THE
NMR
NEWSLETTER

No. 437
February 1995

continued on inside back cover

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Phase Noise: –63dBc (0.5Hz–15KHz)

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Switching: 1–20μs

Output: +3 to +13dBm; 50ohm
Spurious Outputs: –70dBc
Phase Noise: –63dBc (0.5Hz–15KHz)

Freq. St'd: OCXO, TCXO, Ext.
Interface: BCD par. or GPIB
Price: $7,155.00*

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Range: 0.1–310 MHz
Resolution: 1Hz
Switching: 1–20μs
Phase Continuous: 1Hz–100KHz steps

Output: +3 to +13dBm; 50ohm
Spurious Outputs: Type 1 –70/65 (typ/spec) Type 2 –65/60dBc
Phase Noise: –68dBc (0.5Hz–15KHz) –63dBc

Freq. St'd: OCXO, TCXO, Ext.
Interface: BCD par. or GPIB
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PTS 500

Range: 1–500 MHz
Resolution: 0.1Hz–100KHz (opt)
Switching: 1–20μs

Output: +3 to +13dBm; 50ohm
Spurious Outputs: –70dBc
Phase Noise: –63dBc (0.5Hz–15KHz)

Freq. St'd: OCXO, TCXO, Ext.
Interface: BCD par. or GPIB
Price: $8,385.00*

PTS 620

Range: 1–620 MHz
Resolution: 0.1Hz–100KHz (opt)
Switching: 1–20μs

Output: +3 to +13dBm; 50ohm
Spurious Outputs: –70dBc
Phase Noise: –63dBc (0.5Hz–15KHz)

Freq. St'd: OCXO, TCXO, Ext.
Interface: BCD par. or GPIB
Price: $9,255.00*

PTS 1000

Range: 0.1–1000 MHz
Resolution: 0.1Hz–100KHz (opt)
Switching: 5–10μs

Output: +3 to +13dBm; 50ohm
Spurious Outputs: –70dBc (0.1–500 MHz), –65dBc (500–1000 MHz)
Phase Noise: –60dBc (0.5Hz – 15KHz)

Freq. St'd: OCXO, TCXO, Ext.
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Resolution: 1Hz
Switching: 1–5μs
Phase Continuous: 2 MHz band, even or odd steps

Output: +3 to +13dBm; 50ohm
Spurious Outputs: –65/–60dBc (typ/spec)
Phase Noise: –70dBc (0.5Hz–15KHz)

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FORTHCOMING NMR MEETINGS

Symposium on Advances in NMR Applications, Boston, MA, **March 26, 1995**; Contact: Victoria Davies at Nalorac, 837 Arnold Drive, Martinez, CA 94553; (510) 229-3501; Fax: (510) 229-1651. See Newsletter 437, 12.

Symposium on *In Vivo* Magnetic Resonance Spectroscopy VIII, North Falmouth, Massachusetts, **March 25 - 26, 1995**; Contact: Radiology Postgraduate Education; Room C-324, University of California School of Medicine, San Francisco, CA 94143-0628; Phone: (415) 476-5731; Fax: (415) 476-9213; For registration, call (415) 476-5808.

36th ENC (Experimental NMR Conference), Boston, MA, **March 26 - 30, 1995**; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87501; (505) 989-4573; Fax: (505) 989-1073.

Keystone Symposia on Molecular and Cellular Biology, Frontiers of NMR in Molecular Biology - IV, Keystone, Colorado, **April 3 - 9, 1995**; Organizers: S. W. Fesik, T. L. James, and G. Wagner; Contact: Keystone Symposia, Drawer 1630, Silverthorne, CO 80498; Phone: (303) 262-1230; Fax.: (303) 262-1525.

International School of Biological Magnetic Resonance, 2nd Course: Dynamics and the Problem of Recognition in Biological Macromolecules, Erice, Trapani, Sicily, Italy , **May 19 - 30, 1995** ***(Note the new dates.)***; Contact: Prof. O. Jardetzky, Stanford Magnetic Resonance Laboratory, Stanford University, Stanford, CA 94305-5055; Phone: (415)723-6270; Fax: (415) 723-2253; or, Prof. J.-L. Lefèvre, ESBS, CNRS-UPR9003, Univ. Louis Pasteur, Blvd. Sébastien Brant, F67400 Illkirch Graffenstaden, France; Phone: (+33) 88-655269; Fax.: (+33) 88-655343; See Newsletter 437, 19.

12th International Meeting on NMR Spectroscopy, Sponsored by the Royal Society of Chemistry, Manchester, England, **July 2 - 7, 1995**; Contact: Dr. J. F. Gibson or Ms. G. B. Howlett - See Newsletter 415, 5; Phone: (44-71) 437-8656; Fax: (44-71) 437-8883.

ISMAR 1995, Sydney, NSW, Australia, **July 16-21, 1995**; Contact: Dr. W. A. Bubb, Dept. of Biochem., Univ. of Sydney, Sydney, NSW 2006, Australia. Phone: +61-2-351-4120; Fax: +61-2-351-4726; Email: ismar95@biochem.su.oz.au. See Newsletter 437, 20.

NMR Symposium at the 37th Rocky Mountain Conference on Analytical Chemistry, Denver Colorado, **July 24-27, 1995**; Contact: Dr. Alexander J. Vega, DuPont Central Research and Development, P.O. Box 80356, Wilmington, DE 19880-0356; Tel. (302) 695-2404; Fax: (302) 695-1664; e-mail: vega@esvax.dnet.dupont.com. See Newsletter 432, 34.

37th ENC (Experimental NMR Conference), Asilomar Cnference Center, Pacific Grove, California, **March 17 - 22, 1996***[sic]*; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87501; (505) 989-4573; Fax: (505) 989-1073.

38th ENC (Experimental NMR Conference), Orlando, FL, **March 23 - 27, 1997***[sic]*; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87501; (505) 989-4573; Fax: (505) 989-1073.

Additional listings of meetings, etc., are invited.

THE NMR NEWSLETTER

(formerly the TAMU NMR Newsletter)

B. L. Shapiro, Publisher
The NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

Tel. (415) 493-5971
Fax.(415) 493-1348

Plus ça change . . .

Effective with this issue, this publication will henceforth appear under its new name, as above. Texas A&M University has decided to complete its association with the Newsletter, which will now continue privately, into the indefinite future - for a long time, I hope.

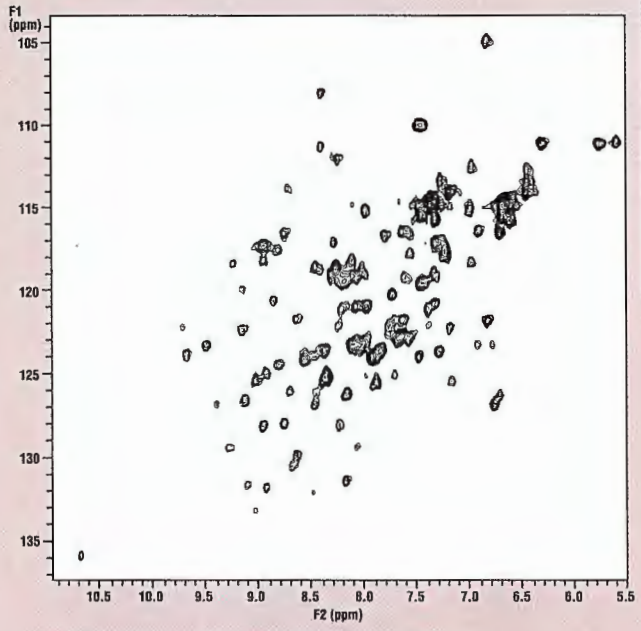
It must be emphasized that the only change (other than a few cosmetic matters) is the name. The Newsletter policies and operation will continue as in the past, except that all aspects will be handled here in Palo Alto, at the same address and telephone numbers. Subscription, sponsorship, and advertising funds which have already been paid for the October 1994 - September 1995 Newsletter year will, of course, be honored. No changes or interruptions in the publication schedule are expected.

When the 'new' operation is fully in place, the issues should in fact appear a week or more earlier in the month than is now the case, because of a shorter printing time expected. (The newly increased postage rates will probably have no visible impact on transit time during the current millenium.)

Let me take this opportunity to thank you - the advertisers, sponsors, and subscriber/participants - for your interest in and loyalty to the Newsletter over its 437 issues during 36+ years. Some of you have been involved with the Newsletter for two decades or more, and there are even a few - perforce an ever-decreasing number - who have been contributing to and receiving the Newsletter since its inception in the fall of 1958. We share in what must be a useful activity, which I feel has also managed to persist with only a minimum of formality, stuffiness, and ossification. I look forward to our continuing.

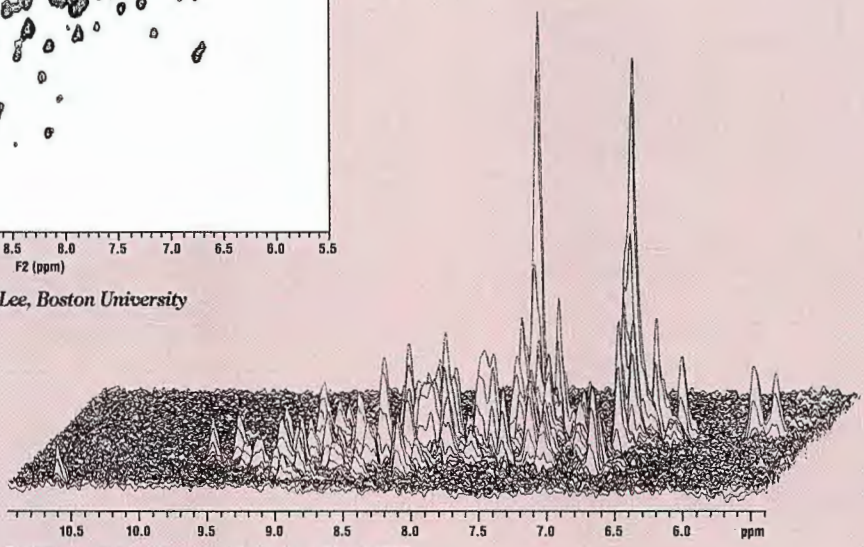
Barry Shapiro
30 January 1995

The World's First 10mm Triple Resonance PFG Probe



Sample courtesy of Jonathan Lee, Boston University

2D ^{1}H-^{15}N gradient HSQC experiment performed on a 350 µM sample (1.8 ml) of a ^{13}C, ^{15}N-labeled 13 kDa protein in 90% H_2O with 100 mM NaCl obtained using a UNITY*plus* 600 and a 10 mm $^{1}H\{^{15}N/^{13}C\}$ Biotriple•nmr PFG probe. The total acquisition time was 2 hours for 256 increments with a relaxation delay of 1.5 sec.



Pulse sequence courtesy of R. Andrew Byrd, NCI

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- **5-fold reduction in data acquisition time relative to a 5 mm probe**
- **25% more sensitivity than an 8 mm probe**
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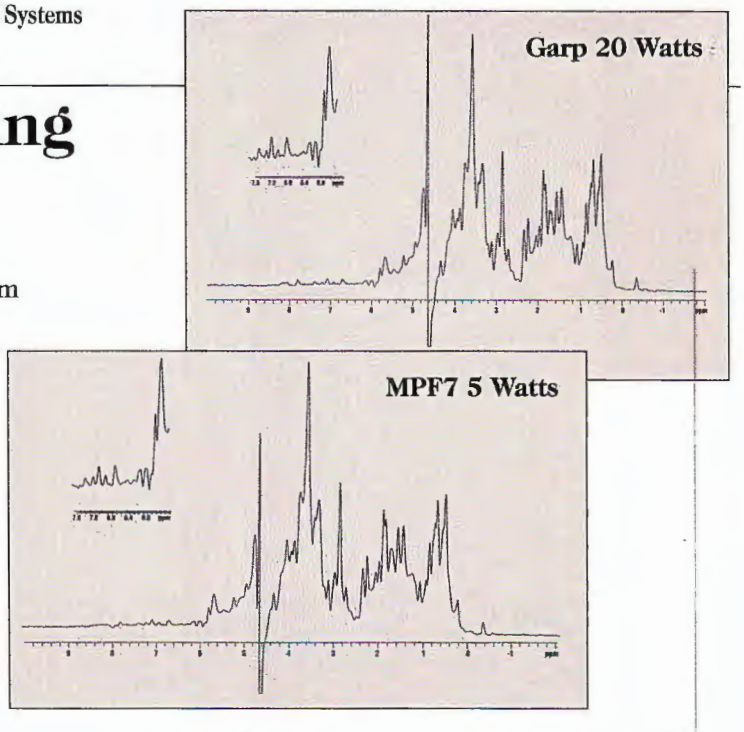
*International Conference on Magnetic Resonance in Biological Systems

Ultrabroadband Decoupling

^{1}H-^{13}C Gradient HSQC

Obtain the maximum decoupling field strength with the minimum power using the powerful Unity*plus* waveform generator. Triple resonance spectra obtained utilizing (A) a GARP broadband decoupling sequence[1] and (B) a MPF7 broadband decoupling sequence[2] at a decoupler power 6dB less than that used in spectrum (A). Both spectra were acquired using a Unity*plus* 600 spectrometer equipped with a waveform generator and a Triple•nmr PFG probe.



[1] Shaka, A.J., Barker, P.B., Freeman, R., *J Magn. Reson.*, 64, 547 (1985).
[2] Fujiwara, T., Nagayama, K., *J Magn. Reson.*, 77, 53 (1988).

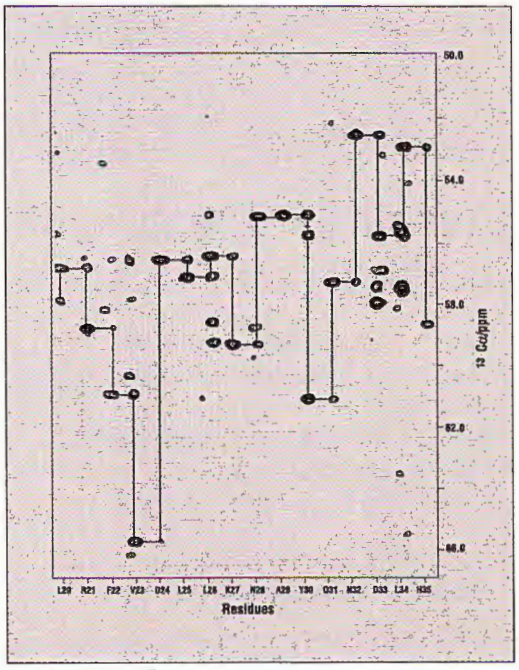
Deuterium Decoupling with Deuterium Lock

Perform deuterium-locked quadruple resonance experiments such as $^{1}H\{^{13}C, ^{15}N, ^{2}H\}$ with ease with Varian's Triple•nmr probe, a four channel UNITY*plus* system, and the UNITY*plus* Adaptive Lock.

This plot displays the resultant sequential connectivities for helices A and B of the *Trp*-Repressor/DNA Complex. Utilizing the experiment above, L. Kay and co-workers* have obtained 100% of the intra-residue and 94% of the inter-residue correlations for the 37 kDa complex.

Spectrum provided by Toshio Yamazaki, Weon Tae Lee, Matt Revington, Cheryl Arrowsmith and Lewis Kay from the University of Toronto and the Ontario Cancer Institute, Toronto, Canada.

*Yamazaki, T., Lee, W.T., Mattiello, D.L., Dahlquist, F., Revington, M., Arrowsmith, C., and Kay, L.E., "An HNCA Pulse Scheme for the Backbone Assignment of ^{2}H, ^{13}C, ^{15}N-Labeled Proteins: Applications to a 37 kDa *Trp*-Repressor Complex," *J. Amer. Chem. Soc.* (submitted).



^{2}H, ^{13}C, ^{15}N - labeled *Trp*-Repressor/DNA Complex (37 kDa) HNCA with constant time carbon evolution combined with ^{2}H decoupling

Monsanto St. Louis NMR Center

Monsanto Company
700 Chesterfield Parkway N.
St. Louis, Missouri 63198
Phone: (314) 694-1000

December 15, 1994 (received 12/24/94)

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

Dear Barry:

TRIED: Triple-Resonance Isotope-Edited Spectroscopy

We would like to inform the TAMU NMR community of a new method for metabolite identification developed in our laboratory. This experiment uses triple-resonance isotope-edited (TRIED) spectroscopy to detect submicrogram amounts of metabolites in the presence of milligram quantities of interfering matrices.

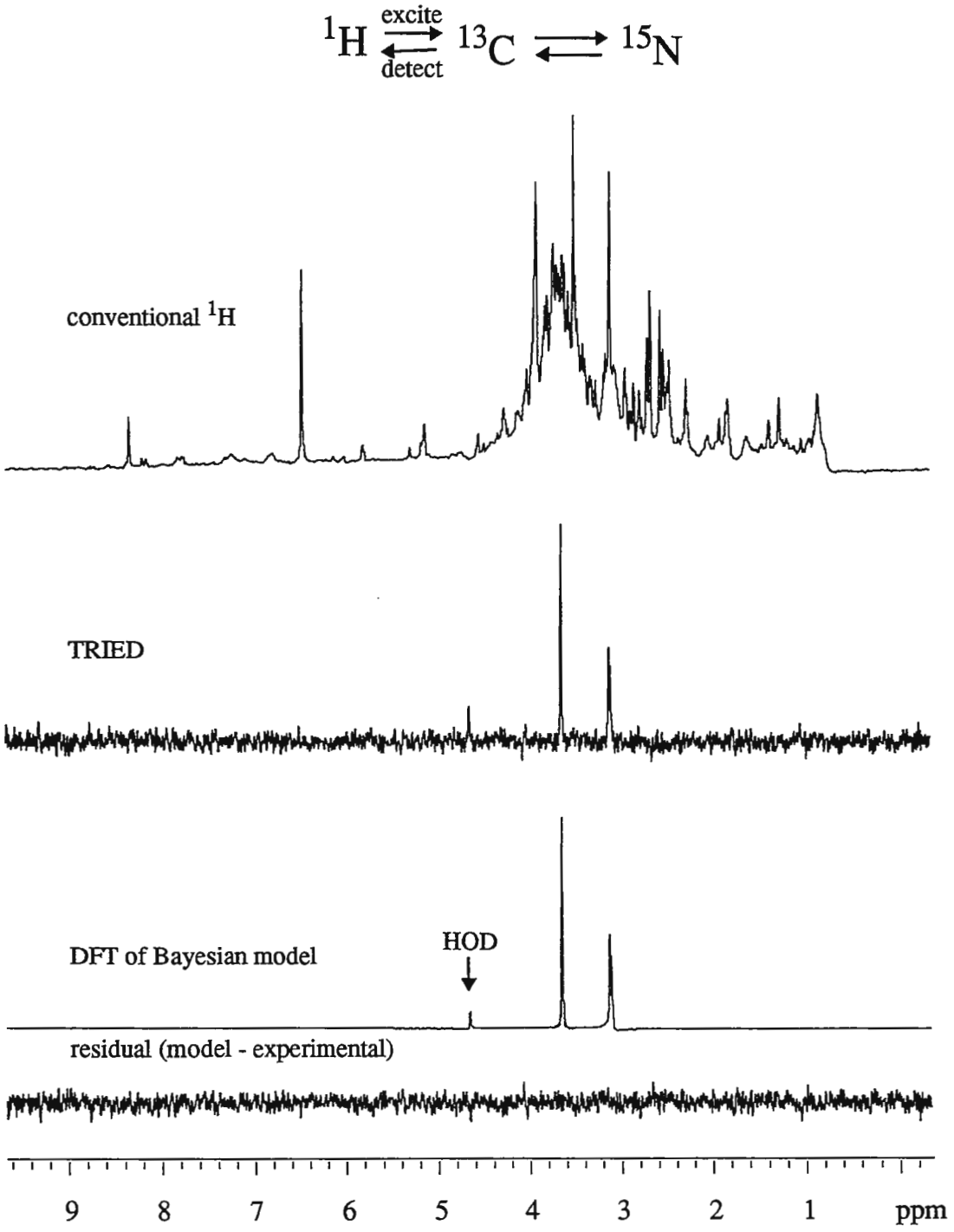
This proton-detected technique requires ^{13}C-^{15}N labeled chemical bonds, and filters the magnetization to remove both single-labeled and unlabeled (natural abundance) impurities. A schematic of the polarization transfer pathway is shown above the conventional proton spectrum of 7 mg crude plant matrix spiked with approximately 3ug of triple-labeled (C2, N, C3) glyphosate. Data were acquired at 500 MHz on a Varian Unity spectrometer with a 3mm Nalorac triple resonance probe using simple solvent presaturation.

Below the conventional spectrum is a TRIED spectrum of the same sample collected in little over an hour. Other than centrifugation to remove solid materials, no sample purification was performed. Bayesian probability theory applied to the TRIED time-domain data detects only the glyphosate protons and a small residual HOD signal. The Fourier transform of the residual of the Bayesian analysis is shown at the bottom.

In our experience TRIED is quite useful in the detection of low level metabolites, especially as the high cost of radioactive labeling continues to become increasingly unattractive.

Sincerely,

William C. Hutton Janice K. Gard John J. Likos Joel R. Garbow


$^{1}H \rightleftarrows^{\text{excite}}_{\text{detect}} {}^{13}C \rightleftarrows {}^{15}N$
conventional ^{1}H
TRIED
DFT of Bayesian model
HOD
residual (model - experimental)
9
8
7
6
5
4
3
2
1
ppm

December 23, 1994
(received 12/28/94)

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

Dear Barry:

Effect of Glycosidic Torsion Angle on ^{13}C Shifts of Nucleotides

With indirect detection techniques, measurments of ^{13}C shifts of oligonucleotides even at natural abundance has become readily available. The analysis of these shifts in conformational terms would provide additional structual information. While the effect of sugar pucker has been examined in this light (e.g. LaPlante, et. al. (1994) *Biochemistry*, **33**, 2430) the dependence of shifts on glycosidic torsion angle is less well understood, largely due to the absence of suitable model compounds for analysis. Some of the recently characterized G-tetraplex model systems provide an opportunity to do this, having G bases that are alternatively in ***syn*** and ***anti*** orientation relative to sugars that are all in the C2′ endo configuration in both instances (Wang et. al., (1991) *J. Mol. Biol.*,**222**, 819). This property allows isolation of the effect of glycosidic bond angle alone. Shift effects of substantial magnitude are observed with rotation from ***anti*** to ***syn***. Average changes for four residues of each type are +5.0 ppm for C1′, -7.0 for C2′, +4.0 for C3′ and +1.5 for C4′. These shifts are most likely related to bond length and bond angle changes which have been indicated in crystal structures of mononucleotides with these base orientations. Shifts observed for the ***syn*** cases are generally beyond the range of those for the respective carbon sites observed in B-DNA type structures. Thus these shifts may be a useful marker for ***syn*** base orientation, although any sugar pucker shift contributions also need to be taken into account in the full analysis. The C8 carbon of the guanine residue also shows a trend of +2.4 ppm when the base goes ***syn***. In RNA the persistence of these trends for C1′ and C8 of G bases are supported by results from Varani and Tinoco ((1991) *J. Amer. Chem. Soc.*,**113**, 9349). There is also theoretical support for the effect on C8 from Ghose et. al. ((1994) *J. Amer. Chem. Soc.*,***116*** 8827). It is likely that these trends extend to other purines and possibly pyrimidines, although presently data for such cases are not available.

Sincerely yours,

David Live

Department of Pure and Applied Chemistry
The University of Strathclyde Glasgow G1 1XL Scotland
Tel/Fax +44-141-776-1718
email cbas25@vaxa.strath.ac.uk

9th January 1995

(received 1/17/95)

Dr. Barry Shapiro
TAMU NMR Newsletter
966 Elsinore Court
Palo Alto CA 94303 USA

Patience Rewarded Again!!

Dear Barry,

When cholesta-4,6-dien-3-one is irradiated with UV light it is transformed into a dimer. First reported in 1944 (1) this compound was studied by Jeger and co-workers in 1962 (2), who recognized that the junction between the two steroid nuclei involved the 4(5)- double bond of one nucleus and the 6(7)-double bond of the other forming a cyclobutane ring. These workers made no assignment of stereochemistry however.

Molecular modelling studies show that out of the eight possible ways of joining the two residues together, one involves much less steric repulsion than the others. This structure (A) has the beta face of the 4(5) bond joining the alpha face of the 6(7) bond. The new bonds formed are thus 4β-7′α and 5β-6′α.

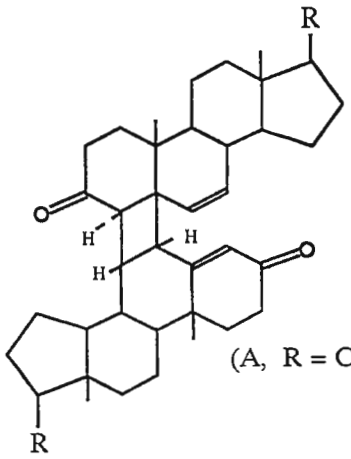
The proton and carbon nmr spectra of this compound are consistent with this idea; the jmod spectrum shows 25 out of the expected 28 signals for methylene and unprotonated carbons, and all of the expected 26 signals for methyl and methine carbons. The proton spectrum has four significant single proton signals at δ=5.83 (s), 5.65 (dd, J=10.1, 2.4 Hz), 5.53 (dd, J=10.0, 2.1Hz), and 3.82 (d, J=10.0), assigned to the 4′, 7, 6, and 4α hydrogens respectively.

Yours sincerely

Peter Bladon

Peter Bladon

(1) M. I. Ushakov and N. F. Kosheleva, *J. Gen. Chem. (USSR),* 1944, **14,** 1138..
(2) H. P. Thronsden, G. Cainelli, D. Arigoni, and O. Jeger, *Helv. Chim. Acta,* 1962, **45,** 2342.



(A, R = C_8H_{17})

PROGRESS IN DIGITAL FILTERING

ON-THE-FLY IN-LINE DIGITAL FILTERING ON THE AVANCE™

All spectrometers in the *AVANCE* continuum utilize real time oversampling and digital filtering for sampling rates of 400 kHz or less. Dedicated very fast digital signal processors (DSPs) are placed in-line on the Receiver Control Unit (RCU), which is located in the *AVANCE* VME acquisition bus, and receives the digitized signal from the ADC. The DSPs on the RCU are extremely fast and can execute up to 100 million mathematical operations per second (not just 100 MIPS). In this manner oversampling, digital filtering, and on-the-fly decimation can be utilized for all high resolution and CP/MAS acquisitions on the *AVANCE* series; all the benefits of oversampling and digital filtering, such as improved dynamic range, steep filter cutoffs, flat baselines, improved signal-to-noise, etc., are provided at all times, without the need for increased data storage or additional operator-intensive manipulations.

Bruker has invested heavily into fundamental digital filtering research, and has developed a unique and novel window function with extremely steep cutoffs. Figure 1 shows various window functions that have been described in the literature. As can be seen, the proprietary *AVANCE* window function provides much steeper cutoffs, and thus, suppression of unwanted signals, than traditional window functions such as the Blackman window function. This is essential for optimal data quality and absence of artifacts.

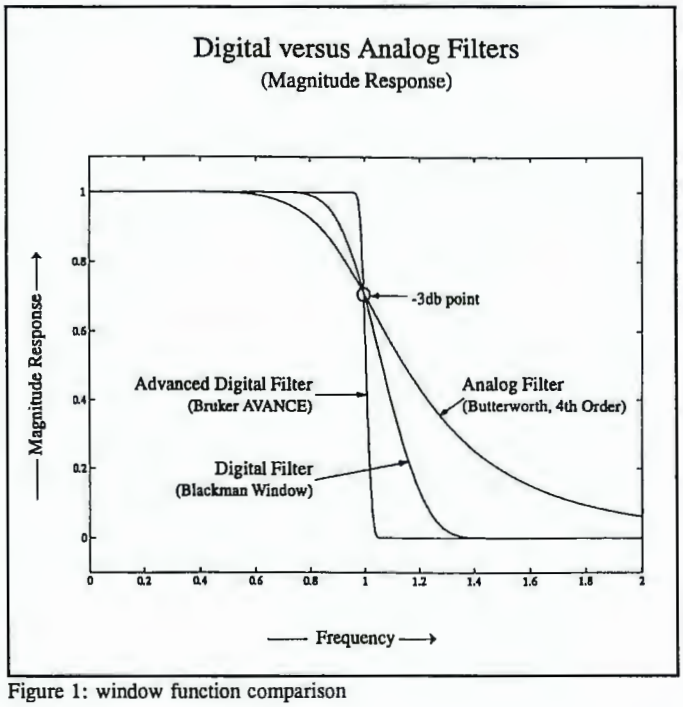
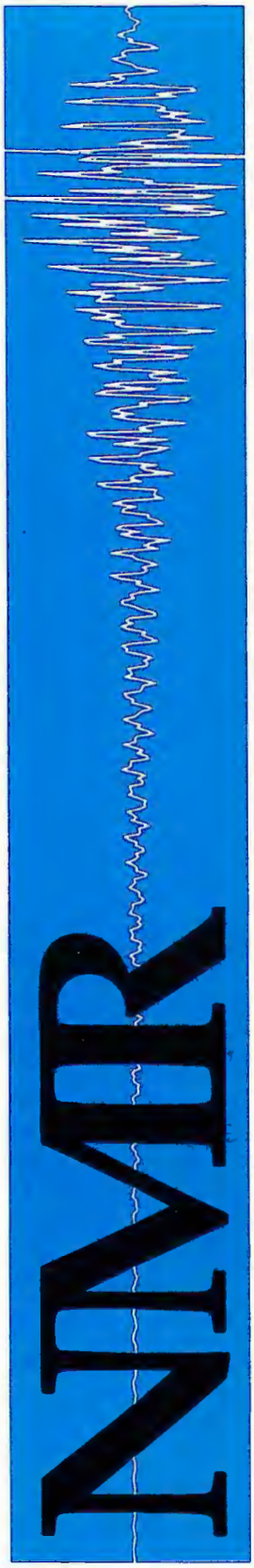


Figure 1: window function comparison



BRUKER

NMR

DIGITAL NOTCH FILTER

In response to customer demand, Bruker now provides a digital notch filter on the *AVANCE* series. Figure 2 shows the spectrum of lysozyme A) with and B) without the digital notch filter. The digital notch filter applied in the time domain can be utilized for the suppression of unwanted signals, for instance water, or other high intensity peaks.

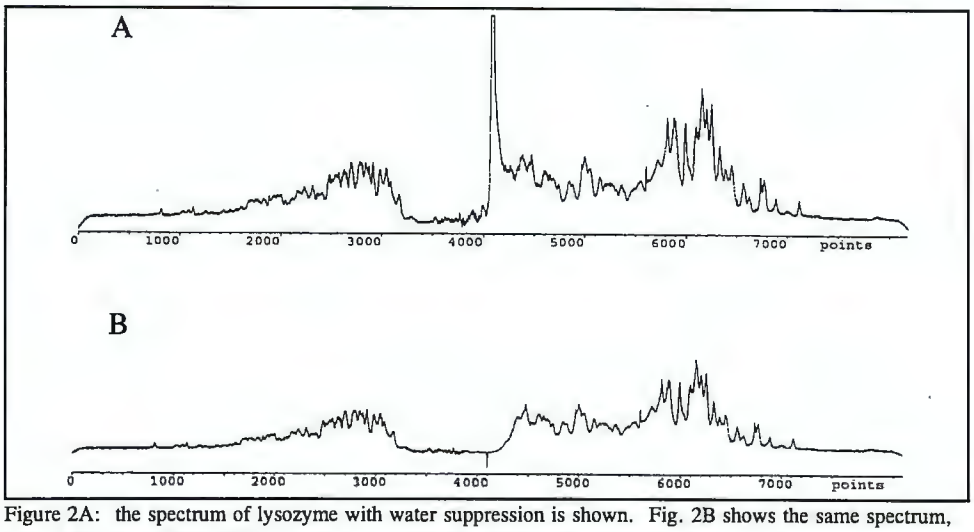


Figure 2A: the spectrum of lysozyme with water suppression is shown. Fig. 2B shows the same spectrum, after digital notch filter (200 Hz band stop), centered on the water resonance, was applied.

OFF-LINE DIGITAL FILTER SOFTWARE FOR AM, AMX AND AVANCE CUSTOMERS

Many customers have inquired about the ability to utilize digital filtering off-line, on spectrometers not yet equipped with on-line real-time digital filters, or simply to become familiar with the applications and benefits of digital filtering. Bruker suggests to utilize the Signal Processing Toolbox available within the program MATLAB (from The MathWorks, Inc. in Natick, MA, phone: (508)653-1415). The MATLAB Signal Processing Toolbox provides an easy user interface for creating various digital filters, including finite impulse response (FIR) and infinite impulse response (IIR) digital filters. The effect of the number of coefficients (tabs) on the quality of the digital filter, and on computational times can be explored. Moreover, various published window functions are available.

Bruker customers can transfer their AM or AMX data to an off-line Silicon Graphics workstation, or utilize the SGI host computer of an *AVANCE* spectrometer. MATLAB also runs on Macintosh and PC computers and can be used in conjunction with Bruker's popular WIN-NMR™ software packages on these platforms. Data transfer from WIN-NMR or UXNMR to MATLAB is easy and can be done in binary or ASCII form. After the application of digital filters, the results can easily be transferred back to UXNMR or WIN-NMR for Fourier transformation, further processing and plotting.

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Prof. B.L. Shapiro
TAMU NMR News letter
966 Elsinore Court
Palo Alto, California
CA- 94303 , USA

December 30, 1994
(received 1/9/95)

IN-VIVO ^{31}P NMR IN PLANT TISSUES

Dear Barry,

With the addition of a Bruker AMX-400 with micro-imaging and multi-nuclear NMR capabilities to our centre, we initiated work on imaging in oil containing seeds such as pea-nut and sunflower in order to map the oil and water distribution. It provided interesting information on the use of NMR imaging in the study of plant physiology. Encouraged by such observations, we have now started work on in-vivo ^{31}P-NMR investigations on plant tissues with special reference to root-tips from germinating seeds.

The physical environment plays a crucial role in plant life right from the seed germination stage. We have monitored the intracellular changes taking place in soybean root tips brought about by thermal stress using ^{31}P-NMR spectroscopy. Indirect and direct heat shocks (brought about by maintaining the root tips at various temperatures between 296-328 K for two hours in the probe itself and by instantaneously raising the temperature of the root tips from room temperature to 323 K by placing them for 5 minutes in water bath maintained at those temperatures) produce significantly different changes at intra cellular level as exhibited in the appearence of the respective temperature dependent ^{31}P-NMR spectra. In the case of indirect heat injury, the temperature dependent ^{31}P-NMR spectra exhibit progressively reduced intensities in the Adenosine Triphosphate(ATP) peaks suggesting a gradual depletion of the ATP levels due to heat stress. The direct heat injury, on the other hand brings about drastic changes in the ^{31}P-NMR spectra of heat treated root tissues. There is a total collapse of the ATP signals indicating a sudden inactivation of mitochondrial electron transport chain. Secondly, the sugar phosphate peaks disappear with a corresoponding growth in the inorganic phosphate peaks. The direct heat injury occures only above 320 K.

The results correspond to the reduction of efficiency of respiration in the tissues and a breakdown of the mitochondrial electron transport chain. Sudden heat shocks can produce effects similar to those of anaerobic conditions.

With best wishes for a very happy new year,

Yours sincerely

(G.A. NAGANAGOWDA)

(C.L. KHETRAPAL)

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SUNDAY, MARCH 26, 3:30 TO 5:30 P.M.

The agenda includes a presentation of recent results by leading NMR experimentalists concerning applications of pulsed field gradient and classical NMR techniques to both large and small molecular systems. The results obtained with 3, 5, 8, and 10mm probes will be of interest to all liquid state NMR spectroscopists. The Symposium will be held Sunday afternoon prior to the start of ENC. Request a detailed program or RSVP by contacting Nalorac's ENC Coordinator, Victoria Davies.

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

Your reference and date	Our reference	Office telephone	Date
		31 15 786041	21-Dec-94. (received 12/30/94)
Subject		Sub-division	

^{1}H signal intensities in PRESS as a function of echo time and field strength.

Significant changes in Myo-Inositol (mI) concentration has been observed in patients with chronic hepatic encephalopathy, with diabetes mellitus, and with Alzheimer disease.
In-vivo ^{1}H spectra obtained with multi-pulse sequences are J modulated, implying that the peak areas depend besides on the concentration and on T_1, T_2, and T_R also on the echo time T_E, the line width, the coupling constants, and for strongly coupled spin systems also on the chemical shifts. The aim of this study is to determine the signal intensities of mI as a function of T_E in the ^{1}H PRESS sequence at 1.5, 4.0, 6.3 and 7.0 T, in order to be able to select an optimal T_E.
The J coupling constants and resonance frequencies were determined from a spectrum of a mI solution in D2O at 7.0 T. The complexity of the J-modulation patterns, and hence the mI peak intensities as a function of T_E depend on B_0. Therefore for 1.5, 4.0, 6.3 and 7.0 T the signal strength was determined as a function of T_E. Because the effect of the PRESS sequence cannot be calculated analytically, a computer simulation program was used, solving the Liouville von Neumann Equation. A complete PRESS sequence with soft pulses would require several weeks of calculation time on a SUN SPARC-2 workstation, therefore soft RF pulses were replaced by hard ones. It is shown elsewhere (1) that if the bandwidth of the soft pulses is much larger than the total spectral bandwidth of the coupled spin system, this is a reasonable approximation. The effect of the PRESS sequence (90-t_1-180-t_2-180-acquire) was calculated for $17.45<T_E<217.45$ ms in equidistant steps of 5 ms. t_1 was kept constant to 7.45 ms for all field strengths, t_2 was varied, relaxation effects were neglected, a Lorentz filter was applied. The absolute value of the signals of H-1,2,4,6 were integrated, because these are most suited to quantify mI in vivo.
Signal loss will especially occur for those echo times where multiplet components are in anti-phase, while linewidths are larger than the separation between the multiplet components, as is the case in vivo; the effect increases with field strength due to in-vivo susceptibility effects.
The figure shows the simulation results as a function of the total echo time $2t_2$. Experiments at 7.0 T were in good agreement with the simulations. The shortest echo times give the strongest signals for all field strengths, because dephasing due to J modulation is still very small. At higher field strengths in principle several echo times are possible: smaller than 25 ms, between 60 and 100 ms and between 180 and 220 ms. However, in vivo transverse relaxation prohibits the use of the longer echo times.

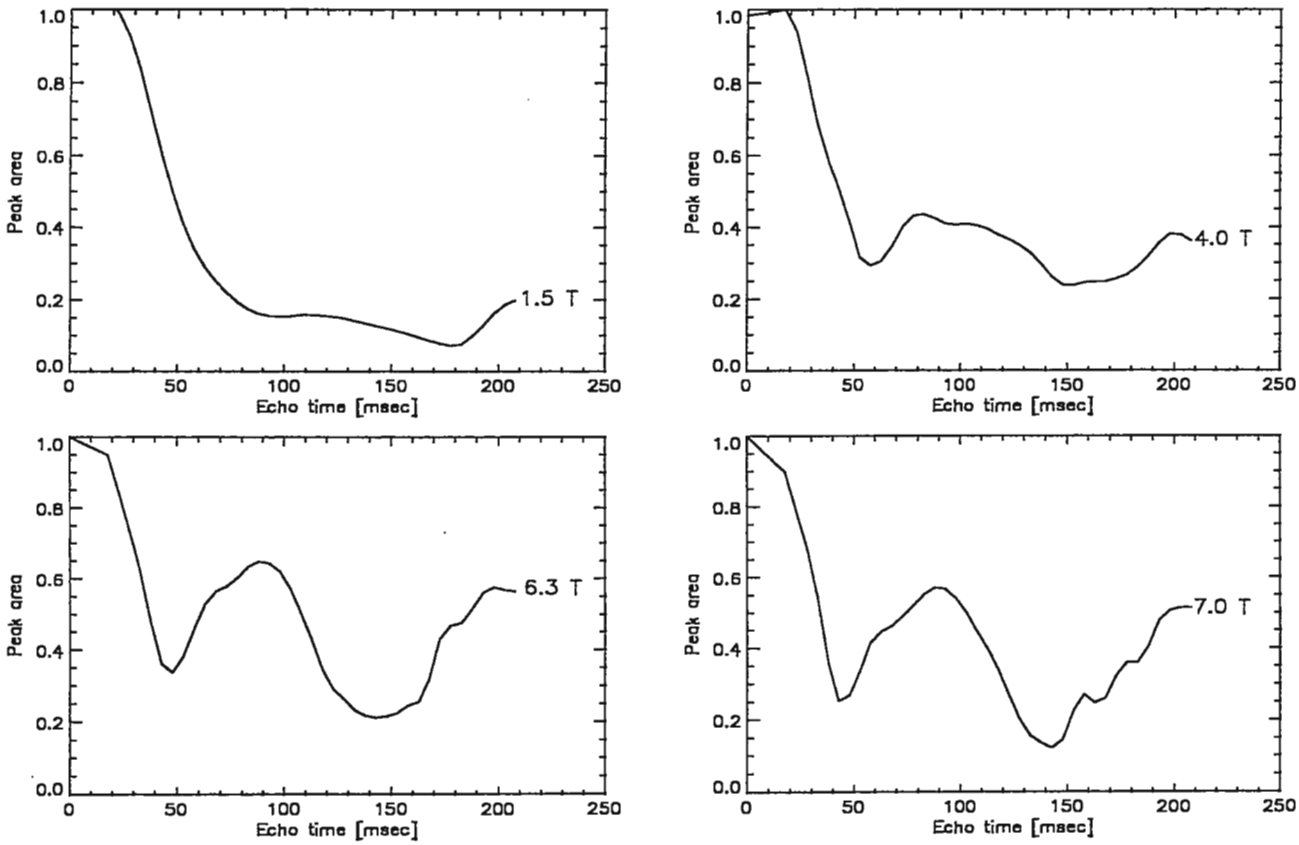
At low field strengths only short echo times are appropriate. For short echo times the signal amplitudes decrease faster with T_E at higher field strength. Increasing the linewidth lowers the minima at T_E~50 ms and ~140 ms.

References:

1. J. Slotboom, A.F.Mehlkopf, W.M.M.J.Bovée. J.Magn.Reson.**A108**, 38-50, 1994.

Wim Bovée

Hans Slotboom



Simulated PRESS intensities of H 1,3,4 and 6 of mI as a function of T_E. Line widths at half height :at 1.5T - 4.1Hz, at 4.0T - 6.5Hz, at 6.3T - 7.6 Hz and at 7.0T - 12.5 Hz.

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750	51	15	60	3.8
600	51	10	120	3.4
500	51	10	150	3.2
400	54	8	365	2.8
360	54	8	365	2.8
300	54	3	365	2.8
270	54	2.7	365	2.8
200	54	2	365	2.8
100	54	1	365	2.8
500	89	15	120	3.4
400	89	10	180	2.8
360	89	10	365	2.8
300	89	3	365	2.8
270	89	2.7	365	2.8
200	89	2	365	2.8
100	110	1	119	2.8

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International School of Biological Magnetic Resonance, 2nd Course: Dynamics and the Problem of Recognition in Biological Macromolecules

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Erice, Trapani, Sicily, Italy

NOTE Date Change!!! ⟶ **19-30 May 1995**

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NOTE some program changes ⟶ **Program and Lecturers**

Basic Principles	
Introduction	Oleg Jardetzky, Stanford University, USA
Basic Principles of NMR	Hartmut Oschkinat, EMBL Heidelberg, Germany
Basic Principles of Protein Crystallography	Rudolf Ladenstein, Karolinska Inst., Stockholm, Sweden
Solid State NMR	Stanley Opella, University of Pennsylvania, USA
Isotopic Labeling of Biomolecules	John L. Markley, University of Wisconsin, USA
Basic Theory of Relaxation	Robert G. Shulman, Yale University, USA
Internal Dynamics and Empirical Determination of Spectral Density Functions	Jean-François Lefèvre, Louis Pasteur University, France
Hydrogen Exchange and Internal Dynamics	Oleg Jardetzky, Stanford University, USA
Molecular Recognition	
Recognition Processes Studied on Oligomeric Enzymes & a DNA Binding Protein	Rudolf Ladenstein, Karolinska Inst., Stockholm, Sweden
Protein A and G Interactions with Antibodies	Gordon C. K. Roberts, University of Leicester, UK
Structure of Glycoproteins	Gerhard Wagner, Harvard Medical School, USA
Antigen and Superantigen Recognition by MHC Class II Receptor	Theodore Jardetzky, Northwestern University, USA
Enzyme-Ligand and Inhibitor Interaction	Gordon C. K. Roberts, University of Leicester, UK
Ligand Design	Martin Karplus, Harvard University, USA
Structural and Dynamical Consequences of Ion Binding on Metalloproteins	Sture Forsén, University of Lund, Sweden
NMR Studies of Protein-Membrane Interaction	Stanley Opella, University of Pennsylvania, USA
Inhibitor-Protease Interactions	Tad Holak, Max-Planck-Institut, Munich, Germany
Solution Structure of LSIII, a Neurotoxin from the Venom of *Laticauda semifasciata*	Jeffrey C. Hoch, Rowland Institute, USA
Molecular Dynamics	
Simulating Protein and Nucleic Acid Molecular Dynamics	Michael Levitt, Stanford University, USA
Dynamics of Peptides Observed by NMR and Other Physical Methods	Rudolf Rigler, Karolinska Inst., Stockholm, Sweden
Structure and Dynamics of Glycogen	Robert G. Shulman, Yale University, USA
H/D Fractionation Studies of Protein Structure and Dynamics	John L. Markley, University of Wisconsin , USA
Nucleic Acids and Protein-Nucleic Acid Interactions	
Plasticity of DNA Structure and Mutagenesis	Jean-François Lefèvre, Louis Pasteur University, France
Structure and Dynamics of RNA	Cornelius Hilbers, University of Nijmegen, NL
Interaction between *trp* Repressor and *trp* Operator	Oleg Jardetzky, Stanford University, USA
NMR Studies of Protein-Nucleic Acid Complexes	Rolf Boelens, Utrecht University, NL
Protein Folding	
Pathways of Protein Folding	Christopher M. Dobson, Oxford University, UK
Simulations of Protein Folding: From Native to Denatured State and Back Again	Martin Karplus, Harvard University, USA
Thermodynamic Studies of Folding	Walter Englander, University of Pennsylvania, USA
Kinetic Studies of Folding	Walter Englander, University of Pennsylvania, USA

PURPOSE OF THE SCHOOL

The School will be devoted to the analysis of the dynamic behavior of biological macromolecules by Nuclear Magnetic Resonance and the implication of dynamics on the mechanism of recognition between macromolecules or macromolecules and small substrates. The subjects listed above will be explored in detail during the course. Students are encouraged to submit abstracts and some student research will be selected for presentation in workshops.

NMR has reached the stage where both three-dimensional structure of macromolecular complexes and dynamics can be studied quite accurately. An integrated approach between these two aspects should be utilized more and more in future research. The proposed course will bring together the interesting features of such an integrated approach.

VENUE

The Ettore Majorana Centre for Scientific Culture was founded in 1963 in the pre-medieval mountain town of Erice near Palermo as a Conference Centre, taking its inspiration from the Italian Physicist, Ettore Majorana. The Centre's lecture halls are located in two restored monasteries and the ancient Palazzo Ventimiglia. School participants are housed in the Centre Institutes or local hotels and meals are taken at local restaurants.

GENERAL INFORMATION

Prospective participants should apply to either:

Prof. Oleg Jardetzky *or* **Prof. Jean-François Lefèvre**

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fax: +33/88 65 53 43
phone: +33/88 65 52 69
lefevre@bali.u-strasbg.fr

stating: (1) date and place of birth, nationality, qualifications and present position; (2) address, fax and phone numbers and email address; and (3) list of publications.

Applicants interested in submitting unpublished results should send the title and an abstract of about 200 words. Selected papers will be presented and discussed in special sessions.

The total fee, including full board and lodging (arranged by the School) will be US $1,000. Limited financial aid available. Participants should arrive by 5 p.m. on the 19th.

THE CLOSING DATE FOR RECEIPT OF APPLICATIONS IS MARCH 20, 1995. NO APPLICATION FORM IS REQUIRED.

Attendance will be limited to ~75 students, to be selected by the Co-Directors. Further details will be mailed with the acceptance letter.

Oleg Jardetzky
Co-Director of the School

A. Zichichi
Director of the Centre

Jean-François Lefèvre
Co-Director of the School

ISMAR '95

TWELFTH CONFERENCE OF THE INTERNATIONAL SOCIETY OF MAGNETIC RESONANCE

THE UNIVERSITY of SYDNEY
SYDNEY NSW 2006
AUSTRALIA
DEPARTMENT of BIOCHEMISTRY

Secretary: Dr Bill Bubb
Office: + 61-2-351-4120
FAX: + 61-2-351-4726
E-mail: ismar95@biochem.su.oz.au

29 November, 1994

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

Dear Professor Shapiro,

Plans for ISMAR-95 to be held in Sydney, Australia in July, 1995 are well advanced.

The program will commence at the Sydney Opera House on Sunday 16 July, with a mixer and special session to commemorate the 50th anniversary of the discovery of NMR, and continue at the University of Sydney from Monday 17 until Friday 21 July. Speakers who have accepted invitations include:

Paul Callaghan (Palmerston, NZ)
Melinda Duer (Cambridge, UK)
Ray Freeman (Cambridge, UK)
Erwin Hahn (Berkeley, USA)
James Hyde (Milwaukee, USA)
Lewis Kay (Toronto, Canada)
Ray Norton (Melbourne, Australia)
Alex Pines (Berkeley, USA)
Hal Swartz (Hanover, USA)
Keith Thulborn (Pittsburgh, USA)
Warren Warren (Princeton, USA)
Kurt Wüthrich (Zürich, Switzerland)
David Doddrell (Brisbane, Australia)
Richard Ernst (Zürich, Switzerland)
Maurice Goldman (Gif-sur-Yvette, France)
Robin Harris (Durham, UK)
Jean Jeener (Brussels, Belgium)
Carolyn Mountford (Sydney, Australia)
John Pilbrow (Melbourne, Australia)
Charles Springer (New York, USA)
Takehiko Terao (Kyoto, Japan)
Kamil Ugurbil (Minneapolis, USA)
John Waugh (Cambridge, USA)
Nino Yannoni (San Jose, USA)

The deadline for submission of abstracts and normal registration is 1 April, 1995. The social program will include a cruise on Sydney Harbour and dinner in Sydney's historic Rocks area. Details of these events as well as information on satellite meetings and travel opportunities in Australia are provided in the registration brochure, copies of which may be obtained from me at the above address.

Yours sincerely,

W.A. Bubb.

Bill Bubb
for the ISMAR-95
Organising Committee

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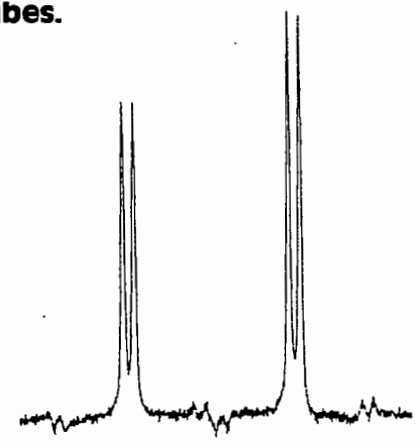
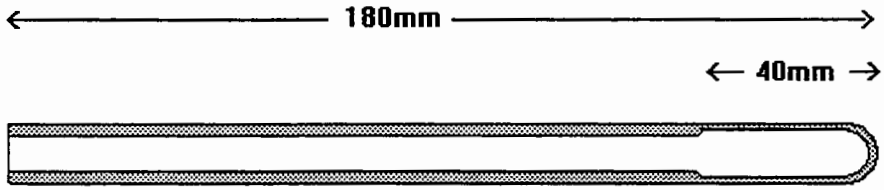
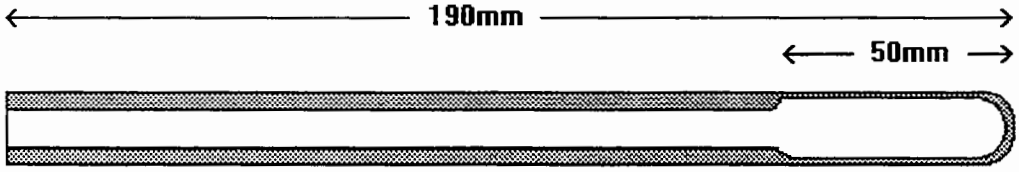


Fig.1a Fig.1b

The spectra of 20mm sucrose in D_2O were obtained with a single scan without apodization prior to Fourier transformation on a Bruker AMX-600 spectrometer at 298 K. By using Shigemi high quality 5mm standard tube (Fig.1a) and the Shigemi highly sensitive thin wall 5mm tube (Fig.1b), the spectra confirms a sensitivity enhancement of about 10%.



PST-001 and PST-002



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	PST-002	0.21	40/15	4.96 + 0.00 - 0.01	4.54 ± 0.01	$13.00	$12.00
8	ST8-001	0.25	40/ 8	8.00 + 0.00 - 0.01	7.52 ± 0.01	$31.00	$28.00
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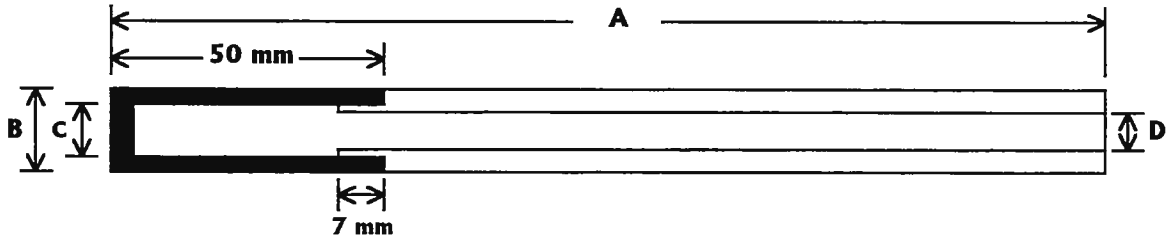

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Professor B. L. SHAPIRO
966 Elsinor Court
Palo Alto
California 94303 - Etats Unis

Dear Dr Shapiro

Theix, 4 January 1995
(received 1/11/95)

STUDY OF WATER PROTONS IN GELATIN : THE SOL AND GEL STATES

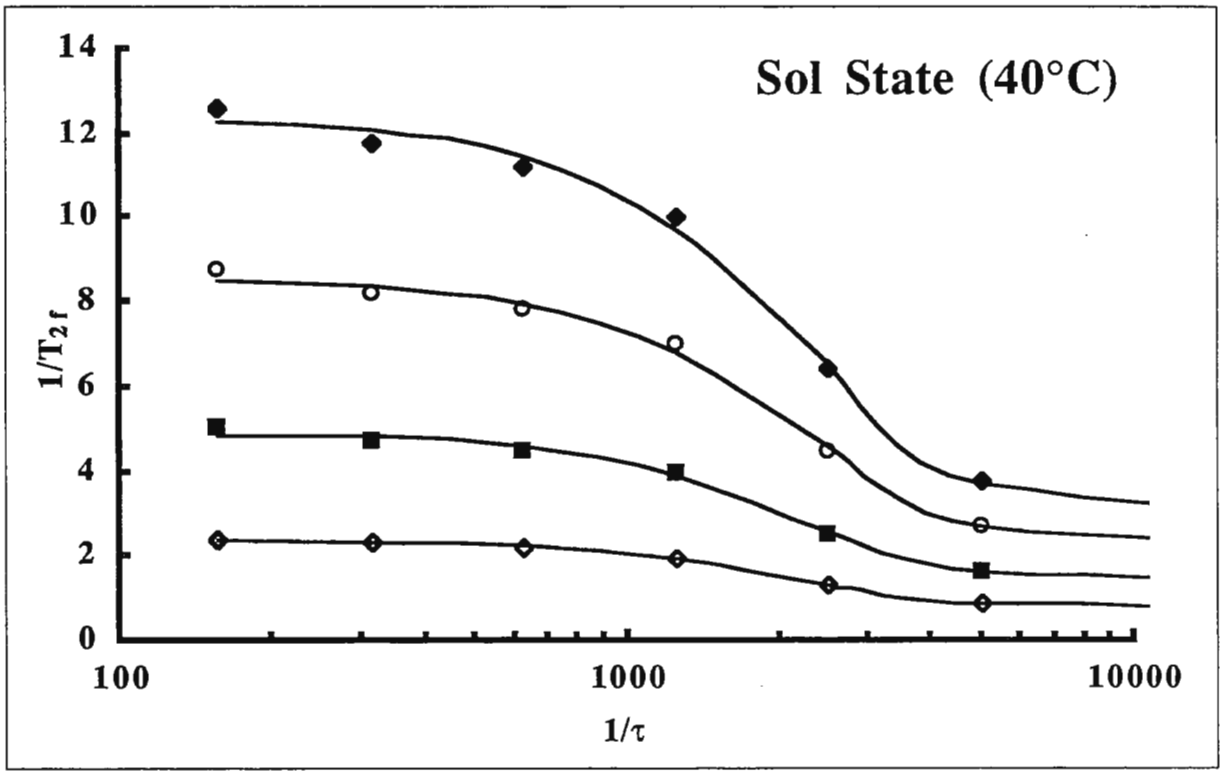
To study water dynamics in gelatin sol and gel states, the transversal water proton relaxation rates ($1/T_2$) were measured at different Larmor frequencies (20, 300 and 400 MHz). The CPMG pulse sequence was used with different pulse spacings (τ) varied between 0.5 and 10 ms. Four gelatin concentrations (5, 10, 15 and 20 % w/w) were used. Samples were thermostated at 10°C for gel state and at 40°C for sol state.

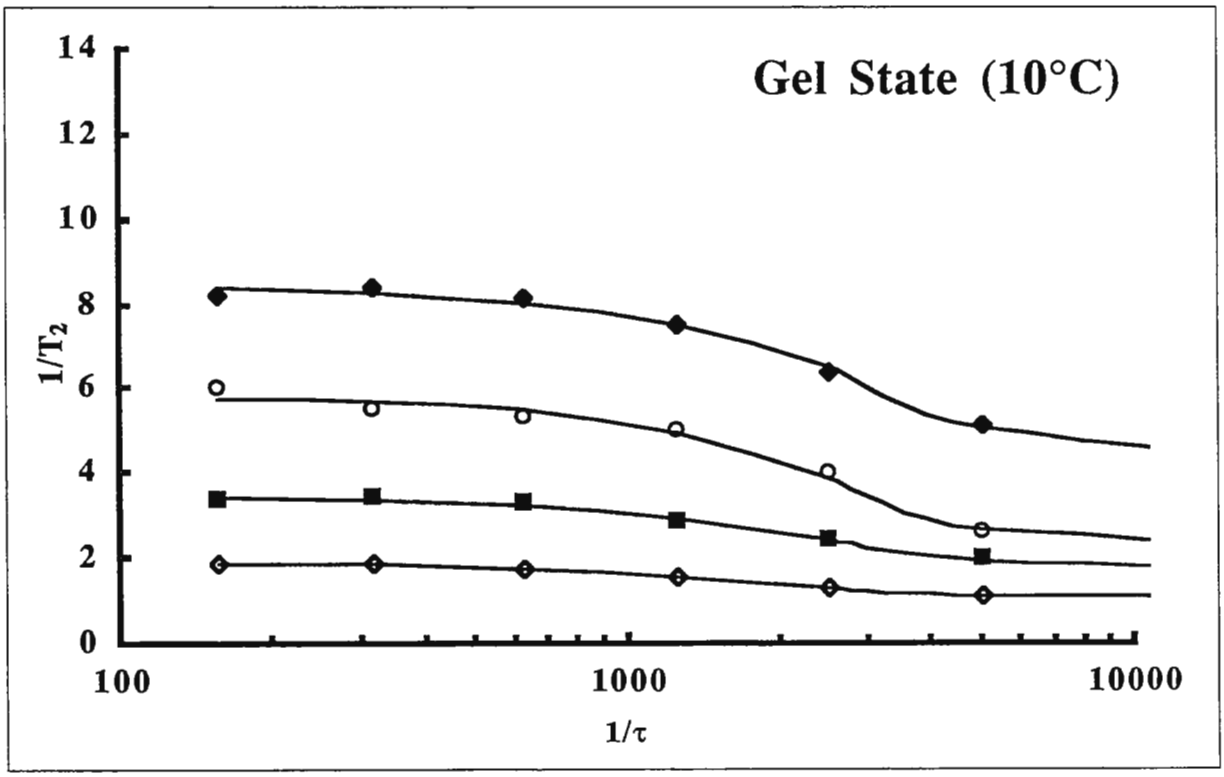
In sol state, two T_2 were always observed. The slow component, T_{2S} was unaffected by τ values while the fast component T_{2f} was τ dependent. In gel state, only one T_2 was detected. Its variation as a function of τ was less affected than in sol state and only detectable at high frequencies.

The proton relaxation measurements give informations about the state of gelatin. Indeed the τ dependence of T_2 values is in agreement with a chemical exchange process. The observation of one or two exponential components could be explained by diffusive exchange ; diffusion coefficient and T_2 are reduced by gelation.

Sincerely yours,

A. TRAORE L. FOUCAT J.P. RENOU





The dependence of transversal water proton relaxation rate $1/T_2$ (s^{-1}) on Log($1/\tau$) for four gelatin concentrations (20% (♦), 15% (O), 10% (■) and 5% (◊) w/w) in sol and gel states at 300MHz.

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Chemagnetics

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Unique COAX™ and APEX ™ RF design:	Increased sensitivity performance across the complete frequency range, allows tuning capacitors to be placed at the base of the probe for easy tuning, and eliminates temperature effects.
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Specifications @ 8.45 T: [3, 11]

Probe Outer Diameter	68 mm	^{13}C 90° pulse width	≤2.0 µs
Rotor Diameter	4.0 mm	^{1}H 90° pulse width	≤2.0 µs
Spinning Speed (ZrO_2 rotors)	1-18 kHz [4]	^{31}P 90° pulse width	≤2.0 µs
"X" Channel Frequency Range	^{15}N-^{31}P	^{15}N 90° pulse width	≤4.0 µs
"H" Channel Frequency Range	^{19}F-^{1}H [5]	^{13}C sensitivity [7]	200:1
Temperature Range	-150°C to + 250°C	^{13}C sensitivity [8]	40:1
Sample Volume	52 µL	^{15}N sensitivity [9]	10:1
^{13}C linewidth [6]	≤0.1 ppm	^{31}P sensitivity [10]	750:1

[1] Available in proton/fluorine tuning at proton frequencies ≥ 360 MHz
[2] Available as an upgrade to standard probe.
[3] Specifications are indicated for performance on Chemagnetics CMX spectrometers and compatible magnets systems. Some magnet systems may have bore restrictions which prevent the use of the Chemagnetics VT stack.
[4] Higher speeds can be obtained using rotors with reduced inner diameter.
[5] Available on probes with proton frequencies ≥ 360 MHz
[6] Adamantane sample, ^{13}C, MAS, single pulse.
[7] HMB, 12 scans, ^{13}C, CP/MAS, methyl carbon.
[8] Glycine, 4 scans, ^{13}C, CP/MAS, alpha carbon.
[9] Glycine, 8 scans, ^{15}N, CP/MAS.
[10] Chiraphos, 4 scans, ^{31}P, CP/MAS
[11] Specifications at other field strengths available on request.

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The NMR Newsletter - Book Reviews

Book Review Editor: **William B. Smith,** Texas Christian University, Fort Worth, TX 76129

"Special Applications"

Guest-Edited by **Dr. H. Pfeifer** and **Dr. P. Barker**

NMR Basic Principles and Progress, (P. Diehl, E. Fluck, H. Gunther, R. Kosfeld and J. Seelig, eds.), 1993; Springer- Verlag New York, Vol. 29 - ISBN 0-387-56438-1, 178 pp.

This volume entitled "Special Applications" concerns itself with Quadrupole effects in the solid-state and NMR studies of synthetic polymers in solution as well as the solid phase. The first chapter contains a description of the basic theory of solid state magnetic and electric interactions. First and second order electric quadrupole effects and the dipole-dipole chemical shift are explored and their impact on the NMR lineshape is discussed. The effects of spinning the sample at the magic angle and varible angle, dynamic angle and double rotation are also addressed. Nutation spectroscopy, spin-lattice relaxation behavior and quantition in the MAS experiment are covered. The theoretical treatment and the mathematical expressions are excellent; however, the presentation is difficult to read and the flow is severely mared by what we can only attribute to a poor job in translation from the native German into English.

The chapter by N. J. Clayden entitled "Solid State NMR Of Synthetic Polymers" includes discussions on compositional analysis, conformational analysis, the determination of morphological phenomena such as orientation, crystallinity, domain size and phase identification, and polymer dynamics. The author describes the use of solid state NMR from the perspective of an industrialist in dealing with questions of when to use solid state NMR in preference to IR or other analytical techniques. His criteria include the uniqueness of the technique, its scientific benefit and cost. He describes the application of solid state NMR to the above mentioned topics from this perspective.

In the discussion of compositional analyses by solid state NMR, the author admits that this technique is not that of first choice. The analysis of composition by solid state NMR usually results when a material is insoluble and not amenable to high resolution NMR and when standards are not available. It is possible (although not straight forward) to obtain quantitative data from solid state NMR without standards. The author deals with several of the problems encountered with this analysis including spinning sidebands, the non-quantitative effects of cross polarization and unresolved resonances. He then shows examples of both quantitative analysis in the curing of methacrylates and with a valuable discussion of the analysis of cross-linking. He discusses the analysis of plasma polymers to illustrate the value of spectral editing and deconvolution.

Conformational analysis performed by NMR spectroscopy originates from the fact that the chemical shift tensor is dependent on the immediate structure around the nucleus. The author deals with the situations which are amenable to NMR analysis. He discounts the ability of solid state NMR to define conformations in the absolute sense, preferring to rely on such techniques as X-ray diffraction for that information. Even for structural analysis of amorphous polymers, the author emphasizes that caution must be exercised in interpreting the data because intrachain effects are dominant in determining the chemical shift tensor.

The chemical shift tensor is also useful for the determination of orientation as is the quadrupolar lineshape. Studies using ^{13}C and ^{19}F chemical shift tensors and ^{2}H quadrupolar tensor are presented in terms of their relative merits and liabilities. The liabilities, which include overlapping lines, dipolar broadening effects and sensitivity limitations, have

been overcome in various ways. However, the sum effect is that other techniques are usually more suited to this analysis than solid state NMR.

A very valuable discussion of the determination of the morphological aspects of heterogeneous polymer systems is given. It describes the use of the various relaxation measurements to determine whether phase separation exists in a material. A discussion of the quantitative use of these relaxation experiments for the determination of the level of crystallinity in several semi-crystalline polymers is presented as an example. Spin diffusion among the proton spin system was utilized for the quantitative determination of domain size in two phase systems by use of the Goldman-Shen experiment. These morphological analyses have found great application in industry.

Correlations between the molecular dynamics of a polymeric material and its mechanical properties as determined by, for example, dynamic mechanical spectroscopy, are very important for a molecular understanding of the relationship between the chemistry of a material and its performance. An interesting, albeit limited, discussion of the resistance to these studies by traditional materials scientists is presented. This is followed by several examples which utilized solid state NMR relaxation times and lineshape analyses to map the temperature dependence of molecular motions for correlation with properties. The relaxation studies were usually carried out with ^{1}H or ^{13}C NMR spectroscopy and the lineshape analyses with ^{2}H NMR. Dynamic information which is available from these experiments is unrivaled by any other technique and invaluable for the modeling of polymeric systems.

In summary. this chapter, although in my opinion, too optimistic concerning the quantitative aspects of solid state NMR, presents a very useful discussion of the attributes of solid state NMR for the analysis of synthetic polymers.

The final chapter by A. Bunn entitled "Solution NMR of Synthetic Polymers" is a workbook of how to perform solution state NMR of synthetic polymers. In the introduction, he defines several texts which could be used for the theoretical aspects of NMR but the author's intention is to describe the strengths that NMR brings to a polymer analytical laboratory.

The first topic discussed concerns techniques used to obtain the spectrum. A useful table of solvents and conditions for dissolving polymers is presented. Instrument parameters which ensure quantitative spectra are discussed as well as topics of data manipulation.

This information is followed by case studies of several classes of polymers, including polyolefins, polyesters, polyamides, polysulfones, polyethers, polyvinyl chloride and polystyrene. Spectral assignments, especially with regard to sequence effects in copolymers, provide a valuable reference for these materials. These studies are used to illustrate points concerning the quantitative analysis and the analysis of other structural aspects, such as tacticity and end group analysis, for these systems.

This final chapter provides a very useful and readable compilation of ^{13}C NMR spectra and information for a wide variety of polymers. While it has no pretensions of being a theoretical treatment of solution state NMR topics, it does contain a wealth of practical and useful information on obtaining high resolution NMR spectra of polymers and is well worth a thorough examination by serious practitioners.

Patrick Smith
Analytical Sciences
Michigan Divison
Dow Chemical USA

Ahmed Ellaboudy
Analytical Sciences
Texas Operations
Dow Chemical USA

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U.S.A.

(received 1/17/95)

Prof.ke-rh

ESF Meeting Wildbad-Kreuth 25.-30. 6. 95

"NMR in Molecular Biology"

Dear Barry,

I would like to draw your attention to a conference on Biomolecular NMR that will be held in Wildbad Kreuth, Germany, June 25 - 30. The scope of the meeting is as follows:

Knowledge of the structures and dynamics of biological macromolecules is the key to understanding their function. NMR spectroscopy is one of the most powerful and most widely used physical methods in this field.

The aim of this conference is to cover the whole range of activities in the field of biomolecular NMR. The meeting will start with contributions concerned with new developments in NMR and computational techniques designed to examine increasingly large biomolecules. Then, there will be a series of presentations of results obtained from structural and dynamical studies of biomolecules, and discussion of their significance for understanding function. Finally, the contributions that NMR is making to the fields of macromolecular recognition and protein folding will be discussed.

A poster session will be organised.

We would also like to encourage young researchers to give 5 - 10 minute talks on their results in a special session during the meeting.

The following scientists have accepted our invitation to give a lecture:

C. Altona, *Leiden, NL*
A. Bax, *Bethesda, USA*
B. Bechinger, *Munich, D*
I. Bertini, *Florence, I*
T. Creighton, *Heidelberg, D*
R.R. Ernst, *Zürich, CH*
J. Feigon, *Los Angeles, USA*
S. Fesik, *Abbott Park, USA*
C. Griesinger, *Frankfurt, D*
W. van Gunsteren, *Zürich, CH*
R. Huber, *Munich, D*
R. Kaptein, *Utrecht, NL*
L. Kay, *Toronto, CAN*
B. de Kruijff, *Utrecht, NL*
J.Y. Lallemand, *Gif-sur-Yvette, F*
E.D. Laue, *Cambridge, GB*
J.L. Markley, *Madison, USA*
D. Mierke, *Worcester, USA*
S. Opella, *Philadelphia, USA*
H. Oschkinat, *Heidelberg, D*
C. Redfield, *Oxford, GB*
M. Rico, *Madrid, E*
H. Rüterjans, *Frankfurt, D*
G. Varani, *Cambridge, GB*
F. van de Ven, *Nijmegen, NL*
P. Wright, *La Jolla, USA*
K. Wüthrich, *Zürich, CH*

One of the basic ideas of this conference is to enhance the exchange of ideas by inviting only a small number (approx. 130) of the best scientists and by offering many opportunities for discussion during the meals etc.

I would appreciate it if you could bring this notice also to the attention of the readers of your NMR Newsletter.

Best regards

H. Kessler

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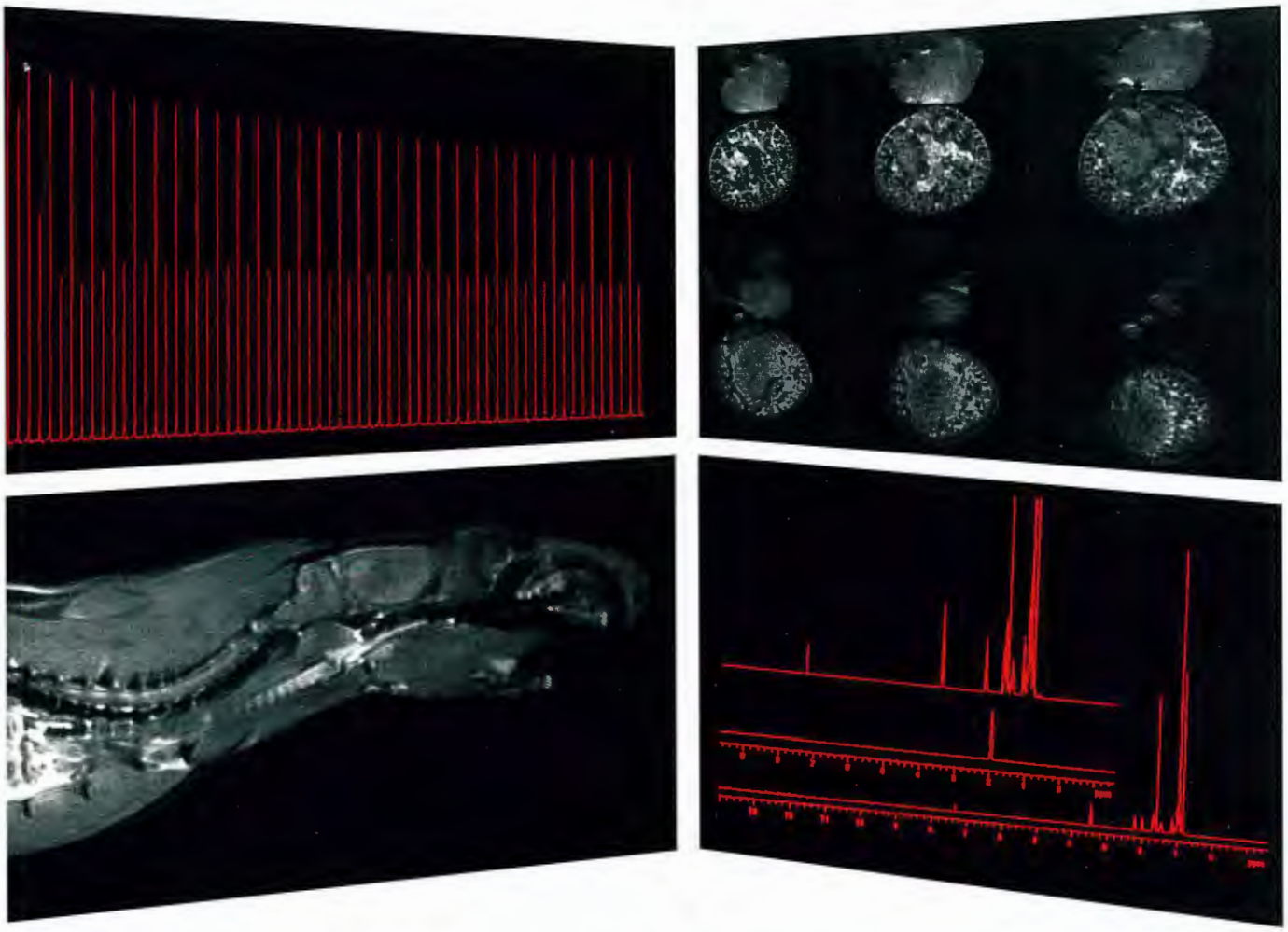

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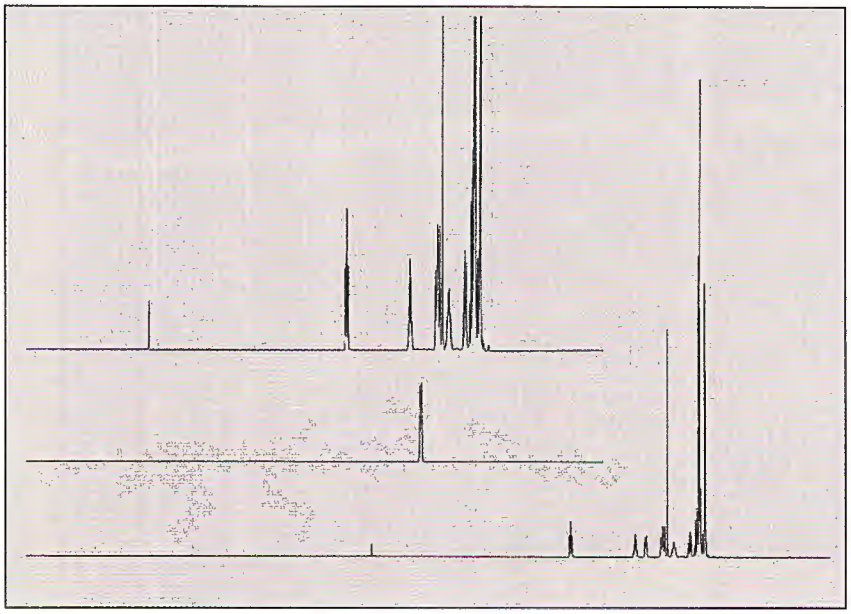

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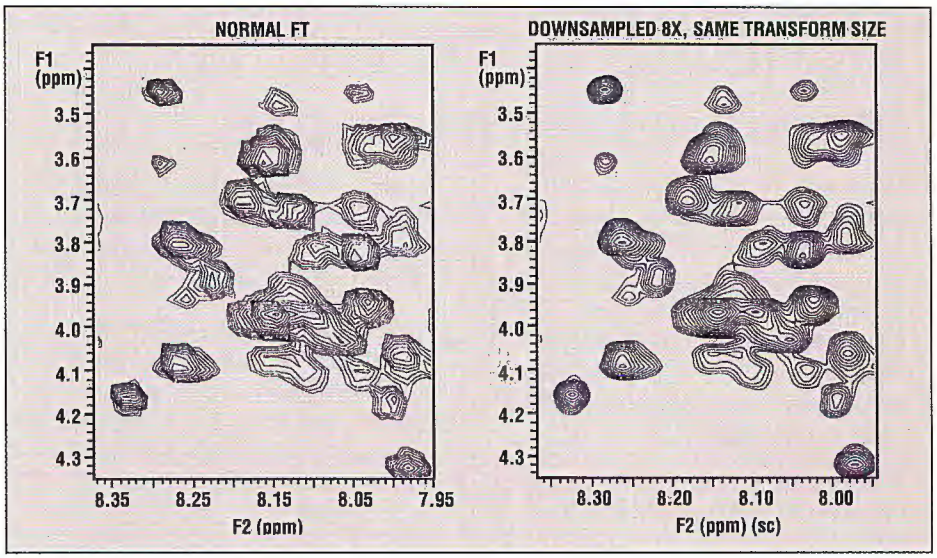

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TAMU NMR Newsletter
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Palo Alto, CA 94303
U S A

2515

Zürich, January 10, 1995
(received 1/20/95)

LAW AND ORDER IN DISORDERED SYSTEMS STUDIED BY PROTON–DRIVEN AND RF–DRIVEN ^{13}C–^{13}C POLARIZATION TRANSFER

Dear Barry,

You know that in amorphous materials it is often difficult to find hidden traces of law and order. Proton–driven and rf–driven ^{13}C–^{13}C polarization transfer (spin diffusion) can help, as has been shown by a recent study on amorphous actactic polystyrene where orientational correlations among the phenyl rings have been discovered in a very restricted distance range of 5 Å only.[1] This finding is in contrast to X–ray and neutron scattering measurements where order appeared to extend over distances of 20–30 Å.[2 3]

In the course of this study, it was found that for the quantitation of short–range order rf–driven polarization transfer is optimal, while for the detection of long–range order proton–driven polarization transfer is to be preferred. The spin diffusion rate constant,

$$W_{ij} = \frac{\pi}{2} b^2_{eff,ij} F_{ij}(0) ,$$

depends on the effective dipolar coupling constant $b_{eff\ ij}$ between spins i and j, which is a measure for the spatial arrangement of the nuclei, and on the zero–quantum spectrum $F_{ij}(\omega)$, which is an integral function of the surroundings of the two spins. The function value $F_{ij}(0)$ is, in general, difficult to compute due to the complexity of its dependence unless a detailed model of the material is available.

An example of $F_{ij}(0)$ for proton–driven spin diffusion as a function of the resonance frequency pair (Ω_i,Ω_j) of the two isochromats i and j is shown in Fig.1 for amorphous atactic poly(1–^{13}C–styrene). Its strong dependence on the two frequency variables is obvious. It can be used for the correction of experimental spin–diffusion rate constants in the laboratory frame. The $F_{ij}(0)$ values have been computed from the measured single quantum spectra $f_i(\omega)$ and $f_j(\omega)$ (extracted from a 2D separated local field spectrum), assuming that the zero–quantum spectrum can be computed by the convolution

$$F_{ij}(\omega) = [f_i(\omega)*f_j(-\omega)]$$

for uncorrelated broadening of the two single-quantum spectra. This assumption is not always valid. The correction has therefore to be applied with caution.

Fortunately, in rf-driven polarization transfer, $F_{ij}(0)$ is nearly constant and the measured W_{ij} rate constants become a direct indication of local order. For this reason rf-driven polarization transfer is preferred for the study of local order in disordered materials, such as glasses or amorphous polymers. On the other hand, for the test of long-range order, long spin-diffusion time intervals (of 100 ms and more) are needed, and rf-driven transfer with the necessary strong rf fields would fatally damage a probe assembly. Here, proton-driven transfer is preferred since no limitations of duration exist. The 2D spin-diffusion spectrum becomes asymptotically independent of W_{ij} (the variations of $F_{ij}(0)$ are irrelevant) and the 2D spectrum directly interpretable. In this way, the two techniques neatly complement each other for the measurement of molecular order on different length scales.

Best regards.

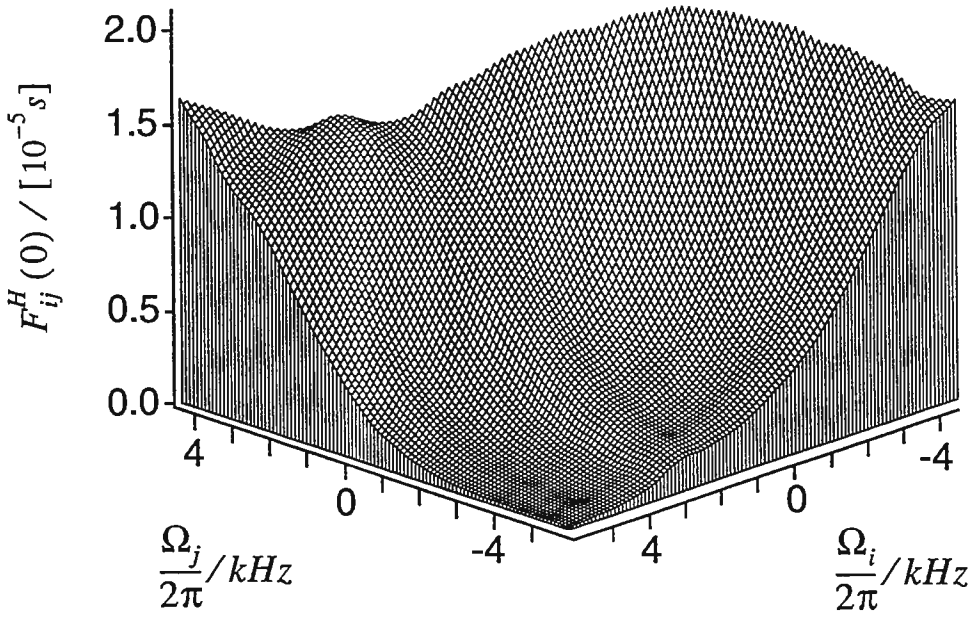
Sincerely yours,

Pierre Robyr

Marco Tomaselli

Richard R. Ernst

1. P. Robyr, M. Tomaselli, J. Straka, C. Grob-Pisano, U.W. Suter, B.H. Meier, and R.R. Ernst, Mol. Phys. (in press).
2. G.R. Hitchell and A.H. Windle, Polymer **25** (1984) 906.
3. B. Gabrys, O. Schärpf, and D.G. Pfeiffer, J. Polym. Sci. **B31** (1993) 1891.



Zero-quantum spectrum intensity at frequency zero under proton-driven polarization transfer conditions for pairs of ^{13}C isochromats with resonance frequencies Ω_i and Ω_j in poly(1-^{13}C-styrene). The zero-quantum spectrum intensities were computed from the respective single-quantum spectra.

LOUISIANA STATE UNIVERSITY
AND AGRICULTURAL AND MECHANICAL COLLEGE
Department of Chemistry

January 12, 1995
(received 1/17/95)

Dr. B. L. Shapiro
TAMU NMR Newsletter
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Palo Alto, CA 94303

Multimedia & Teaching: Remote Operation of an ARX300

Dear Barry:

Last night, I gave a short lecture to the LSU Student Affiliates chapter of the American Chemical Society. This chapter is very active and has won an Outstanding Chapter award from the ACS for the past two years. So, they deserve the very best, and that means a high-tech lecture on NMR.

At LSU, we have been curious about the possibilities of remote operation of our new ARX300 with a Silicon Graphics Indy computer. Discussions with Bruker were very helpful, but they warned us of slow performance for screen updates to non-SGI computers. The problem, they say, originates from the the original UXNMR graphics code, and may be fixed in the future. In practice, we found remote operation to a non-SGI computer to be barely adequate for demonstration purposes.

As is standard, the ARX300 was installed in the basement, and the lecture room for the 40 students is on the 2nd floor. The chemistry building is wired with an ethernet trunk line and thin-wire drops. The equipment used in the lecture room consisted of: a color LCD display panel (InFocus Panel Book 550 with 640x480 resolution), a high intensity overhead projector, and a Macintosh 520 Powerbook (16-level gray scale LCD display, 12 Mbyte RAM, ethernet, and a port for a second monitor which was connected to the InFocus Panel Book). The x-windows server software was eXodus (release 5.0.4) from White Pines running with 6Mbyte of memory partition.

There were some difficulties making eXodus and UXNMR compatible. eXodus was set to "rooted screen", command processor REXECC, and the logon command line was "setenv DISPLAY $$ME$$ && xterm" (this enabled xterm

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logon). Also, eXodus was set as follows: middle and right SGI mouse buttons were assigned to option-mouse and command-mouse, the virtual screen size was set to 1280x1040, screen colors were set to 256, and backing store support was enable. Fonts required by UXNMR that were not initially available in eXodus were redefined in the eXodus font alias files to available Adobe fonts. Then, logon to the SGI unix shell was normal. In the SGI unix shell, an SGI display manager was enabled with the command "4Dwm &". Then, UXNMR (version 940510) was run and a display appeared on the lecture hall screen in about 30 seconds. Surprisingly, the colors choices for the Mac520 video out were adequate, mostly variations of greens and blue-greens (not the putrid pale green seen with a Mac6100 and a 17" CRT). The LCD overhead display panel resolution of 640x480 is a big problem; the eXodus scroll bars do allow one to access all of the UXNMR window, but screen updates are a few seconds. Resizing (reducing) the UXNMR window is only a partial solution as data display becomes erratic and buttons are hard to read.

This first demo consisted of acquiring a ^{1}H FID, processing, and plotting a spectrum of a previously loaded and shimmed menthol sample. To give you an appreciation of the screen update rate, with a total recycle time of 2 s and 8 transients accumulated, we could observe about 2 or 3 intermediate FID displays (real and imaginary components separately displayed with the "unshuffle" command). Manual phasing is extremely tedious; instead, automatic phasing was used. Screen updates for plot expansions were ok for this 8k complex data set (SI=16k).

In summary, we like the fact that a laptop computer could provides x-windows emulation. However, the slow screen update is a problem, as well as the limited sized of the LCD display panel. Nevertheless, the demo seemed to be well received.

Regards,

Les Butler Marcus Nauman David Vargas

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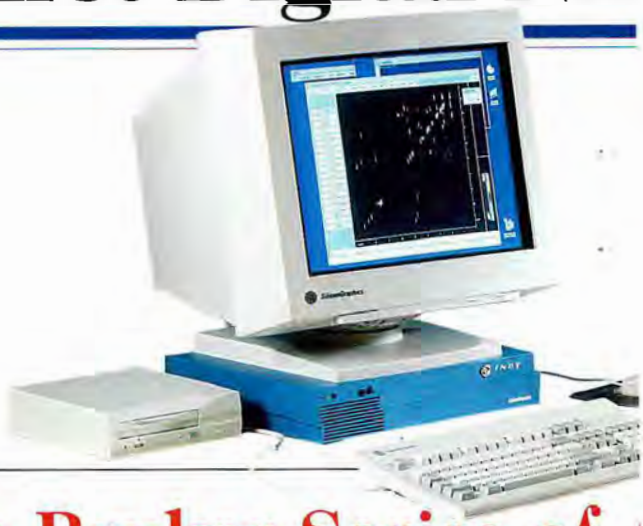

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The AVANCE design is fully modular for easy access, exchange of sub-assemblies and addition of upgrades such as additional rf channels. Extensive use of built-in system diagnostics facilitates localization of system faults, often remotely via ETHERNET or modem. Although the AVANCE is marketed in the DPX, DRX, DMX and DSX standard configurations, there is really a continuum of possibilities from one configuration to another.

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Digital filtering with oversampling and data decimation provides near perfect exclusion of peaks and noise outside the spectral width. The result is a clean spectrum, flat baseline, improved dynamic range and increased sensitivity. In many cases, especially for 2D and 3D experiments, digital resolution is also improved since only the spectral region of interest need be recorded.

Digital Lock for Unprecedented Stability

The AVANCE digital lock combines quadrature lock detection with digital signal processors and intelligent feedback control to provide superior results, especially for water suppression, 2-D, 3-D and gradient spectroscopy. Even under ideal environmental conditions performance is measurably improved.

Digital Signal Routing for Flexible, Automatic Configuration

The AVANCE digital signal router places the configuration of the entire system under full computer and software control. This allows complete flexibility to interconnect the hardware as needed without manual switching or re-cabling. Experimental configurations can also be stored and recalled for easy repetition and modification at a later time.

R Spectrometers

BRUKER

Industry Standard UNIX Workstation for Ease of Operation

AVANCE spectrometers may be controlled by any one of several industry standard UNIX workstations, including the popular SGI INDY R4000 SC. In all cases, the system operates under the X-11 windows environment with MOTIF tool kit, making it quick to learn and easy to use.

VANCE™ Spectrometers

xibility for the Future Built In

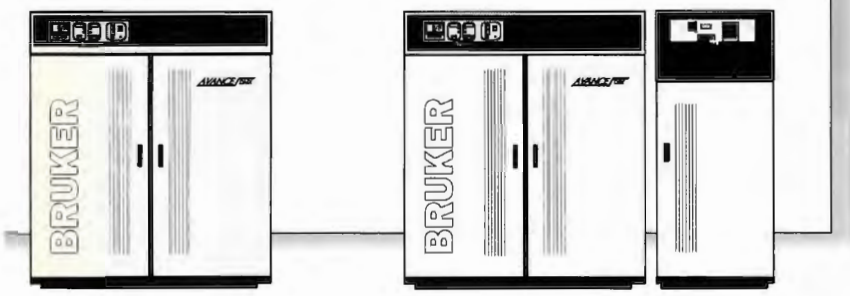
DMX

Same as DRX, plus:

- 750 MHz
- Wideline Solids
- CRAMPS Solids
- Widebore Magnet
- Solids Imaging
- Multiple Receiver Channels

DSX

Same as DMX but configured for solids only.



Solids, Imaging and More

A full range of NMR capabilities is available for the AVANCE, including microimaging, CPMAS, wideline and CRAMPS. A variety of options for gradient spectroscopy is also available, including both single and three axis magnetic field gradients and rf field gradients. Gradient shapes are calculated on the fly, providing the equivalent of an infinite wave form memory. Systems may be equipped for completely automated analysis of up to 120 liquid samples and 20 CPMAS solid samples.

Choice of Magnets and Probes

More than 30 years of experience and innovation in cryo-magnet technology guarantee maximum reliability, minimum drift, high stability and ultra-long helium hold times for Bruker cryo-magnets, which range from 100 to 750 MHz in field and 52 mm to 150 mm in bore diameter. Bruker also provides the widest range of NMR probes in the industry, including dual, quadra-nuclear, broadband and inverse probes with sample diameters from 2.5 mm to 20 mm. Specialized probes are also available for micro-imaging, CIDNP, LC-NMR, a full range of solids, and many other applications.

Comprehensive Applications Support

Specialists are available in Bruker offices throughout the world to provide answers to applications questions in person, on the telephone, or by E-mail. Updated information on applications and developments is also available from applications notes, from the "Bruker Report" periodical and from a Bruker on-line FTP server.

UXNMR Software for Full Acquisition and Processing Power

The powerful UXNMR software provides full control of all spectrometer capabilities, including a powerful, intuitive pulse programming language. A wide range of processing options is also included, including 2-D volume integrals, NMR imaging and maximum entropy.

QUICKNMR for Convenient, Routine Operation

The intuitive QUICKNMR software provides easy access to a wide variety of pre-tested experiments, including 1D, 2D and gradient applications. It is an ideal user interface for routine users and for new user training.

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Call today to learn more about how Bruker is advancing the limits of NMR spectroscopy with digital precision and performance. Call your nearest Bruker representative, and find out why everything else is just analog. Your Bruker representative will be happy to recommend a configuration that is optimum for your needs – today and tomorrow.

Everything else is just analog.℠

How to select the Digital NMR Spectrometer for your needs today...and tomorrow.

FEATURE	AVANCE™ SERIES	OTHERS
HOST COMPUTER		
Industry standard UNIX Work-station	Yes	
X-11 Windows and MOTIF	Yes	
Workstation interface to spectrometer	dedicated ETHERNET	
DIGITAL FEATURES		
Oversampling and digital filtering on the fly	Yes, via dedicated DSP processor	
Real time data decimation	Yes, via dedicated DSP processor	
Digital lock with real-time quadrature detection	Yes, via dedicated DSP processor	
Real-time gradient calculation	Yes, via dedicated DSP processor	
PROBES		
GRASP with Z-gradient	Yes	
GRASP with X, Y and Z-gradients	Yes	
RF GRASP	Yes	
2.5 mm micro-sample probes	Yes, including inverse triple resonance	
8 mm probes	Yes, including inverse triple resonance	
Quadra-nuclear inverse probes	Yes	
SOLIDS		
Pneumatic sample ejection	Yes	
Automatic sample changer	Yes	
Broadband triple resonance CPMAS	Yes	

Compare these AVANCE features to those of other systems, then contact your Bruker representative to help you select the AVANCE system configuration that's right for you.

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Molecular Sciences Department
Central Research Division
Pfizer Inc
Eastern Point Road
Groton, CT 06340

Central Research
NMR Spectroscopy

January 9, 1995
(received 1/12/95)

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

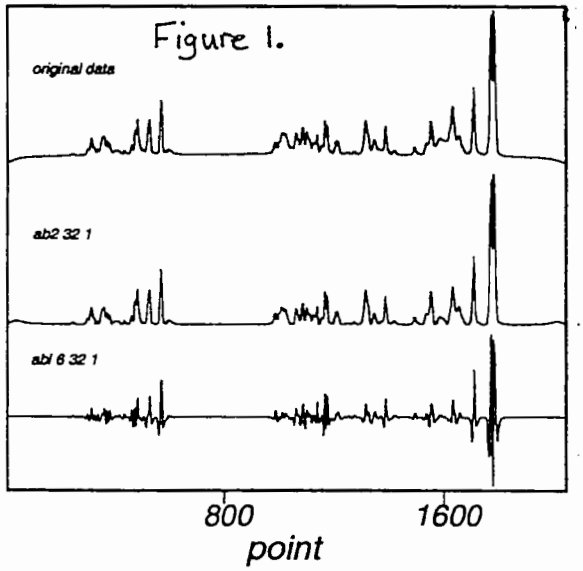
Bruker-to-Felix Data Transfer...Again!

Dear Dr. Shapiro,

Once upon a time there lived in the NMR woods a spectrometer manufacturer who insisted that a single ADC design was far superior to other receiver designs, and that spectroscopists should learn to live with the perils of poor baseline incumbent on that design. And so we did. And each day, we would acquire our data, process it, and baseline correct the data. And day-by-day, our ability to collect and baseline correct the data improved, so that by 1992-1993 it was possible to produce baseplanes that rivaled those found on other manufacturer's instruments. And we were happy, and lived in peace.

Then came the news that digital filters were upon us, and poor baselines were a thing of the past. We were excited, and many thoughts surfaced: could our old instruments be retrofitted? would we be able to afford the new design? could we get rid of water (read solvent) forever? But alas, it was not to be. And, in a moment of sheer marketing brilliance, we discovered that the new spectrometer produced data that could not be simply imported to our third party software packages. Would Felix be rendered mute?? The irony was, the first pass through data conversion led us to a baseline that was **far worse** than any we had previously encountered (Figure 1, 'original data'). A future filled with Bruker-only processing software loomed ominously on the horizon.

Then, a hero from the past emerged, known only by the initials 'abl'. With swift strokes of digital deftness, the rolling hills of digital-filtered doldrums were deftly de-emphasized (Figure 1, 'abl 6 32 1'). But at what cost? Now the signals of interest were horribly mutilated past the point of any discernible resemblance to a lorentzian.



The solution to our problem was found not in the massive digital architecture of modern processing packages, but in an algorithm so simple that it was ridiculed for its ignorance (Figure 1, 'ab2 32 1'). The algorithm asked of each processed data point 'what is the lowest point in your region?' and, much the way a convolution filter goes about its business, this low-point subtraction quickly edits out the broad unwanted features introduced by the digital filter conversions. Once again, peace returned to the forest, but it was a tenuous peace, ragged at the ends, unstable, and prone to descent into chaos.

The ages past, and our new algorithm gained respect for its diligence and simplicity. New uses were found, much as for any new, unexploited tool (Figure 2). We discovered that as the search space for the algorithm decreased to be less than the peak width, the algorithm was able to act as a resolution enhancement tool, actually creating space between barely resolved peaks (see Figure 2, as the number of points decreases from 32 down to 8). Yet something was still rotten in the forest.

One day, an honored visitor from a foreign land asked to see the raw data that was causing all the tension and noticed that the tail of the fid was actually increasing at the end! Excited by this discovery, the king and queen of the forest issued an edict: 'Hear-to-for and forever, no weighting function can be imposed that truncates the end of the fid.' The forest people were crushed, since they knew that without the ability to truncate the fid, no useful ω_2 weighting was possible. Would this be the final processing insult, the one that would negate any signal to noise advantage that digital filters imposed in the first place? That night, no one slept.

As morning broke the forest people assembled and one said: "Last night I had the strangest dream. Two trees appeared to me, shrouded in forest mist, one the obvious out-of-phase component of the other. The out-of-phase component lay down on the forest floor and the overhead sun traced the perfect phase diagram circle that results from identical real and imaginary components. But when the imaginary tree departed it left behind a hideous imperfect ellipse. Then I woke."

In utter silence, the forest elders gently pried the imaginary component of the data away from the real component and set it on fire (Figure 3). In moments it had vanished into the air, and the delicate task of reconstructing the imaginary with a hilbert transform, followed by inverse transform, was complete. And the king and queen of the forest issued a final edict: 'Hear-to-for and forever, if weighting is to be employed on a digital-filtered fid, the fid must be transformed, the imaginary rebuilt, and the inverse transform employed before apodization. Only then will harmony prevail in the forest.'

Figure 2.

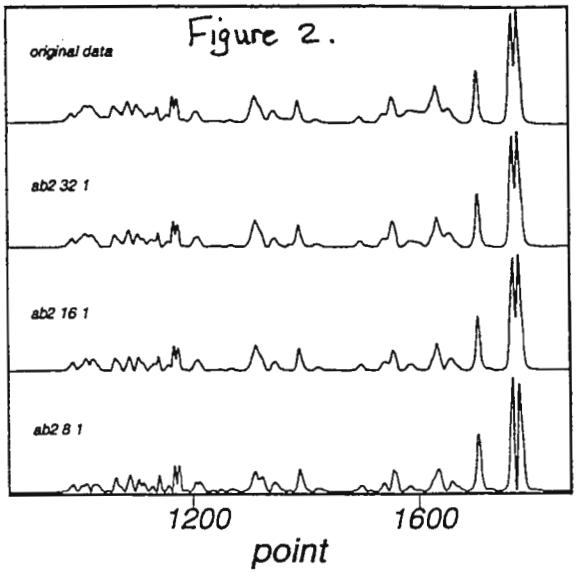
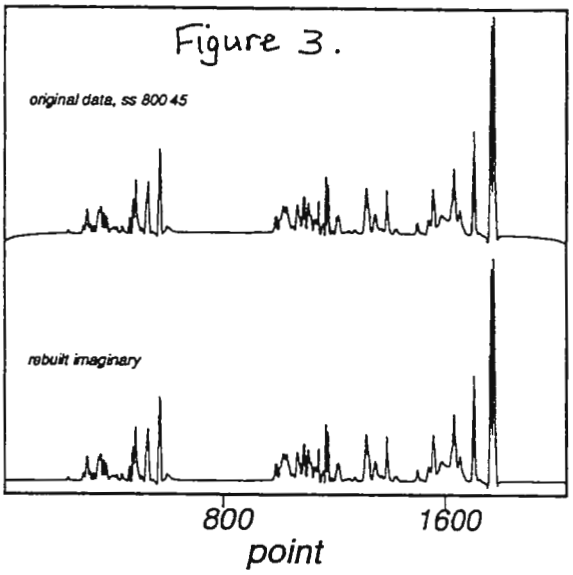


Figure 3.



This contribution is dedicated to Dr. Earl Whipple on the occasion of his retirement from Pfizer Central Research.

Sincerely,

Walt

Walter Massefski, Jr.
203-441-5962
203-441-4734 (FAX)
email: wwm@pfizer.com

STAFF NMR SPECTROSCOPIST: The City University of New York (CUNY) seeks qualified applicants for a Research Associate position, available immediately in the Chemistry Department of our new College of Staten Island campus. The NMR spectroscopist will instruct, assist, and collaborate with departmental users in spectrometer operation, new-experiment development, and offline data processing, with an emphasis on multidimensional high-field NMR geared toward polymer and biopolymer applications. The successful applicant will join our current support staff, consisting of a Facility Manager, electronics technician, and computer specialist. Instrumentation includes a Varian Unityplus 600 MHz high-resolution spectrometer, Unityplus 300WB and Unity 200 instruments equipped for both solid- and solution-state experiments, and both SUN and SGI workstations for advanced data analysis and molecular modeling. Requirements for this position include a Ph.D. in chemistry or related fields; a thorough familiarity and track record with 3D/4D techniques for solution NMR and macromolecular structure determination; a working knowledge of the chemistry of polymers and biopolymers; and the ability to solve problems in conjunction with a diverse group of scientists. This position offers a salary of $25,000 - $40,000, independent research opportunities, and excellent fringe benefits. Applicants should submit a resume and three letters of recommendation to **Dr. Ruth E. Stark, Department of Chemistry, College of Staten Island, 2800 Victory Boulevard, Staten Island, NY 10314-6600.** The City University of New York is an affirmative action/ equal opportunity employer.

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A position is available immediately to study protein folding, dynamics and conformation by NMR. Multi-dimensional NMR techniques are used to characterize systems including α-lactalbumin, triple helical collagen-like peptides and pro-subtilisin. NMR facilities in the Chemistry department at Rutgers University include a Unity Plus 500 MHz Varian spectrometer and a new 600 MHz spectrometer arriving in September. Candidates should have experience in NMR of biological macromolecules. A curriculum vitae with the names of three references should be sent to:

Professor Jean Baum	Phone:	(908)445-5666
Dept. of Chemistry	Fax:	(908)445-5312
Rutgers University	E-mail:	baum@rutchem.rutgers.edu
Piscataway, NJ 08855-0939		

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Center for Structural Biology

FACULTY POSITIONS: NUCLEAR MAGNETIC RESONANCE

The Center for Structural Biology of the College of Medicine, University of Florida currently has openings for faculty conducting innovative research emphasizing nuclear magnetic resonance. The Center is associated with the University of Florida Brain Institute (UFBI) and with the National High Magnetic Field Laboratory (NHMFL), jointly run by Florida State University, the University of Florida, and the Los Alamos National Lab. The Center is an interdisciplinary program with emphasis on understanding of biological function by determining high-resolution structures of large biological molecules and assemblies, studying cell structure and function, and the morphology and physiology of the whole organism. Within the Center, advanced spectroscopic, diffraction, and imaging techniques (nuclear magnetic resonance, optical microscopy, and electron microscopy; X-ray crystallography is being planned) are used to derive molecular-based information related to cellular, tissue, and organism-level structure and function. The Center houses NMR spectrometers (Varian Unity 300 and Unity 600) used for macromolecular structure determination and microscopy, as well as an imaging spectrometer (12 T, 40 cm system to be installed in 1977) for animal research. Also, the Center uses a 4.7 T, 33 cm animal system and a 3 T whole-body system (to be installed in 1995) for research. In addition, Center faculty use prototype magnets and spectrometers located at the NHMFL Tallahassee site, including a wide-bore 600 MHz and a 720 MHz high-resolution spectrometer, with other magnet systems operating at higher fields.

Faculty are being recruited in two areas: 1) high-resolution macromolecular NMR spectroscopy and 2) MR imaging and spectroscopy in living systems. Interested persons are invited to apply for tenure-track faculty positions, at any level, with direct association to the National High Magnetic Field Laboratory. Applicants at the Assistant Professor level need to have an established program with extramural funding. Successful candidates will conduct innovative research emphasizing NMR and will use the facilities of the Center for Structural Biology, with additional support provided through the facilities of the NHMFL and UFBI. Opportunities exist for collaborative research in areas such as biochemistry, cell biology, cognitive neuroscience, pharmacology, or physiology

Applicants much have a Ph.D. Degree and a minimum 1 year postdoctoral experience. Submit a C.F. with statement of research interests and three letters of reference by February 15, 1995. All correspondence should be sent to Thomas H. Mareci, Ph.D., Director, Center for Structural Biology, College of Medicine, University of Florida, Box 100245, Gainesville, FL 32610-0245. The University of Florida is an Affirmative Action-Equal Opportunity employer, and applications from minorities and women are strongly encouraged. Gainesville is an attractive University community in North-central Florida with good low-cost housing, quality public schools, and many outdoor activities.

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1%	Orthodichlorobenzene in Acetone-d_6 (min. 99.9%D)	^1H	Resolution
0.1% 0.01%	Ethylbenzene TMS in Chloroform-d (min. 99.8%D)	^1H	Sensitivity
0.2 mg/ml 0.1% 1%	Gadolinium Chloride DSS (Sodium 2,2-dimethyl-2-silapentane-5-sulphonate) Water in Deuterium Oxide	^1H	Homogeneity
1%	Chloroform in Acetone-d_6 (min. 99.9%D)	^1H	Line Shape
5%	Chloroform in Acetone-d_6 (min. 99.9%D)	^1H	Line Shape
40%	p-Dioxane in Benzene-d_6 (min. 99.9%D)	^{13}C	Sensitivity/ Resolution
0.05%	Trifluorotoluene in Benzene-d_6 (min. 99.6%D)	^{19}F	Sensitivity
0.0485 Molar	Triphenylphosphate in Chloroform-d (min. 99.8%)	^{31}P	Sensitivity

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Urbana, IL 61801

Telephone: (217) 244-0564
Fax: (217) 244-8068
mainzv@aries.scs.uiuc.edu

January 11, 1995 (received 1/17/95)

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

NMR Newsletter Database

Dear Barry:

I have been working on a way to index The NMR Newsletter. Information from all issues, 1958 to date, have been entered in a Paradox for Windows database. The database consists of the issue number, month, and year, title, and authors. I plan to make this information available by posting two sets of text files to an anonymous ftp site (**aries.scs.uiuc.edu, cd NMRNewsletter**) and gopher site (**gopher vixen.cso.uiuc.edu 70** or **xgopher vixen.cso.uiuc.edu 70**, or if using **mosaic: gopher://vixen.cso.uiuc.edu//11/UI/DInfo/chemsch/nmr**).

The first set of files will be text files which will contain the information in a format such as is shown below, and will be in issue number order, with titles usually entered as on the issue cover page.

Number: 120 Month: September 1968
Hexafluoro-1,3-butadiene Parameters; 65 Hz 4J(FF)'s; H-C-P Couplings in Phosphiran
S Manatt

Number: 120 Month: September 1968
LAOCN 3 on the IBM 1130 Computer
J Colson, G Penna, D Marr

The second set of files will be the Paradox database exported as a text delimited file. The text delimiter, and the database file structure information will be shown in the file header, with instructions for importing into the program of your choice. I include this option so users can import the database into other programs.

Every file will be headed by the warning shown on the cover of every issue of this Newsletter, as well as an indication of where browsers should go for information if they do not have access to the necessary Newsletters, i.e., **mainzv@aries.scs.uiuc.edu**. I will provide the relevant information, if I have it. The database will go on-line after the ENC meeting in March 1995 in Boston.

Please send any suggestions or comments you have about this project to me.

Sincerely,

Vera V. Mainz

Vera V. Mainz, Director
Molecular Spectroscopy Laboratory
Microanalytical Laboratory

KARL-FRANZENS-UNIVERSITÄT GRAZ
Institut für Organische Chemie
Dr. Heinz Sterk

A-8010 Graz, 14.1.1995
Heinrichstraße 28
Tel. (0316) 380 DW. 5322, 5320

Unser Zeichen:

(received 1/20/95)

Dr. Bernhard Shapiro
TAMU NMR Newsletter
9666 Elsinore Court
Palo Alto, CA 94303

Transfer of Felix-spectra to Winword

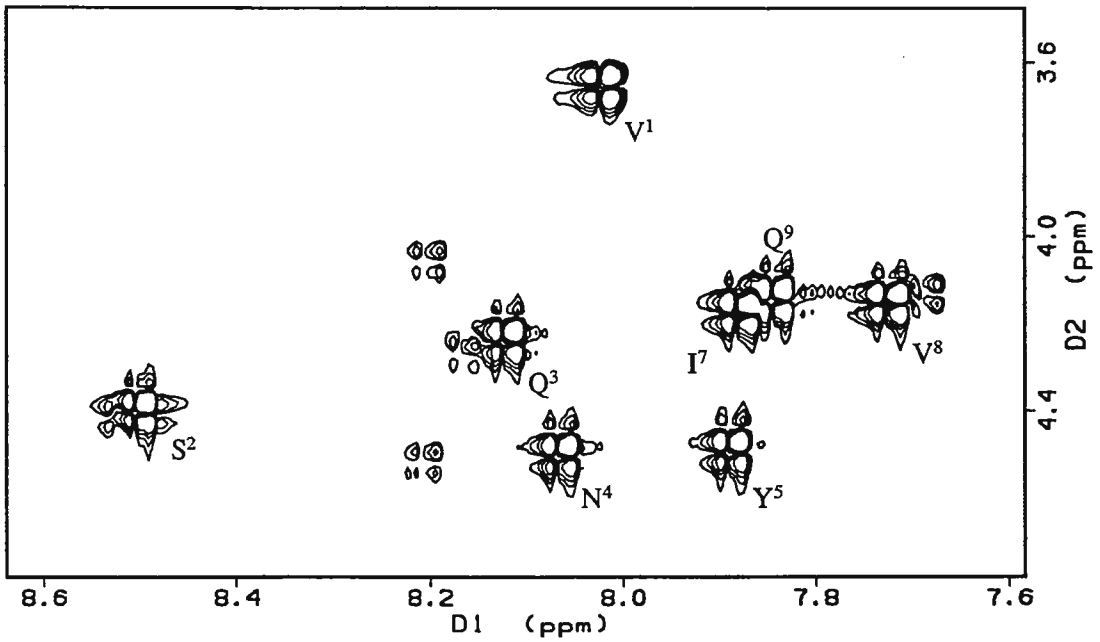
Dear Dr. Shapiro:

In our laboratory we generally use Felix for processing and editing of spectra. In order to use these graphics for publications they have to be transferred to a text editor. We'd like to propose a strategy so simple that almost everyone who ist not yet so dedicated to do this by computer manipulation can make use of it and can avoid the sometimes cumbersome glueing procedure.

Transfer procedure:

1. Prepare the spectrum in Felix the way you'd like to show it.
2. Generate a hardcopy plot of the spectrum to a file (Enter hardcopy menu, adjust hardcopy parameters as HPGL, grayscale, size and so on and start hardcopy).
3. Transfer file to DOS-terminal (connect your DOS-terminal by FTP (FileTransferProtocol) or a similar program to the workstation where Felix is running an get your file).
4. Start Winword and import spectrum by using the menu 'import graphic'. Choose 'HP graphic language' for data conversion. All further manipulations like siting annotation and so on operate staight forward.

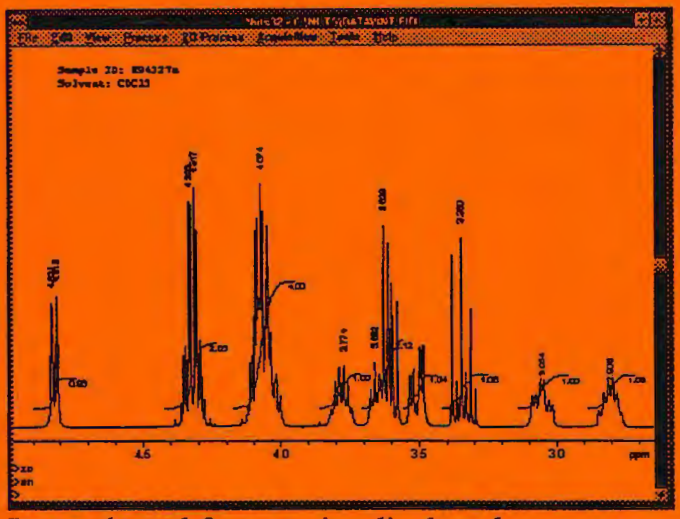
As an example a part of the DQCOSY of the nonapeptide SP-211 in DMSO-d_6:



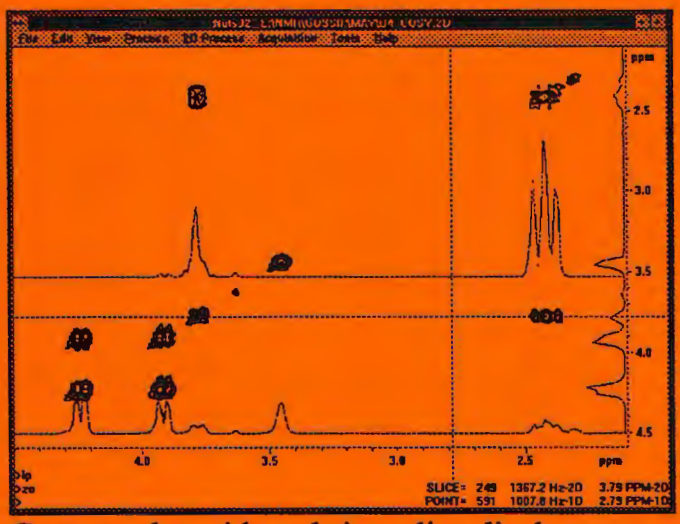
(H. Sterk)

(H. Sengstschmid)

From soup to NUTS *



Integrals and frequencies displayed on screen



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* Title of software review by:
James F. Haw, *Analytical Chemistry*, 66, 1128a (Nov. 15, 1994)

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Volume integration
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Jeffrey A. Reimer
Professor
reimer@garnet.berkeley.edu

Department of Chemical Engineering
Berkeley, California 94720-1462
(510) 642-8011 FAX: (510) 642-4778

Dr. Barry Shapiro
High-Homogeneity *rf* Coils For Solid-State NMR

December 7, 1994
(received 12/24/94)

Dear Dr. Shapiro:

While working with Professor Reimer on my doctorate I have become interested in applications of multiple pulse NMR techniques toward the study of liquid crystalline polymers and polymer blends. I have ascertained that an important consideration for multiple-pulse solid-state experiments is the sample *rf* coil. For example, to avoid beating and attenuation of the multiple-pulse FID the sample must reside in a "sweet-volume" in the inductor wherein the axial *rf* field is highly homogeneous (i.e. the axial *rf* fields are within 2% of the center value). In your basic NMR solenoid, this sweet-volume is only 10% of the coil volume- *yikes* ! How are we to improve the effective fill factor for multiple pulse NMR?

For regular helical coils, appropriate formulae* tell us that the NMR probe $\frac{S}{N}$ increases linearly with sample fill-factor and coil radius to the 1-1.5 power. Thus to increase the $\frac{S}{N}$ for most NMR probes we increase the coil radius, maintaining some proportional length L, until (usually because of a large inductance) either arcing occurs, the tuning capacitance becomes too small, or the ring-down time becomes too long. The effective fill factor of coils for multiple-pulse (or shim) applications may be improved considerably by *shaping* the coil appropriately for a given coil volume. Flattening the wire is a popular practice; is this always necessary? Variable pitch coils have also been examined**; can coils with tapered ends (decreasing radius) work as effectively, or better?

I spent a few days trying to develop an practical understanding of these coil structural features. Using the Biot-Savart Law (for the magnetic field produced by a known current path), I have numerically calculated the axial and transverse field components in coils of variable pitch and taper. I also looked at the effect of wire thickness and shape. All calculations and plots were performed with Mathematica on a Macintosh PowerPC. My results are summarized below and in the attached three figures; a full analysis is being prepared for publication.

1) Very modest amounts of linear taper on a constant pitch coil ($\frac{L}{D} \approx 2$) can increase the sweet-volume by 60%.

Not shown: The enhancement is larger for smaller $\frac{L}{D}$ ratios and turn numbers, see Figure 2.

2) A tapered coil alone is as effective as a coil with only variable pitch. Combining variable radius and pitch doesn't improve the coil above either alone.

Not shown: The transverse field components are 1-3% of the axial field magnitude at the boundaries of the sweet-volume defined by the axial component.

3) Inhomogeneity ($> 1\%$) extends radially from the inner "wall" of the coil with a length scale of about the wire spacing or radius - whichever is larger. Thus, flattening is not necessary, for example, if your wire radius and spacing is equal to or less than your sample tube thickness.

Sincerely***

Michael Gentzler

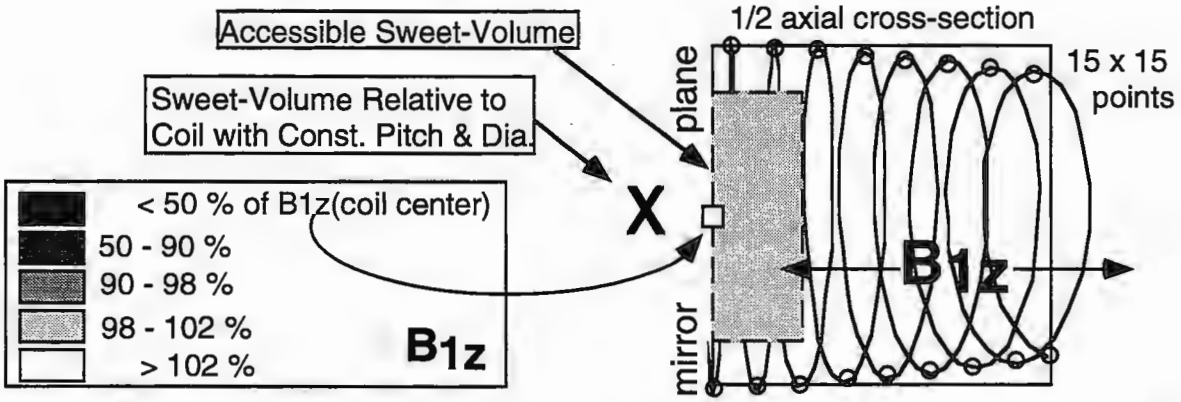
* D.I. Hoult and R.E. Richards, *Jour. Mag. Res.* **24** 71, (1976).

** S. Idziak & U. Haeberlen, *Jour. Mag. Res.*, **50** 281, (1982)

*** Please credit this contribution to the Raychem account.

Figure 1. Axial B_1 Field in a Tapered Coil

(L/D = 2; 16 turns; infinitely thin wire; linear taper)



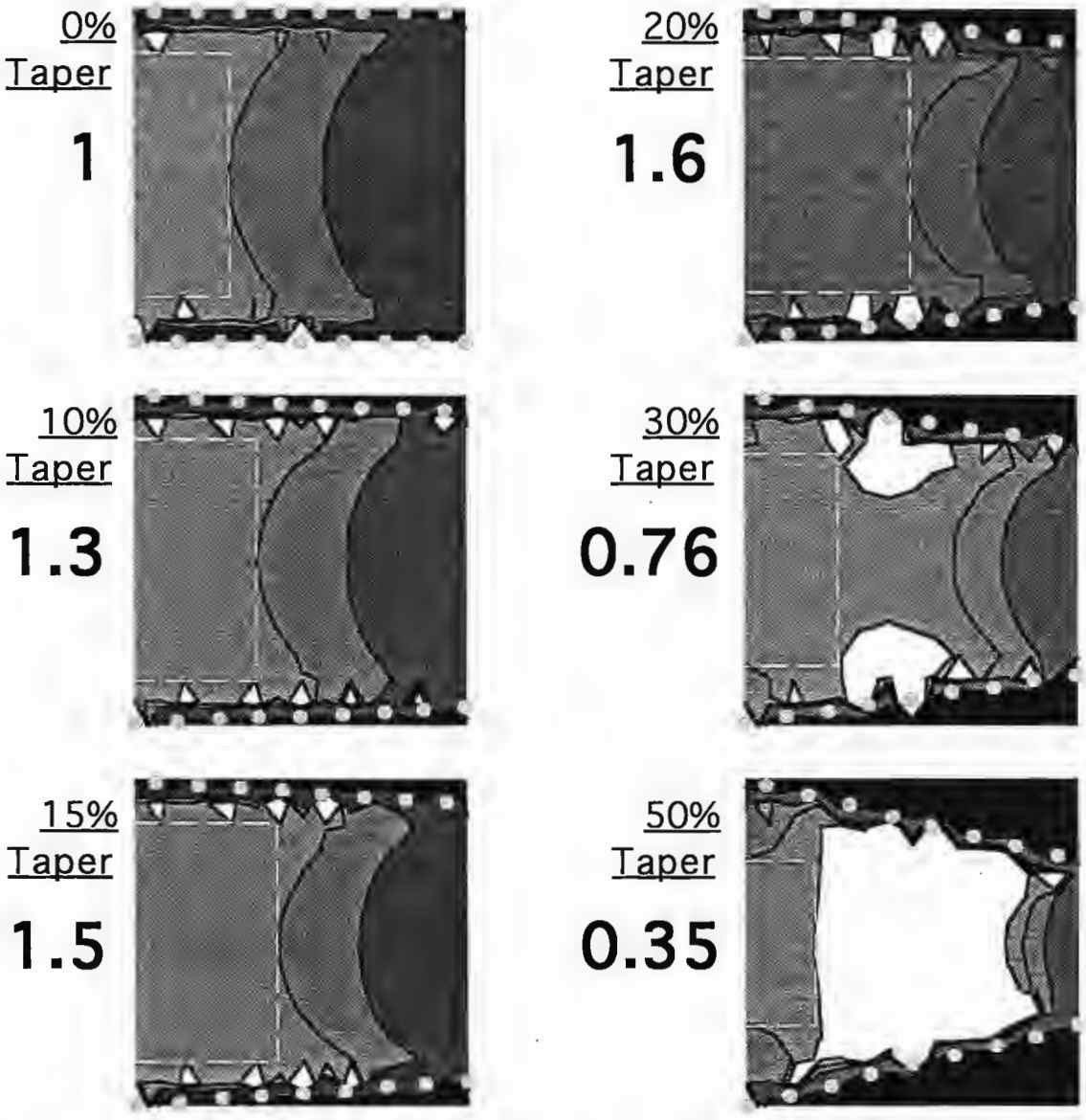


Figure 2. Axial B_1 Field in "Optimized" Coils

(L/D = 1.5 ; 8 turns; infinitely thin wire)

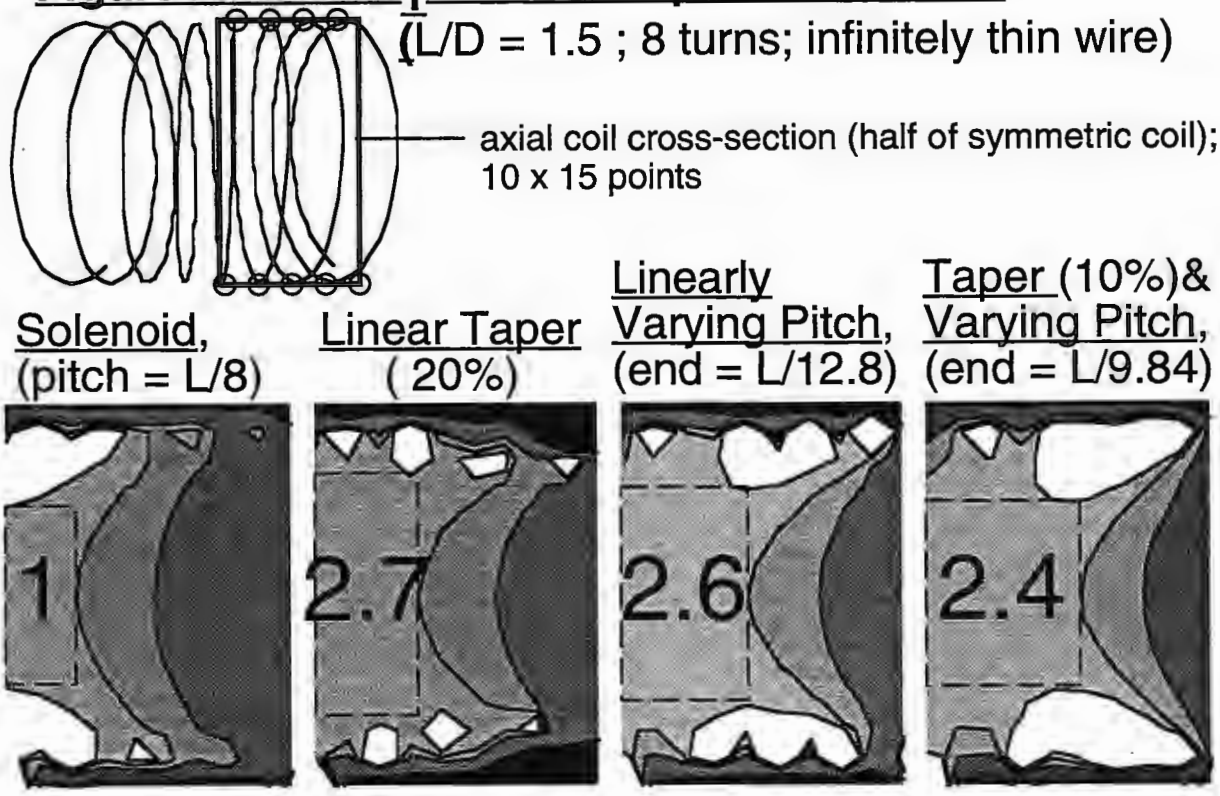
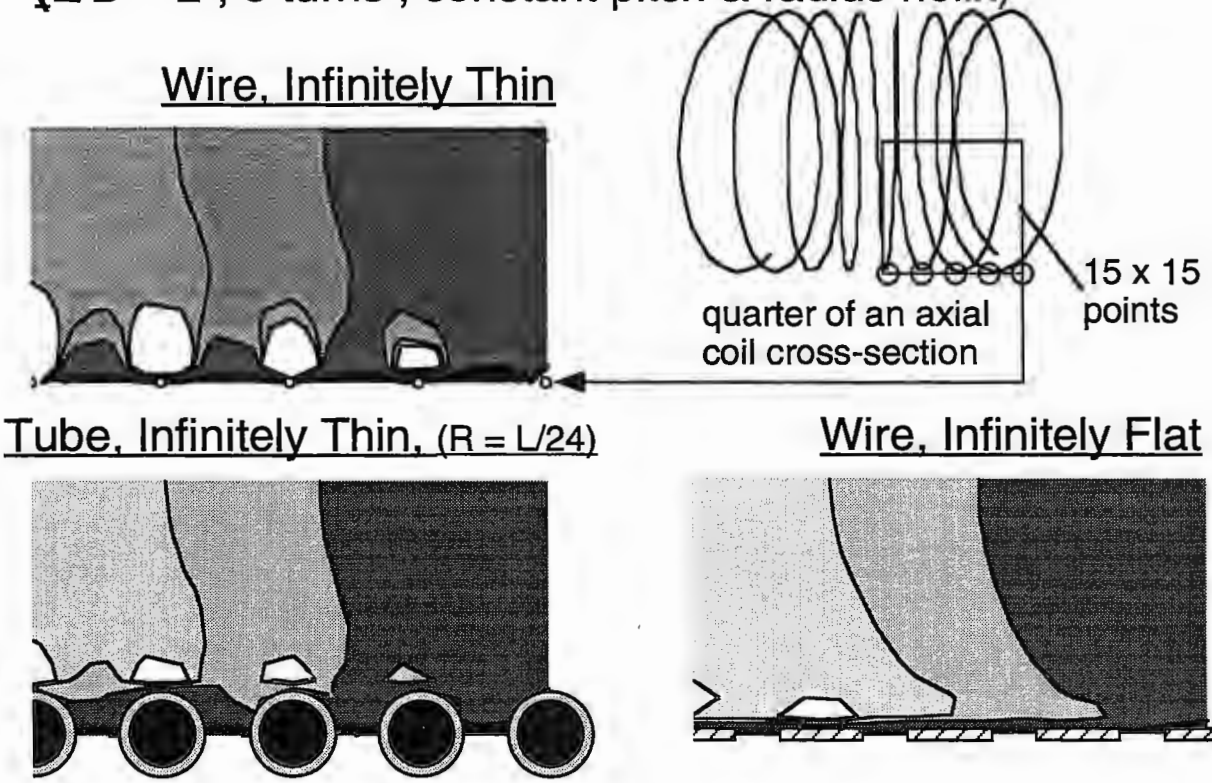


Figure 3. Effect of Wire Shape on Coil Axial B_1 Field

(L/D = 2 ; 8 turns ; constant pitch & radius helix)



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

January 2, 1995
(received 1/7/95)

To Delta or not to Delta? A resounding yes

Dear Dr. Shapiro:

After receiving the dreaded "Ultimatum" notice, my New Year's resolution was to send off my contribution.

I am happy to report that we have moved finally into the 90's. Our JEOL GSX-270 has been outfitted with the DELTA upgrade.

After playing around for approximately four months with the new system, listed below are a few items that might be of interest to other DELTA users out there.

Battery backup: Upon installation of a BACK-UPS 900 (American Power Conversions, West Kingston, RI, USA), the SGI continually went down during battery backup tests. After half a dozen or so phone calls, APC finally informed me that only a SMART-UPS would work with an SGI. Swapping out the units solved the problem. At peak usage the backup unit indicates that 70% of the rated load is in use, which allows for a battery run time of ~15 minutes.

Multiple DELTA: Occasionally multiple copies of DELTA (up to 5) open up with no provocation. This can be avoided by setting up the window to one's liking, and changing Save Windows & Desks (under Desktop-Customize-Windows Setup) to explicitly.

Phase tables: Within pulse sequences if the pulse align (leading, center, trailing) statement is used, the length of the phase tables in that section **must** be of equal length or an error message is generated.

More Delta trivia in my next contribution.

Yours sincerely,

Ashok Krishnaswami

THE NMR NEWSLETTER

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*Fax.(415) 493-1348**

Policies and Practical Considerations

The NMR Newsletter (formerly the **TAMU NMR Newsletter**, the **IIT NMR Newsletter**, and originally, the **Mellon Institute NMR Newsletter**), now in its thirty-seventh year of consecutive monthly publication, continues under the same general policies as in the past. All communication with the Newsletter should be sent to the address above.

1. **Policy**:

The 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 serves its purpose best if the participants impart whatever they feel will interest their colleagues, and inquire about whatever matters concern them. Technical contributions should always contain a significant amount of information that has not already been published or that will appear in the formal literature within a few weeks of the appearance in the Newsletter.

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 is followed by the 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 Newsletter is not, and will not become, a journal. We merely reproduce and disseminate exactly what is submitted. 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 NMR Newsletter by its present or previous names in the scientific literature is *never* permissible. *In order to quote or use material from the Newsletter, it is necessary, in each individual case, to obtain the prior permission of the responsible author 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 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, only one contributor 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 its funding depends on Advertising, Sponsorships, and individual Subscriptions. The **Subscription** fee for the October 1994 - September 1995 year is US$170, with a 50% academic or personal subscription discount. Subscriptions are available for a minimum of the twelve monthly issues which end with a September issue. However, a subscription can be initiated at any time, with the price for more than twelve issues being prorated.

Continued

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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 Newsletter will be included in the next issue if received on or 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" (1.3cm) on all four sides. 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) 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 11 or 12 point type is acceptable if the particular font is not too large. 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. Type smaller than 7 point should not be used.

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.).

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
January 1995

*Telephone: (415) 493-5971. Please confine telephone calls to 8:00AM-10:00PM, *Pacific Coast Time.*
*Fax: (415) 493-1348 (Do not use for technical contributions which are to appear in the Newsletter, for Fax quality is not adequate.)

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Address all Newsletter correspondence to:

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(415) 493-5971* - *Please call only between 8:00 am and 10:00 pm, Pacific Coast time.*

Deadline Dates

No. 439 (April)	24 March 1995
No. 440 (May)	21 April 1995
No. 441 (June)	26 May 1995
No. 442 (July)	23 June 1995

*Fax: (415) 493-1348, at any hour. Do not use fax for technical contributions to the Newsletter, for the received fax quality is very inadequate.

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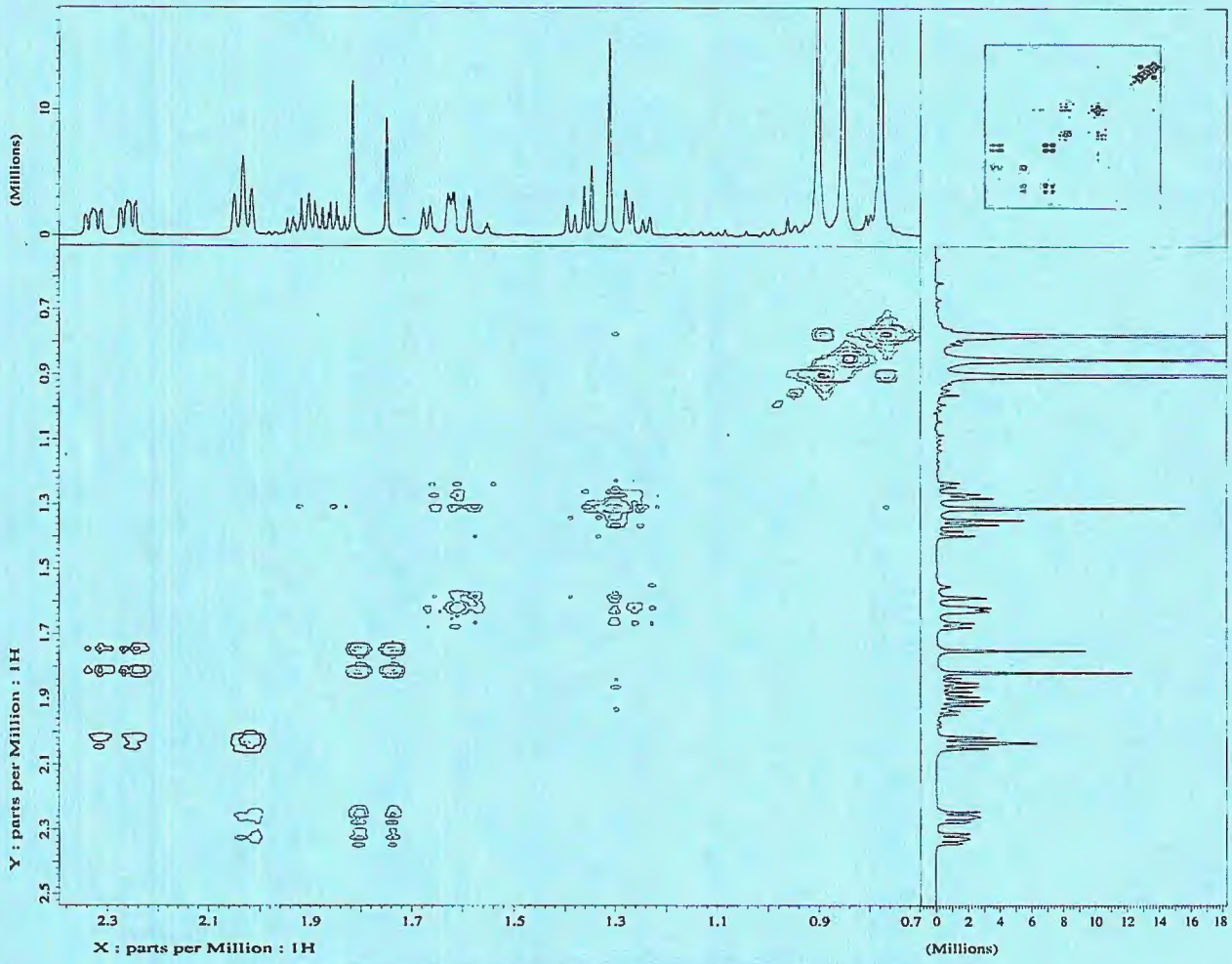

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