labelled protein is shown in Figure A. About 160 cross peaks of back-bone amide groups can be counted out of a total of 209 expected cross peaks (222 amino acid residues minus 12 prolines and one N-terminal amino group). The missing cross peaks are caused by resonance overlap and fast solvent exchange. The selective single ^{15}N labelled protein for Val and Leu and double ^{15}N labelled for Leu and Ile were prepared. The spectra of these samples are shown in Figure B-D. Extra cross peaks were observed in both the selective ^{15}N-Val and ^{15}N-Leu samples. This is surprising as a strain of *E.coli* which was auxotrophic for Asp, Ile, Leu, Phe, Tyr and Val, was used to obtain these selectively labelled samples. Investigation are currently being carried out to solve this problem.

Despite interference problems due to cross-labelling, identification of 52 cross peaks in ^{15}N-^{1}H HMQC spectra was possible. These cross-peaks have allowed us to make some sequential assignments using the ^{15}N-^{1}H 3D HMQC-NOESY and HMQC-NOESY-HMQC spectra of the uniformly ^{15}N-labelled protein. Due to the high helical content of the protein, heavy reliance is placed on the correlations formed within the amide proton region to provide the sequential assignment.

Please credit this contribution to Prof. Gordon C.K. Roberts's subscription.

J.C. Yang R. Badii A. Prescott L.Y. Lian



Figures, HMQC spectra of GST. (A) uniformly 15N labelled, (B) Val-labelled, (C) Leu-labelled, and (D) double Leu and Ile labelled.

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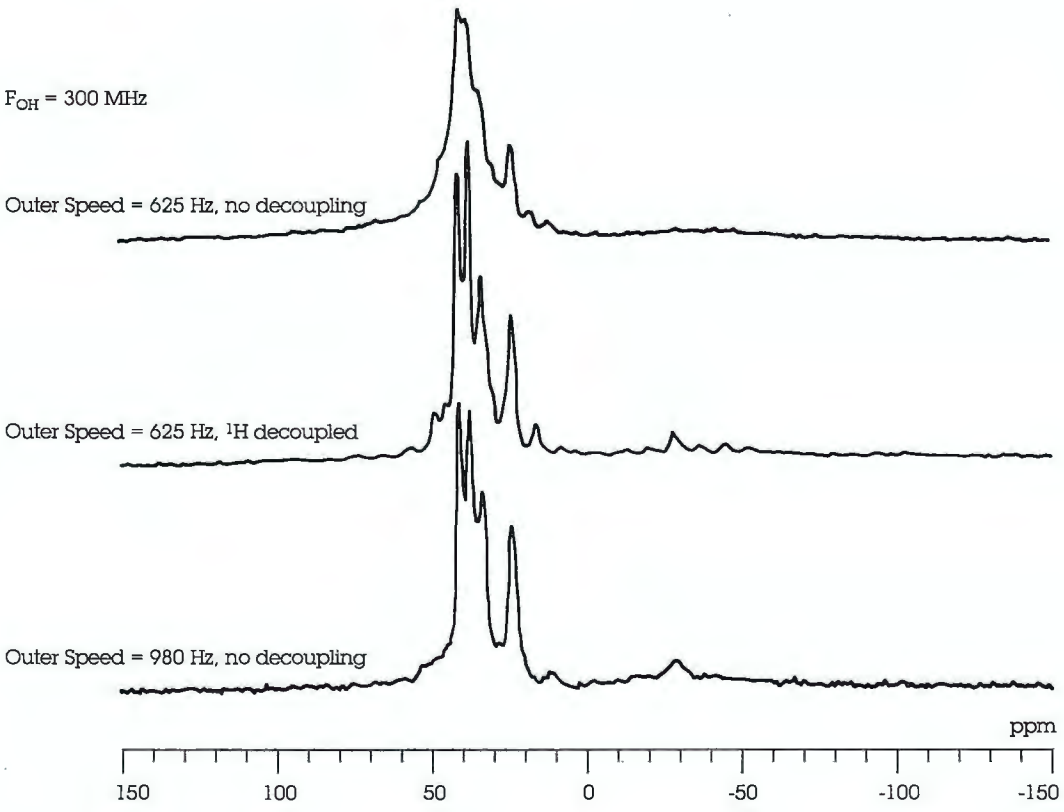

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NSW 2006 Australia

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Dr B. L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto
California 94303 USA

21 August 1992
(received 8/31/92)

RE: Detection Sensitivity in Heteronuclear Multiple Quantum Diffusion Experiments.

Dear Dr. Shapiro,

The apparent self-diffusion coefficient of a solute can be determined using a spin-echo pulse sequence, containing pulsed-linear magnetic field gradients [1].The attenuation of the echo in the presence of these gradients is given by

$$A(\tau)=A_0(\tau)\exp[-\gamma^2G^2D\delta^2(\Delta-\delta/3)]$$

where $A(\tau)$ is the observed amplitude, $A_0(\tau)$ the amplitude in the absence of the pulsed-field gradients, τ is half the echo-time, γ is the magnetogyric ratio, G is the gradient strength, D the self-diffusion coefficient and δ and Δ are the duration and spacing of the gradient pulses, respectively. It can be seen from the equation that the attenuation of the echo will be reduced when nuclei with low γ are observed. In order to attenuate the echo sufficiently for accurate measurements of D, a large value of G must be used. However, this causes eddy currents in conductive components in and around the NMR probe and in the magnet, which interfere with the refocussing and observation of the echo. It is possible to circumvent this problem by observing the effect of the magnetic field gradients on the attenuation of multiple quantum coherences, where the effective γ is the sum of the γ's of the nuclei involved in the coherence. For a two quantum homonuclear coherence the effective magnetogyric ratio is 2γ and thus there is a fourfold increase in the signal attenuation caused by the pulsed-field gradients. This has been used recently by Sotak [2] and colleagues in measuring cell-diffusion of lactate *in vivo*.

Another use of linear magnetic field gradients is in the selection of particular orders of quantum coherence, and this is particularly valuable in 'spoiling' large singlet solvent peaks, such as that from water in ^{1}H- observed spectra. We have recently incorporated this method of coherence-order selection into a diffusion experiment [3]. Multiple-quantum diffusion and coherence gradient-selection experiments with a heteronuclear system, phosphorous acid [$HP(DH)_2O$], was studied with a modified inverse DEPT (IDEPT) pulse sequence. This sequence in valuable for observing the phosphorus nucleus as there is polarization transfer from the proton to the phosphorus population, giving an increased signal to noise ratio. When protons are observed however, there is a decrease in sensitivity as the magnetisation of the less favourable population difference of phosphorus is transferred to the protons.

It can be seen from the Figures that an inverse heteronuclear correlation pulse-sequence (IHETCOR) may be modified for diffusion/coherence selection experiments, and has improved sensitivity when observing protons. This pulse-sequence is shown in Figure 1. Figure 2 shows the results of a ^{1}H NMR 'δ' diffusion experiment, carried out on phosphite in water at pH 7. A spectral width of 1200 Hz was plotted, and A shows a series of 1-quantum spectra obtained with a simple pulsed-field gradient spin-echo experiment. The spectra in B and C were filtered through 0 and 2 quantum coherences, respectively, obtained with the IHETCOR pulse sequence shown in Fig. 1. The four spectra shown in each of the three experiments were obtained with pulsed-field gradient duration values of 3, 9, 15 and 21ms. It can be seen from these spectra that the two quantum coherence selection yields signal attenuation which is much greater, and therefore much more sensitive to detection of changes in D, than in the other experiments (0 and 1 quantum). Furthermore, the 0 and 2 quantum detection has the merit over the 1 quantum detection in that the prominent water signal, evident in the four spectra in A, are effectively removed.

[1] E. O. Stejskal and J. E. Tanner, J. Chem. Phys. 42: 288 (1965).
[2] C. H. Sotak, NMR Biomed. 4: 70 (1991).
[3] P. W. Kuchel and B. E. Chapman, J. Magn. Reson. in press (1992).

Philip W. Kuchel.

PHILIP W KUCHEL

B E Chapman

BOGDAN E CHAPMAN

409-18

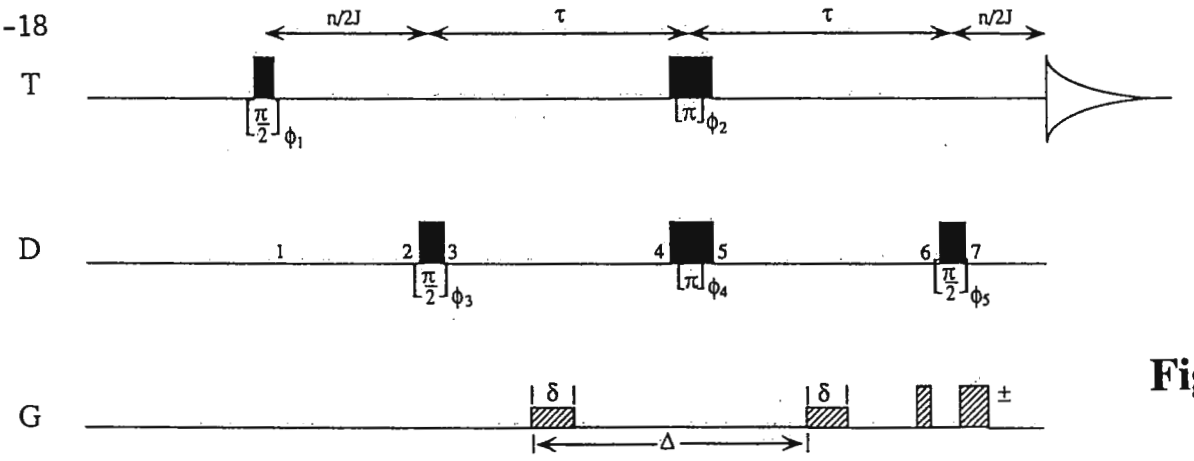

Figure 1.

$\phi_1 = 0$
$\phi_2 = 0$
$\phi_3 = 0123$
$\phi_4 = 1230123030123012$
$\phi_5 = 00002222$
$R_0 = 03212130$ Gradient + - for 1H ++ for X
$R_2 = 01232301$ Gradient + -

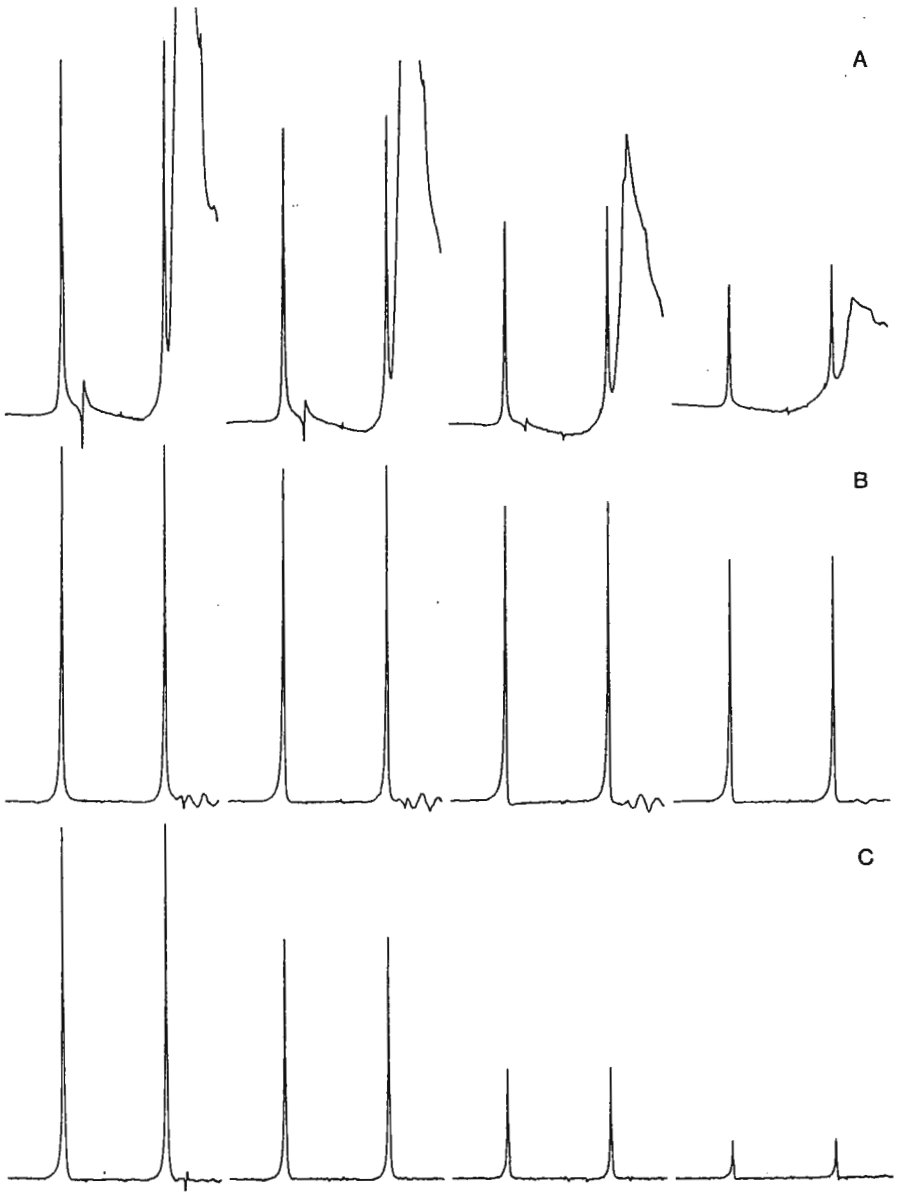

Figure 2.

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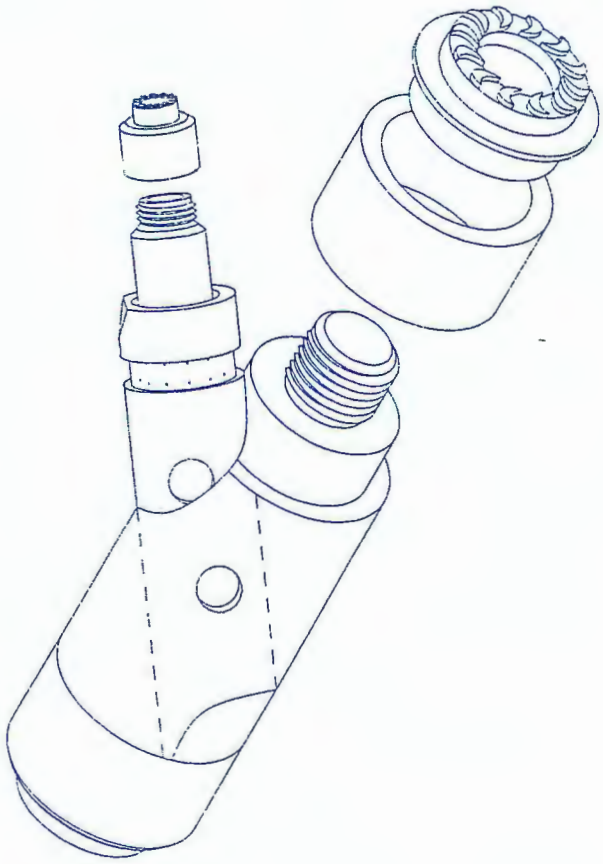
Sample volume	50 µl	**100 µl**
Packing/balancing	hours	**5 minutes**
Typical rotor lifetime	hours	**2 years**
Materials	Vespel	**ZrO_2, Si_3N_4**
Dual spin rate detection	No	**Yes**
Acoustic noise	deafening	**quiet**
VT range		**-140 to +180°C**



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4.7	Double	^{17}O	27	25 µs	800	5
9.4	Single	^{27}Al	104	10 µs	200	6
9.4	Single	^{7}O	54	15 µs	500	6

*Ringdown (20τ) when matched to typical preamp.

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Parameter	Model # 8-36	Model # 12-38	Model # 16-42	Model # 24-68	units
Inside diameter (rf shield)	8	12	16	24	mm
Outside diameter (passive shield)	36	38	42	68	mm
Cooling system	water	water	water	water	
Z Gradient Coils					
Maximum continuous gradient	**6**	**3**	**2.4**	**1.4**	**T/m**
Pulse gradient, 4% duty cycle	**30**	**15**	**11**	**7**	**T/m**
Pulse gradient, 0.5% duty cycle	**80**	**40**	**30**	**20**	**T/m**
Gradient Coefficient, α	1.65	0.6	0.35	0.18	T/Am
d.s.v. for ±5% non-linearity, d_1	4.6	7	9.5	14	mm
d.s.v. for ±15% non-linearity, d_2	6	9.6	13	19	mm
DC resistance, R_E	2.5	2.2	2.2	2	Ω
Inductance, L	85	120	150	270	μH
Time constant, L/R_E	35	55	75	150	μs
Flux leakage, δL /L	0.02	0.02	0.1	0.05	%
Switching efficiency, $\alpha^2 d_2^5/\mu_0 L$	20	25	25	25	%
Switching gradient (50 μs, 50 V)	25	9	4	1.4	T/m
Switching gradient (1 μs, 100 V)	1.2	0.5	0.2	0.07	T/m
Z-offset Shim Coils					
Coefficient	1.5	1	0.8	0.5	mT/A
Resistance	15	15	20	15	Ω
Inductance	200	300	400	400	μH
Z^2 Shim Coils					
Coefficient	20	6	2	0.8	T/Am^2
Resistance	15	15	15	15	Ω
Inductance	120	200	250	400	μH

University of Arkansas for Medical Sciences
Departments of Radiology and Pathology
Biomedical NMR Center
Little Rock, AR 72205

Professor B. Shapiro
TAMU NMR Newsletter
966 Elsinor Court
Palo Alto, CA 94303

(received 9/17/92)

Resolution of Phospholipid Acyl Congeners by ^{31}P NMR

Dear Barry:

Having previously reported the use of ^{31}P NMR to profile amniotic fluid phospholipid (PL) extracts,[1] we were interested in applying detergent solubilization techniques to simplify the assay. In the course of this work we found that we can obtain partial resolution of acyl congeners (varying unsaturation and chain length) of phosphatidylcholine (PC) and other PL's by this technique. Such a PC profile may have some utility in assessing clinical status from amniotic fluid.

Solubilization of the phospholipids was achieved by adding sodium cholate and using methods previously described.[1,2] The figure shows the expanded PC region of the ^{31}P NMR spectrum (acquired on a GE GN300WB spectrometer) from a model compound mixture (D) and from amniotic fluid (A), egg yolk extract (B), and soybean extract (C). Line broadening of 0.8 Hz was used in A only.

An arrow indicates the location of the β,γ-dipalmitoyl PC (DPPC, acyl 16:0) signal in spiked samples. The model spectrum (Fig. 2D) suggests that, at least for C-16 and C-18 acyl chain lengths, the aggregate PC signal can be resolved into three distinct regions: disaturated acyl PC (dsPC, eg, DPPC), saturated-unsaturated acyl PC (suPC, eg, β-oleoyl, γ-palmitoyl PC, POPC or β-palmitoyl, γ-oleoyl PC, OPPC) and di-unsaturated acyl PC (duPC, eg, β,γ-dioleoyl PC, DOPC). The latter two subgroups resonate at 0.02 and 0.04 ppm upfield, respectively, from the former subgroup.

We have tentatively assigned the minor upfield peak in the egg yolk PC spectrum to both duPC and saturated-arachidonoyl PC (sAPC). Although we find oleoyl (18:1) and linoleoyl (18:2) PC congeners indistinguishable in this system, the presence and/or location of the additional (cis) double bonds on the arachidonoyl (20:4) moiety apparently shift this "suPC" signal nearly into the "duPC" region.

We also examined the effect of small chain length differences on chemical shift for several dsPC congeners: dilauroyl PC (DLPC, C-

12), dimyristoyl PC (DMPC, C-14), DPPC (C-16), and distearoyl PC (DSPC, C-18). Although the C-12 PC congener is shifted well upfield, the C-14, C-16, and C-18 congeners are incompletely resolved. In the case of amniotic fluid, PC acyl chains are primarily C-16 +/-2, a restriction which helps to simplify the potentially complex PC profile into 3 broadened regions.

The resolving power of the detergent method is not limited to PC, and has been observed in the spectra of the dipalmitoyl and dioleoyl congeners of phosphatidic acid (PA), phosphatidylglycerol (PG) and phosphatidylethanolamine (PE).

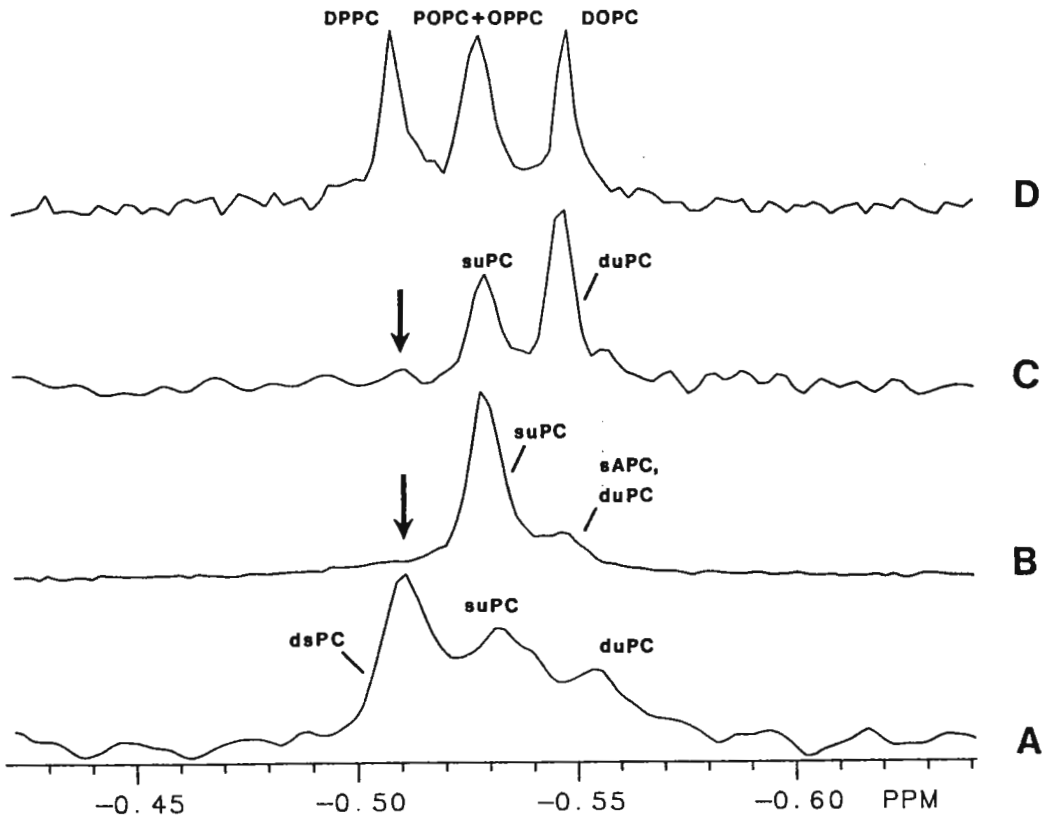
We are currently examining the PC acyl congener profiles for a number of amniotic fluid samples as a function of gestational age. It is known that dsPC, an essential component of mature lung surfactant, increases as a percentage of total PC during gestation, and can be correlated with clinical outcome.

Sincerely,

John M. Pearce

Richard A. Komoroski

1. Pearce et al., Magn. Reson. Med. 21, 107(1991).
2. Pearce and Komoroski, Abstracts, 11th Annual meeting, Soc. Magn. Reson. Med., Aug. 8-14, 1992, p. 3418.



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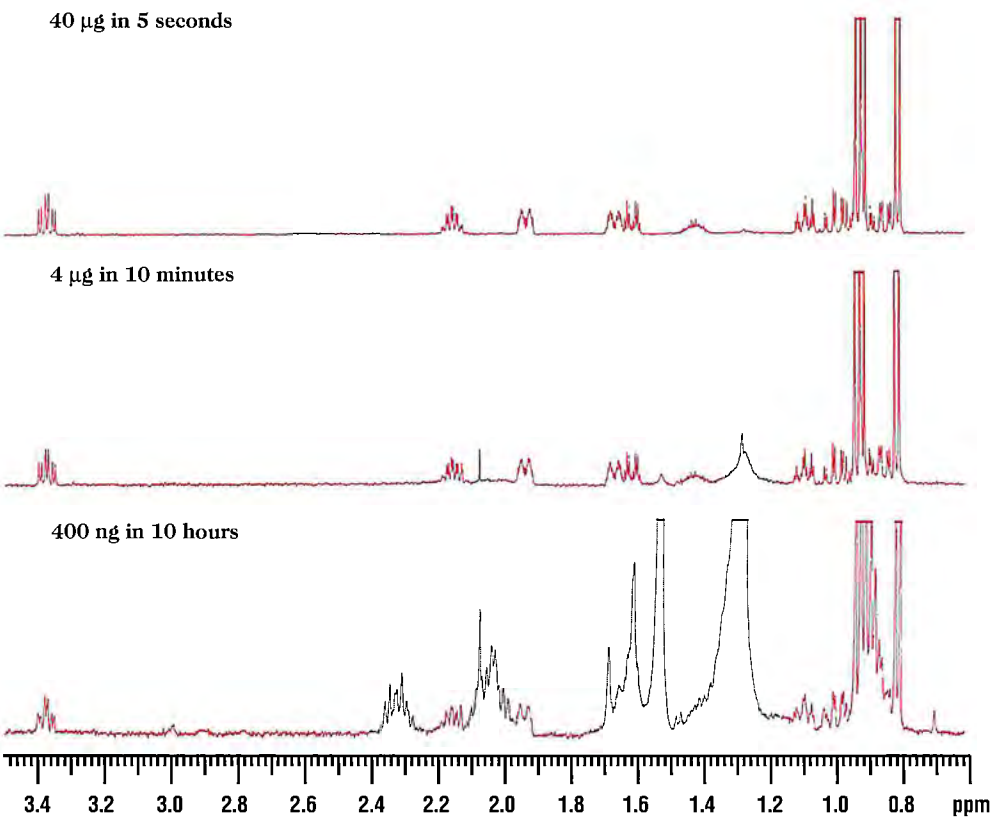

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Prof. B.L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303
USA

Nijmegen, 27 August 1992 (received 9/5/92)

Off-Resonance Nutation NMR.

Dear Prof. Shapiro,

2D nutation NMR experiments of half-integer quadrupolar nuclei can provide the quadrupole coupling constant and asymmetry parameter of the electric field gradient (EFG) tensor at the site of the nucleus. The basic idea of the nutation experiment is to study the evolution of the spin system in the small rf field in the rotating frame. This diminishes the influence of anisotropic interactions which are proportional to the magnetic field, i.e. chemical shifts, while the sensitivity of the high external magnetic field is retained. The shape of 2D-nutation spectra depends on the ratio of the quadrupole frequency ω_Q^{max} and the strength of the radiofrequency field ω_{rf}. Useful information about the quadrupolar interaction of a nucleus can only be obtained if this ratio lies within a certain range. This imposes great restrictions on the usefulness of the nutation experiment especially for nuclei with a low spin quantum number (I=3/2, 5/2). E.g. for a spin I = 3/2 employing an rf field of 50 kHz means that nutation NMR can no longer be used to determine the quadrupole parameters if the quadrupole coupling constant exceeds 1 MHz, as the main features of the spectrum are already concentrated around a frequency of $2*\omega_{rf}$. An interesting new development in all fields of NMR is the application of frequency and phase modulations on modern pulse spectrometers. Modern frequency synthesizers, equipped with direct digital synthesis, are capable of fast phase and (coherent) frequency jumps. In our laboratory a device has been developed that allows phase coherent frequency switching in 200 nanoseconds. Using these techniques we have been trying to overcome the limits of conventional nutation spectra by recording off-resonance nutation spectra, using fast frequency switching techniques. In this experiment the spin system is irradiated with an off-resonant rf-field, whereas the response of the spin system is recorded on-resonance in order to avoid detection problems. In that way the evolution of the spin system is studied in the effective field in the rotating frame. This extends the applicability of nutation NMR to systems with larger quadrupole coupling constants. Moreover, as the resonance offset is an easily controllable parameter, it is straightforward to obtain several nutation spectra with a different effective field on one spectrometer with a single probehead. In principle, irradiating the spin system at large resonance offsets leads to a strong loss of signal into the uninformative zero-frequency signal in the nutation spectra. This is due to the fact that the part of the magnetization

that is projected on the effective field shows no development as a function of pulse length. As previous work has shown it is possible to bring all the magnetization packets of a half-integer quadrupolar nucleus simultaneous in the x-y plane by a frequency-stepped adiabatic half-passage. Using this adiabatic half-passage as a preparation in off-resonance nutation NMR, the magnetization can be brought to a position perpendicular to the effective field in the rotating frame and thus the evolution of the full magnetization can be studied, without the occurrence of a large zero-frequency signal. The effectiveness of this new type of nutation experiment is shown in the figures. Figure 1 shows the normal on-resonance nutation spectrum of $NaNO_2$, recorded with an rf field of 48.5 kHz. As can be seen the spectrum consists of one broad resonance at $2*\omega_{rf}$, and can thus give hardly any information about the quadrupole interaction. In figure 2 the spectrum is recorded with a resonance offset of 200 kHz. Now a well structured spectrum is obtained from which the quadrupolar parameters can be obtained.

Sincerely yours,

Arno Kentgens.

Please credit this contribution to the account of Prof. E. de Boer.

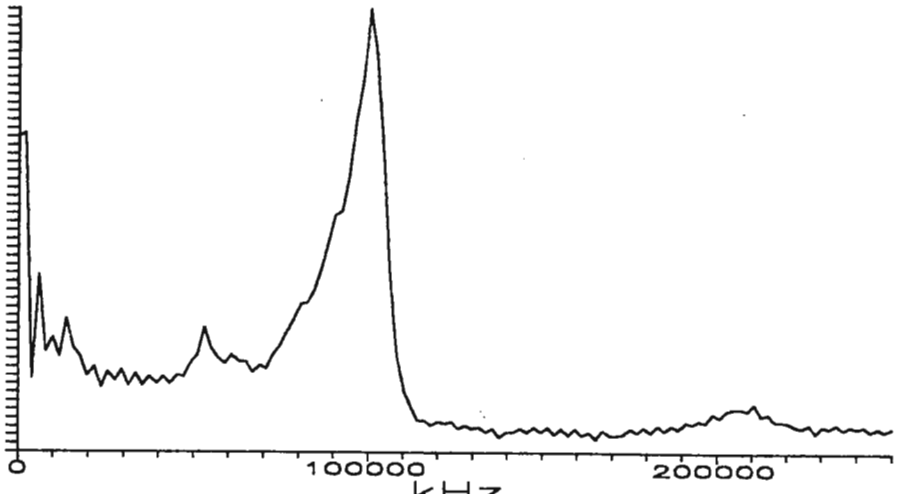

Figure 1. On-resonance Nutation NMR of $NaNO_2$

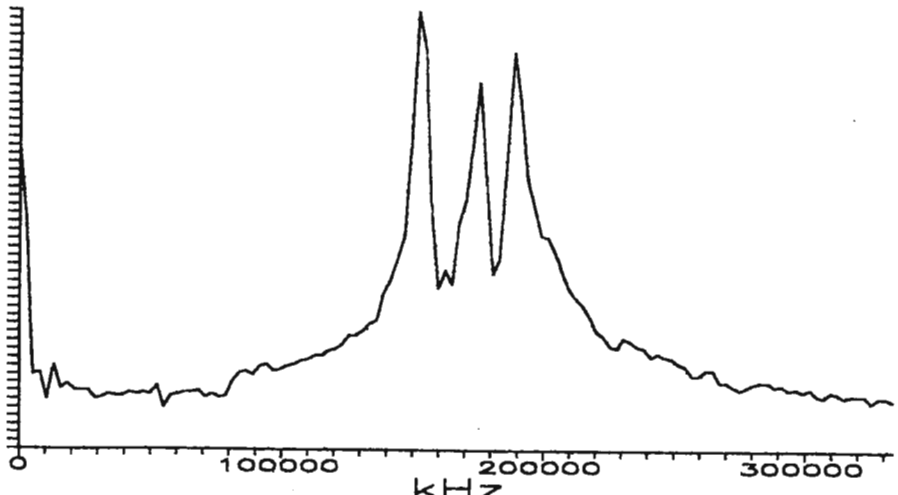

Figure 2. 200 kHz Off-resonance Nutation NMR of $NaNO_2$

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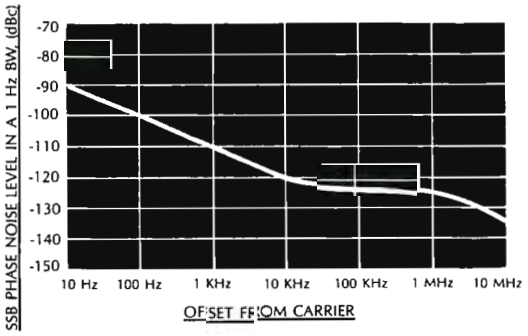
SPECIFICATIONS

Frequency	Range:	0.100 000 0 MHz to 999.999 999 9 MHz
	Resolution:	0.1 Hz to 100 KHz, optional in decades
	Control:	Local by front panel control; remote by TTL-level parallel entry BCD or GPIB (option)
Switching Time		(to within 0.1 radian at new frequency)
	100 MHz–10 MHz digit:	10 µseconds
	1 MHz–0.1 Hz digit:	5 µseconds
Output	Level:	+3 to +13 dBm (1V into 50 Ω), metered in dBm and volts (rms)
	Flatness:	±0.7 dB
	Impedance:	50 Ω
	Control:	Manual by front panel control; remote by analog voltage
Spurious Outputs	Discrete:	-70 dBc 0.1–500 MHz -65 dBc 500–1000 MHz (-55 dBc, 1/2 & 3/2 f_{out})
	Harmonics:	-30 dBc at full output , 1–1000 MHz (-40 dBc at lower level)
	Phase Noise:	-60 dBc (0.5 Hz to 15 KHz) including effects of internal standard
	£(1 Hz):	100 Hz/100 dBc, 1 KHz/110 dBc, 10 KHz/120 dBc, 100 KHz/122 dBc
	Noise Floor:	-135 dBc/Hz
Frequency Standard	Internal:	OCXO or TCXO
		3×10^{-9}/day — 1×10^{-8}/day
		$\pm 1 \times 10^{-8}$/0–50°C — $\pm 1 \times 10^{-6}$/0–50°C
		1×10^{-6}/year — 2×10^{-6}/year
	External Drive:	10 MHz, 0.4 Vrms into 300 Ω; 5 MHz, 0.5 Vrms into 300 Ω
	Aux. Output:	10.000 MHz, 0.4 Vrms into 50 Ω
		(Note: internal or external standard required for operation)
General	Oper. Ambient:	10–50°C, 95% R.H.
	Power:	105–125V, 50–400 Hz, 55W (100, 220, 240V optional)
	Dimensions:	19 × 5.25 × 18 inches (relay rack or bench cabinet)
	Weight:	35 lbs.

For units equipped with a **DDS-TLU OPTION**, specifications are modified as follows:

DDS Option		**H**	**K**
Phase Continuous Switching Range		100 KHz thru 0.1 Hz digits (~1 MHz bandwidth)	10 KHz thru 0.1 Hz digits (~100 KHz bandwidth)
Frequency	Resolution:	0.1 Hz (0.2 Hz, 500–1000 MHz)	0.1 Hz (0.2 Hz, 500–1000 MHz)
	Optional Phase Rotation:	0–360° in .36° steps (in .72° steps, 500–1000 MHz)	N/A
Switching Time		(within phase continuous range) <1 µs transient, 2 µs delay	
Spurious Outputs	Discrete:	-65 dBc 0.1–500 MHz -60 dBc 500–1000 MHz	-70 dBc 0.1–500 MHz -65 dBc 500–1000 MHz
Prices (domestic)		$12,145.00 including 0.1 Hz resolution, manual and remote controls, OCXO frequency standard. Other configurations available; prices are a function of resolution.	



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CHEMISTRY

August 20, 1992
(received 8/24/92)

Influence of Cardiac Pacing on Chloride Potential in Perfused Rat Hearts

Dear Dr. Shapiro:

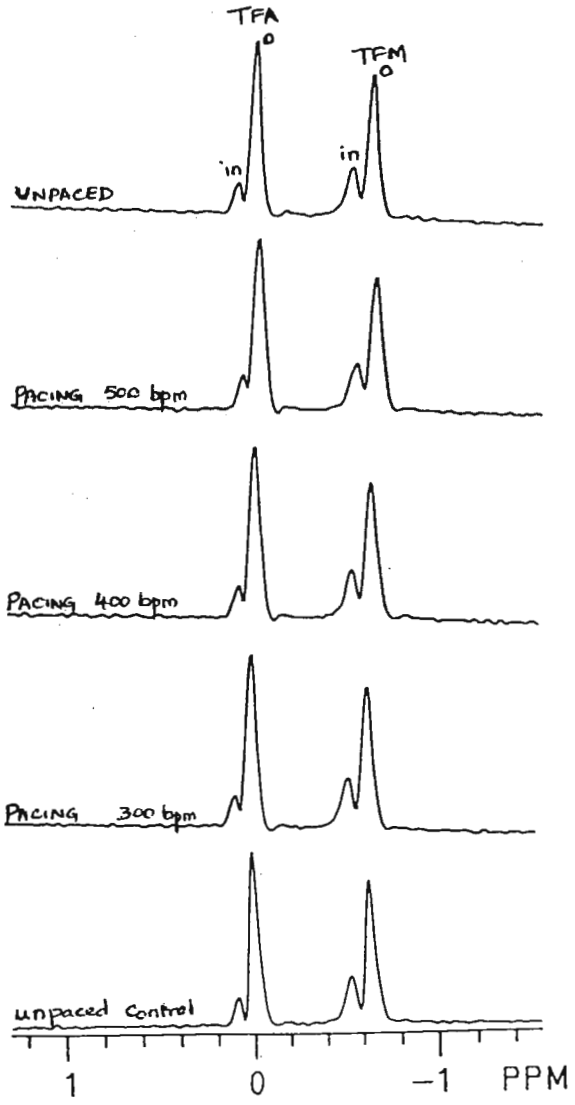
We have recently reported a ^{19}F NMR method, using trifluoroacetate (TFA) and trifluoroacetamide (TFM), to monitor chloride potential in perfused rat hearts [1]. Briefly, TFA distribution ratio reflects the intra and extracellular chloride distribution while TFM distribution ratio is a measure of intra and extracellular volume. The ^{19}F resonance areas of intra and extracellular TFA and TFM are used to calculate chloride potential as shown:

$$E_{Cl} = \frac{RT}{nF} \ln \left[\frac{A_i(TFA)\ A_e(TFM)}{A_e(TFA)\ A_i(TFM)} \right]$$

Our interest was to investigate the influence of pacing on chloride potential in perfused rat hearts. The ^{19}F NMR method was used to investigate changes in chloride potential in perfused rat hearts as a function of varying heart rates.

Rat hearts were perfused with TFA and TFM (3 mM each) and were paced using 3-millisecond pulses at twice voltage threshold (20-30 mV) with a Grass S88B stimulator [2]. Hearts were paced at 300, 400, 500 beats per minute. The ^{19}F NMR spectra were recorded for each pacing rate and also for controls without any pacing. As observed earlier [2], the developed pressure decreased with increasing heart rate (from 300 to 500 bpm).

The figure shown below displays ^{19}F NMR spectra of control and paced rat hearts. There was no significant changes in the areas of TFA and TFM resonances upon pacing. The chloride potential did not change upon pacing (E_{Cl} = -38.3$\pm$2.1 mV). Recently, it was shown that intracellular sodium does not change upon pacing [2]. It would be interesting to apply the ^{19}F NMR method to study the influence of pacing on chloride potential in perfused guinea pig or rabbit hearts, both of which demonstrate a positive staircase response.



References

[1]. Ramasamy R, Zhao P, Gitomer WL, Sherry AD, Malloy CR. **Am. J. Physiol (in press).**

[2]. Butwell NB, Ramasamy R, Sherry AD, Malloy CR. **Invest. Radiol 26, 1079, (1991).**

Sincerely Yours;

Ravichandran Ramasamy A. Dean Sherry Craig R. Malloy Warren J. Goux

Please credit this contribution in the account of Warren Goux.

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Professor Barry Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

September 15, 1992
(received 9/19/92)

Multidimensional Maximum Likelihood Spectral Optimization and its Application to NMR Molecular Modeling

Dear Barry,

(---), I finally received one of those dreaded Ultimata! Anyway, here in Syracuse we are finally about to come out of the cold. After two years without funding on computing projects, my latest proposal received a very fundable score (A sincere **thank you** to my Colleagues!); if there is any money left in Washington after the election, some may find its way to my laboratory.

Meanwhile, here, a greatly reduced staff has been extending the methodology and applicability of 2D and 3D Maximum Likelihood Method (MLM) spectral reconstruction's.

In particular, we have been analyzing the ability of MLM to locate and quantitatively measure small and overlapped crosspeaks in crowded 2D spectral regions. We have shown that MLM greatly assists the spectroscopist in determining NOESY walks through those regions where overlaps make the assignments quite ambiguous. Furthermore, quantitative accuracy of MLM allows measurement of crosspeaks over a 1000:1 dynamic range. Accuracy is high enough to support factorization where crosspeak components are exactly coincident, provided that the spectroscopist can observe portions of multiplets. We are using MLM to assist assignment and solution structure determination for a 24mer RNA hairpin loop molecule (Prof. Philip Borer is the Principal Investigator on that project).

Our first 3D results have also been quite promising.

Warmest Regards,

George C. Levy
Science & Technology Professor

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- Development of new techniques for and novel applications of pure nuclear quadrupole resonance, including ^{14}N NQR.

There are also well-established programs at NRL to explore solid state NMR imaging techniques for the analysis of materials, and to use solid state NMR techniques to study polymer structure and dynamics.

There are two postdoctoral programs at NRL: the National Research Council (NRC) associateship and the Office of Naval Technology (ONT) fellowship. Each program selects applicants on a competitive basis. Stipends currently start at $36K; relocation and professional travel allowances are provided. *The applicant must be a U.S. citizen.* ***Note that there are January and April 1993 deadlines for submission of proposals; <u>now</u> is the time to apply for positions commencing in Spring of 1993.***

Interested individuals should contact one of the following for further details, either by phone or by sending a letter and c.v. to them at Code 6120, Naval Research Laboratory, Washington, DC 20375-5320:

James Yesinowski (202) 767-0415; Joel Miller -2337; Allen Garroway -2323.

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  - Apodization functions
  - Complete FFT modes
  - ICON driven Integrals
  - Peak Picking
  - Line fitting functions
  - T1 and T2 calculations
  - S/N calculation
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  - Integral Setup SAVE files
  - DSP array processor support

- 1D Display:
  - Real/Imaginary/Magnitude
  - Difference display mode
  - Axis/grid
  - Stack plot display
  - Display color selection
  - Copy to Clipboard
  - Lines/Points mode
  - Point shift left/right

- 1D Printing:
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  - Integrals and tables
  - Peak tables
  - Parameter block
  - Logo (PICT format)
  - SAVE as PICT document
  - Print Setup SAVE files

MacFID 2D

SPECIFICATIONS

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TAMU NMR Newsletter

Policies and Practical Considerations

(Slightly Revised October 1992)

The **TAMU NMR Newsletter** (formerly the **IIT NMR Newsletter**, and originally the **Mellon Institute NMR Newsletter**) continues with the same name, under the aegis of Texas A&M University, although the undersigned Editor/Publisher now resides in California. The Newsletter, now beginning its thirty-fifth year of consecutive monthly publication, continues under the same general policies as in the past. All communication with the Newsletter must be directed to the address overleaf.

1. **Policy:**

The **TAMU NMR Newsletter** is a means for the rapid exchange of information among active workers in the field of NMR spectroscopy, as defined broadly, including imaging. As such, the Newsletter will serve its purpose best if the participants impart whatever they feel will be of interest to their colleagues, and inquire about whatever matters concern them.

Since the subscriber/participant clearly is the best judge of what he or she considers interesting, our first statement of policy is "We print anything." (This usually is followed by the mental reservation, "that won't land us in jail or bankruptcy court.") Virtually no editorial functions are performed, although on rare occasions there is the need to classify a contribution as 'not for credit'. I trust that the reasons for this policy are obvious.

The **TAMU NMR Newsletter** is not, and will not become, a journal. We merely reproduce and disseminate exactly what is sent in. Foreign participants should not feel obliged to render their contributions in English.

2. **Public Quotation and Referencing:**

Public quotation of Newsletter contents in print or in a formal talk at a meeting, etc., is expressly forbidden (except as follows), and reference to the TAMU NMR Newsletter by name in the scientific literature is never permissible. *In order to quote results or use material from the Newsletter, it is necessary, in each individual case, to obtain the prior permission of the author in question and then to refer to the material quoted as a "Private Communication".* If your copy of the Newsletter is shared with other readers, it is your obligation as the actual recipient of the Newsletter to see that these other readers of your copy are acquainted with, and abide by, these statements of policy.

3. **Participation is the prime requisite for receiving the TAMU NMR Newsletter:**
In order to receive the Newsletter, you must make at least occasional technical contributions to its contents.

We feel that we have to be quite rigorous in this regard, and the following schedule is in effect: Eight months after your last technical contribution you will receive a "Reminder" notice. If no technical contribution is then forthcoming, ten months after your previous contribution you will receive an "Ultimatum" notice, and then the next issue will be your last, absent a technical contribution. Subscription fees are not refunded in such cases. If you are dropped from the mailing list, you can be reinstated by submitting a contribution, and you will receive back issues (as available) and forthcoming issues at the rate of nine per contribution.

Frequent contributions are encouraged, but no "advance credit" can be obtained for them. In cases of joint authorship, either contributor, but not both, may be credited. Please indicate to whose account credit should be given. Please note that meeting announcements, as well as "Position Available," "Equipment Wanted" (or "For Sale"), etc., notices are very welcome, but only on a not-for-credit basis, *i.e.*, such items do not substitute for a *bona fide* technical contribution. Similar considerations must occasionally be applied to a few (quasi-)technical items.

4. **Finances:**

The Newsletter is wholly self-supporting, and depends for its funds on advertising, donations, and individual subscriptions.

The **Subscription** fee for the October 1992 - September 1993 year is US$170.00, with a 50% academic or personal subscription discount. Subscriptions are available only for the twelve monthly issues which begin with the October issue and run through that of the following September. However, a subscription can be initiated at any time, and the issues back to the previous October will be provided as long as copies remain available.

Companies and other organizations are also invited to consider joining the list of **Sponsors** of the Newsletter. Sponsors' names appear in each month's Newsletter, and copies of the Newsletter are provided to all Sponsors. The continuation of

Continued

this non-commerical Newsletter depends significantly on the interest and generosity of our Sponsors, most of whom have been loyal supporters of this publication for many years. We will be happy to provide further details to anyone interested.

Another major, indeed most essential, source of funds for the Newsletter is **Advertising**. We earnestly encourage present and potential participants of the Newsletter to seek advertising from their companies. Our rates are very modest - please inquire for details.

5. **Practical Considerations**:

a) All technical contributions to the TAMU NMR Newsletter will always be included in the next issue if received before the published deadline dates.

b) Please provide short titles of all topics of your contributions, so as to ensure accuracy in the Table of Contents.

c) Contributions should be on the *minimum* (NOTE!!) number of 8.5 x 11" (21 x 27.5 cm) pages, printed on one side only. Contributions may not exceed three pages without prior approval. Each page must have margins of at least 0.5 - 0.75" (1.3 - 2.0 cm) on all sides. Please observe these limits. Black ink for typing, drawings, etc., is essential. All drawings, figures, etc., should be mounted in place on the 8.5 x 11" pages. We are not equipped to handle pieces of paper larger than 8.5 x 11" (21 x 27.5 cm).

Please do not fold, clip, or staple your pages. Protect the condition of your letters from the ravages of the mails by enclosing what you send in a cardboard or plastic folder, etc.

Foreign subscribers are reminded that regardless of the standard paper length you use, *all material* - letterhead, text, figures, addresses printed at the page bottom, *everything - must not exceed 10" (ca. 25.3 cm) from top to bottom.*

Significant savings of Newsletter pages and total space can be made by exercising close control over the formatting and type sizes of the contributions. **Please consider the following:**

i) For those with computers, try using a smaller type font. The body of this page is printed in 10 point type, which I believe is adequate for most purposes. Even 12 point is acceptable, I suppose. Those who are computerized can also employ non-integral spacing of lines so that sub- and superscripts don't collide with lines below and above.

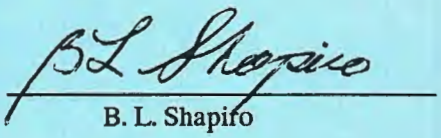
ii) **PLEASE** avoid excessive margins. *Instruct your secretaries to avoid normal correspondence esthetics or practices, however time-honored or 'standard'!* This page has margins on both sides of 0.6" (*ca.* 1.55 cm), which is very adequate. Margins of the same size at the top and bottom are sufficient also, but don't worry if there is more space at the end of your document, for I can often use such spaces for notices, etc.

Also, please avoid large amounts of unused space at the top of letters. Give thought to the sizes of figures, drawings, etc., and please mount these so as to use the minimum space on the page.

iii) 'Position Available', 'Equipment Wanted', and Similar Notices. These are always welcome, but not for subscription credit, of course. Such notices will appear, however, *only* if received with these necessarily rigid constraints: a) Single spaced; b) both side margins 0.6 - 0.7" (1.5 - 1.7 cm.)- NOT WIDER; c) the minimum total height, please, but definitely no more than 4.5" (11.5 cm.) This will let me place such notices wherever a bit of space occurs.

iv) **AVOID DOUBLE SPACING LIKE THE BLACK PLAGUE ! ! !** This is extremely wasteful of space. Even sans computer, small type and 1.5-line (if needed) spacing can be had with a little effort.

6. **Suggestions**: They are always welcome.



B. L. Shapiro

Address for all correspondence:

Dr. Bernard L. Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto, California 94303
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1 October 1992.

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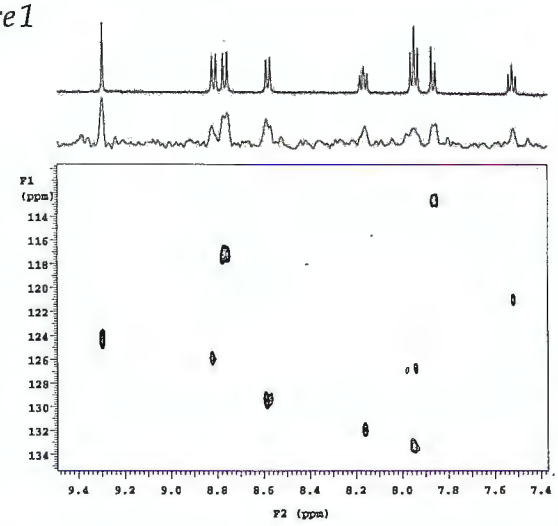
Figure 1: HMQC Spectra of 12µg of cryptolepine obtained in 16 hours with Z•SPEC MID500 probe. Normal ^1H spectrum (256 transients) for the 12µg sample plotted on top.

Figure 2: HMBC Spectra of 35µg cryptolepine obtained in 22 hours with Z•SPEC MID500 probe. Aromatic F_2 window. Normal ^1H spectrum (64 transients) for 35µg sample plotted on top.

Figure 1



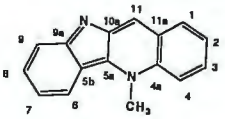


Figure 2

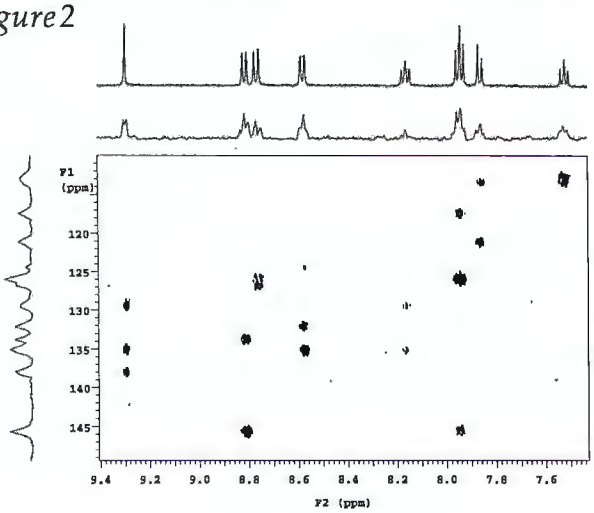
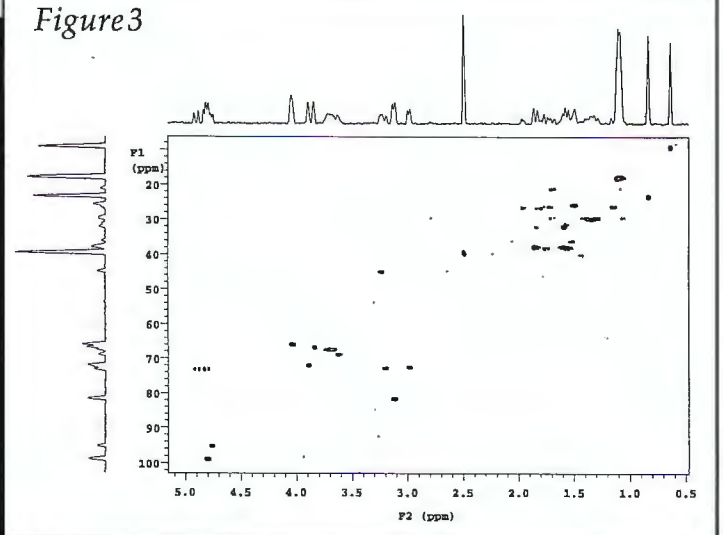


Figure 3



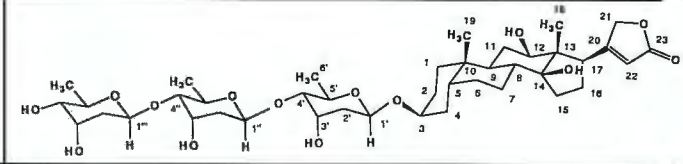


Figure 4

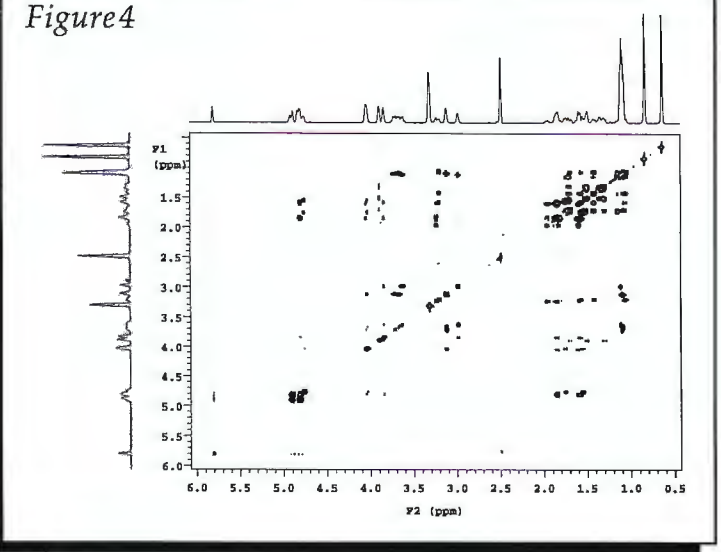


Figure 3: HMQC Spectra of 140µg Digoxin obtained in 14.5 hours with Z•SPEC MID500 probe.

Figure 4: TOCSY Spectra of 140 µg Digoxin obtained in 58 minutes with Z•SPEC MID500 probe.

Please review the following publications for additional examples of results obtained with Z•SPEC Microsample Probes: Micro Inverse-Detection: A Powerful Technique for Natural Product Structure Elucidation, Ronald C. Crouch and Gary E. Martin, *Journal of Natural Products*, **55 (9)**, pg 1343-1347 (1992); Comparative Evaluation of Conventional 5mm Inverse and Micro-Inverse Detection Probes at 500MHz, Ronald C. Crouch and Gary E. Martin. *Magnetic Resonance in Chemistry*. In press.

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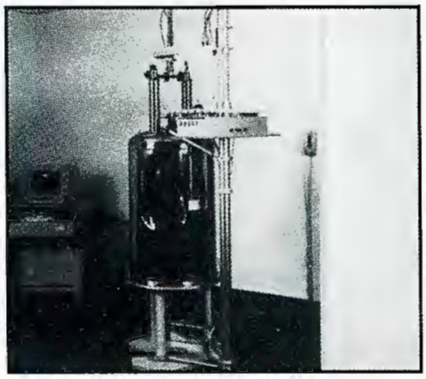

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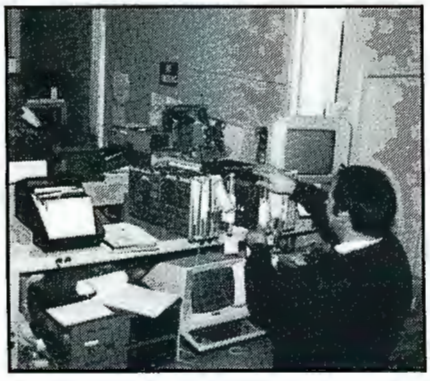
We consider our superconducting magnet service engineers to be the best in the business. Our customers do too. Our engineers routinely handle moving, assembly, pumping, energizing, cryoshimming and complete re-commissioning.



IN-HOUSE REPAIR SERVICE

Our in-house service facility is outfitted with all the necessary equipment to ensure speedy and reliable repair of your system. We also maintain most boards and modules in stock for immediate swap-out.

OUR ENGINEERING STAFF IS EQUIPPED TO HANDLE VIRTUALLY ANY PROBLEM THAT MAY ARISE WITH YOUR NMR SPECTROMETER.

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OUR ENGINEERS ARE NMR PROFESSIONALS!

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Across campus or around the world. We take care of everything from dismantling, packing and moving to re-commissioning, calibration and running specifications.

CONSOLE SERVICE

Our NMR hardware engineers can offer you the benefit of many years of NMR system experience. Regardless of the age or condition of your NMR spectrometer, we can restore it to one hundred percent operating condition.

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Your NMR System Computer is not just a "black box" to MR Resources' Service engineers. Our people are specifically trained in the control, acquisition and processing functions of your NMR's computer system.

MAGNET SERVICE

To keep your cryogen costs down and your system in operation, you must keep your magnet properly maintained. From replacing cracked o-rings to complete cryostat overhauling, we have the expertise you need.

LARGE PARTS INVENTORY

We maintain one of the largest spare parts inventories in the world for most major brands of NMR systems. Components, circuit boards and modules are ready for instant delivery.

SERVICE CONTRACTS

For the ultimate in protection consider an annual service contract. We offer initial system check-out and repair, periodic on-site inspection and, of course, guaranteed service when you need it.

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DEADLINE DATES

No. 411 (December)----- 20 November 1992
No. 412 (January 1993) - 18 December 1992
No. 413 (February) -------- 22 January 1993
No. 414 (March)----------19 February 1993

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Mailing Label Adornment: Is Your Dot Red?

If the mailing label on your envelope of this issue is adorned with a large **red dot** or circle: this decoration means that you will not be mailed any more issues until a technical contribution has been received by me.

Page Length Instruction

Attention overseas subscribers: If you must use paper which is longer that 11", *please* take care that all material (including signatures, addresses - everything!) ends no more than 10" from the top of each of your pages. It is costly to make reductions, and henceforth I reserve the right to chop the excess length off any page, no matter what the result. Beware of the dreaded guillotine! Your cooperation in this matter will be greatly appreciated.

WANTED: *An Advertiser for this inside back cover page!*

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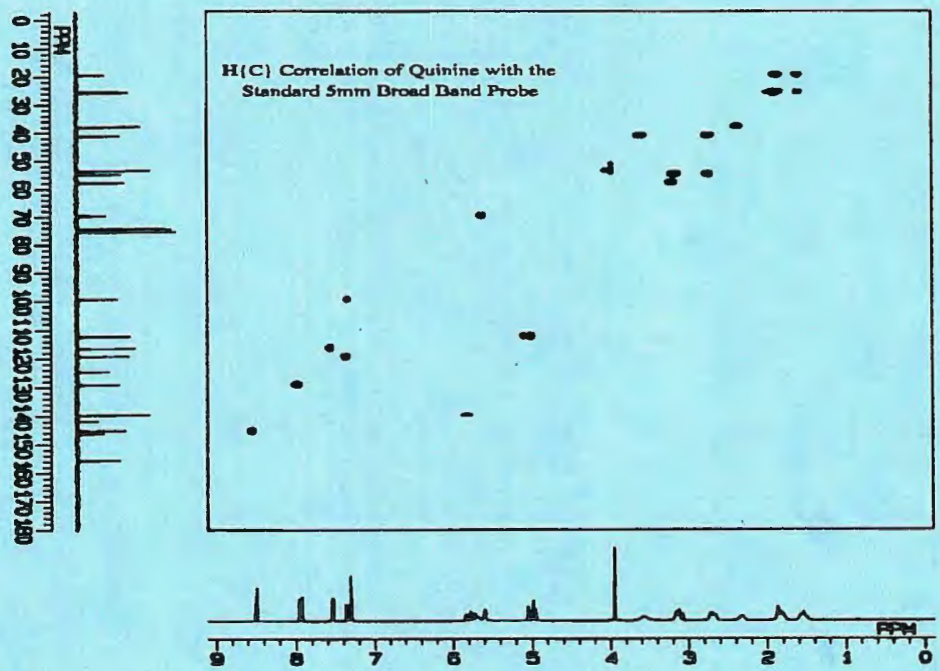

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