TEXAS A&M UNIVERSITY

NMR NEWSLETTER

BRIAN SYKES

NO. 324

SEPTEMBER 1985

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TEXAS A&M UNIVERSITY

NMR NEWSLETTER

AUTHOR INDEX -- TAMU NMR NEWSLETTER, NO. 324, SEPTEMBER 1985

FORTHCOMING NMR MEETINGS (Additional listings are solicited)

Eighth Semi-Annual New Mexico Regional NMR Meeting - October 19, 1985; Western New Mexico University, Silver City, New Mexico; see page 19.

J.H. Goldstein Retirement Symposium - October 25, 1985; Emory University, Atlanta, Georgia; see Newsletter No. 323, page 23.

1985 Eastern Analytical Symposium - November 19-22, 1985; Penta Hotel, New York; see Newsletter No. 321, pages 17-18, and pages 46-47 of this issue.

British Radiofrequency Spectroscopy Group - April 9-11, 1986; Oxford University, Oxford OX1 3QR England; see Newsletter No. 323, page 23.

27th ENC - April 13-17, 1986; Baltimore Hilton; Chairman: R.G. Bryant, Department of Radiology, University of Rochester Medical Center, 601 Elmwood Avenue, Rochester, NY 14642, 716-275-5541; see Newsletter No. 323, page 31.

U.S.-Latin American Workshop on Recent Developments in Organic and Bioorganic NMR - July 7-11, 1986; Campinas, Brazil; see Newsletter No. 323, page 59.

Suggestions for other types of articles, news items, etc., to appear in the Newsletter would be welcomed - please make your wishes known.

★ *Please check to be sure you have received and processed your 1985-86 Newsletter invoice. If we don't have some indication (formal or otherwise) that payment has been made or is in the works by the time the November issue is mailed, your copy will not be sent.* ★

B.L. Shapiro

All Newsletter Correspondence
Should be Addressed to:

Professor Bernard L. Shapiro
Department of Chemistry
Texas A&M University
College Station, Texas 77843 U.S.A.

DEADLINE DATES

No. 326 (November) ---- 25 October 1985

No. 327 (December) --- 22 November 1985

Department of Biochemistry

College of Agricultural & Life Sciences
University of Wisconsin-Madison

420 Henry Mall
Madison, Wisconsin 53706 USA

July 18, 1985

Professor B. L. Shapiro
Department of Chemistry
Texas A&M University
College Station, TX 77843

Subject: Incorporation of a TECMAG, Inc. DECkit-2 X-nucleus Decoupler into a Nicolet NT-200 widebore NMR Spectrometer.

Dear Professor Shapiro:

In order to perform NMR experiments which require X-nucleus decoupling with level control, WALTZ modulation and 90°, 180° phase control on our Nicolet NT-200 spectrometer, I have interfaced the TECMAG, Inc. (Houston, TX) DECkit-2 decoupler control into our present system. The decoupler control unit fits into an empty slot above the room temperature shim power supply. Shown in Figure 1 is the block diagram of decoupler operation illustrating its use with an ^{15}N enriched sample. A 420LA Electronic Navigation Industries R.F. amplifier is used to obtain adequate power output and TEXSCAN filters are used to remove unwanted R.F. frequencies. Phase and level control of decoupler output are obtained with the present NMC program (version #40911) on SP lines from the 293B pulse programmer as shown below:

Command	SP line	Assignment
U	SP-9	F3-level 2
G	SP-8	F3-180° phase shift
F	SP-7	F3-90° phase shift

Several other SP and LEV lines are available for more elaborate control of the decoupler. With a separate frequency synthesizer for F3, the X-nucleus decoupling frequency can be set by the 1280 computer using the F3 command. Shown in Figure 2 are some decoupling results for ^{15}N in $(^{15}NH_4)_2SO_4$ in 50% H_2O/50% D_2O. The modified Redfield 21412 sequence was used to nearly eliminate the water peak.

Please note on another subject that the Department of Biochemistry has for sale a Nicolet Model 1180 computer with 8K memory, X-Y display board and Diablo model 44B disk drive interface board: asking $3,000.

Sincerely,

Ed Mooberry

Ed Mooberry

EM/clw
Enclosure

Telephone: 608-262-3026, 262-3040
Telex: 26 54 52

Fig. 1

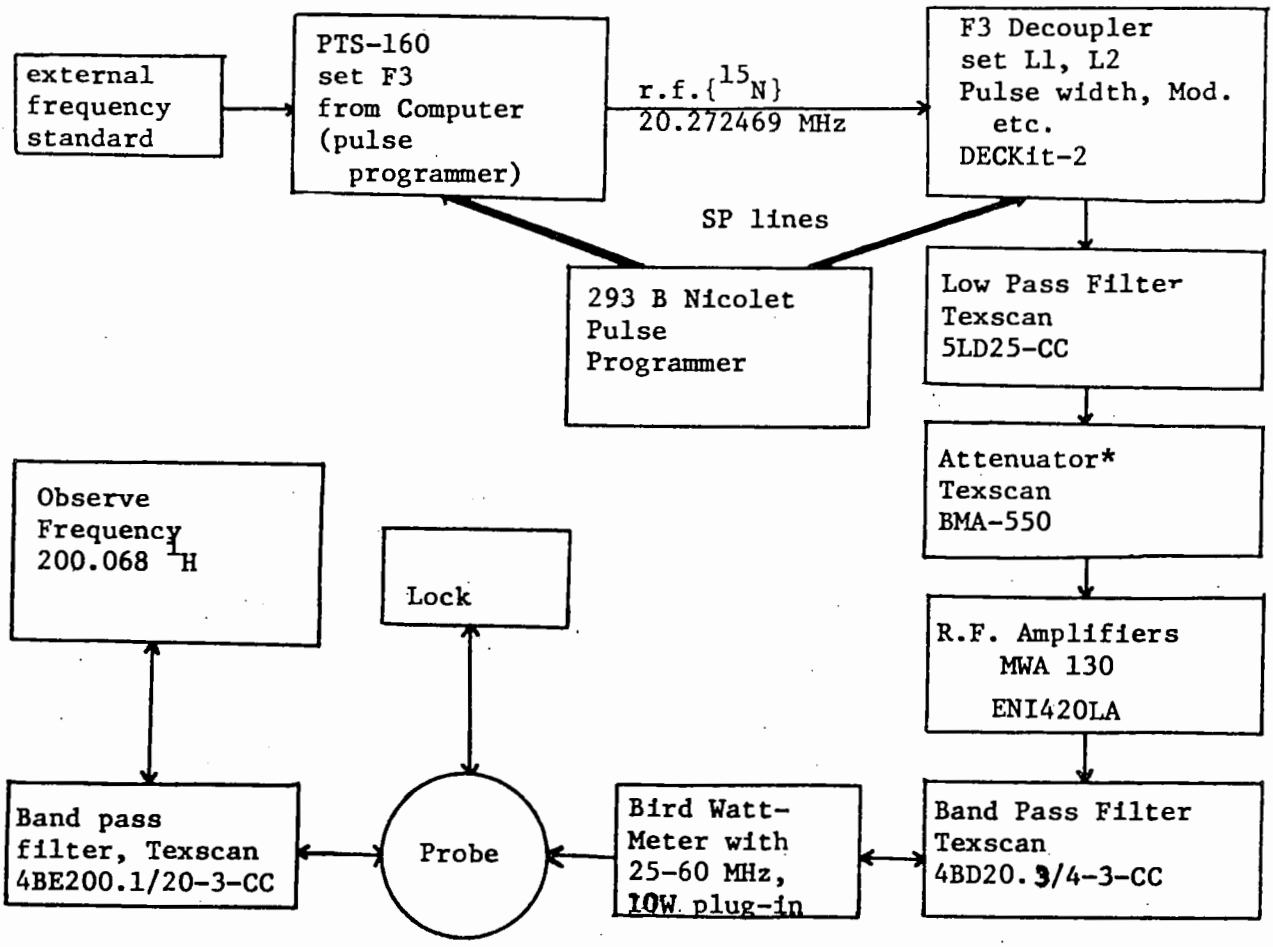
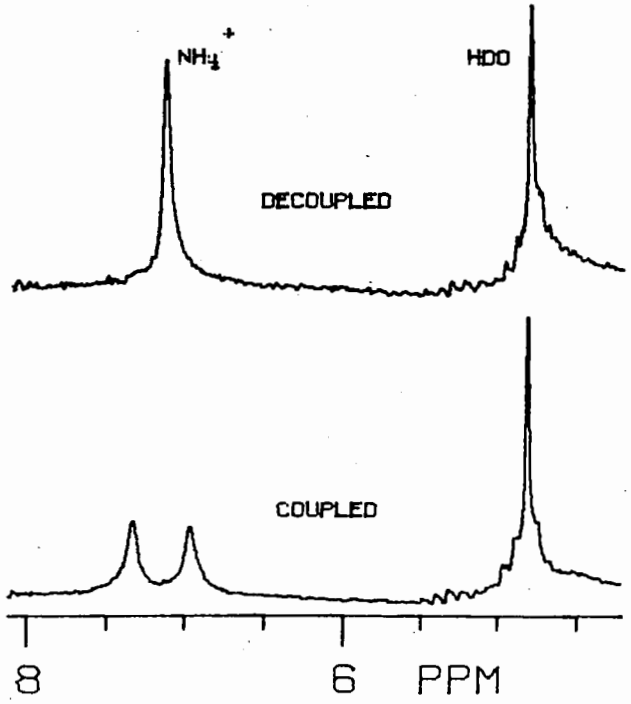


Fig. 2 MODIFIED REDFIELD 21412 SEQUENCE




```
 P1=      541.95 USEC
 P2=      148.05 USEC
 DS=        1.00  SEC

NA =          4
SIZE =     8192
AT =         2.05  SEC
QPD ON =       1
ABC ON
BUTTERWORTH FILTER ON
DB ATT.=       3
ADC =   12 BITS
AI =        -8
SW = +/- 1000.00
DW =      500
RG =       10 USEC
DE=      500 USEC
TL HIGH POWER OFF
F2=      200.087000
BB MODULATION ON
OF=      961.29
SF=      200.087987
EM=        1.00
PA=      999.0
PB=       94.2

SCALE      97.65 HZ/CM
       =      .4881 PPM/CM
```

University of Alberta
Edmonton

Department of Biochemistry

Canada T6G 2H7

474 Medical Sciences Building, Telephone (403) 432-5460

August 1, 1985

Professor Bernard L. Shapiro
Department of Chemistry
Texas A & M University
College Station, TEXAS 77843

"Pulling the Plug"

Dear Barry:

To make way for our new Varian XL-400 spectrometer, we were forced to decommission our Bruker HX-270 spectrometer. After 10 years of days and nights with this our first supercon, it was like losing an old friend. I think the magnet could have gone for some stability record — it never drifted in 10 years and the field offset dial was still mid range, untouched, 10 years later. The enclosed figure shows the first spectrum (bottom) taken on 29 July 1975 (CW) and a quick final look at the same sample on 24 January 1985 (FT). Since we always work in H_2O/D_2O, we had not looked at ODCB in the intervening years.

The spectrometer is alive and well in the chemistry department at UBC.

Best regards,

Brian

Brian D. Sykes

(continued with figure on page 7)

Position Available

NMR Physicist or Engineer with knowledge of NMR electronics and RF technology and interest in probe design/construction. Challenging position with opportunities for instrument development and research collaboration. Academic staff appointment, rank, and salary dependent on qualifications. Application and letters of reference should be sent to: Dr. Oleg Jardetzky; Stanford Magnetic Resonance Laboratory; Stanford University; Stanford, California 94305.

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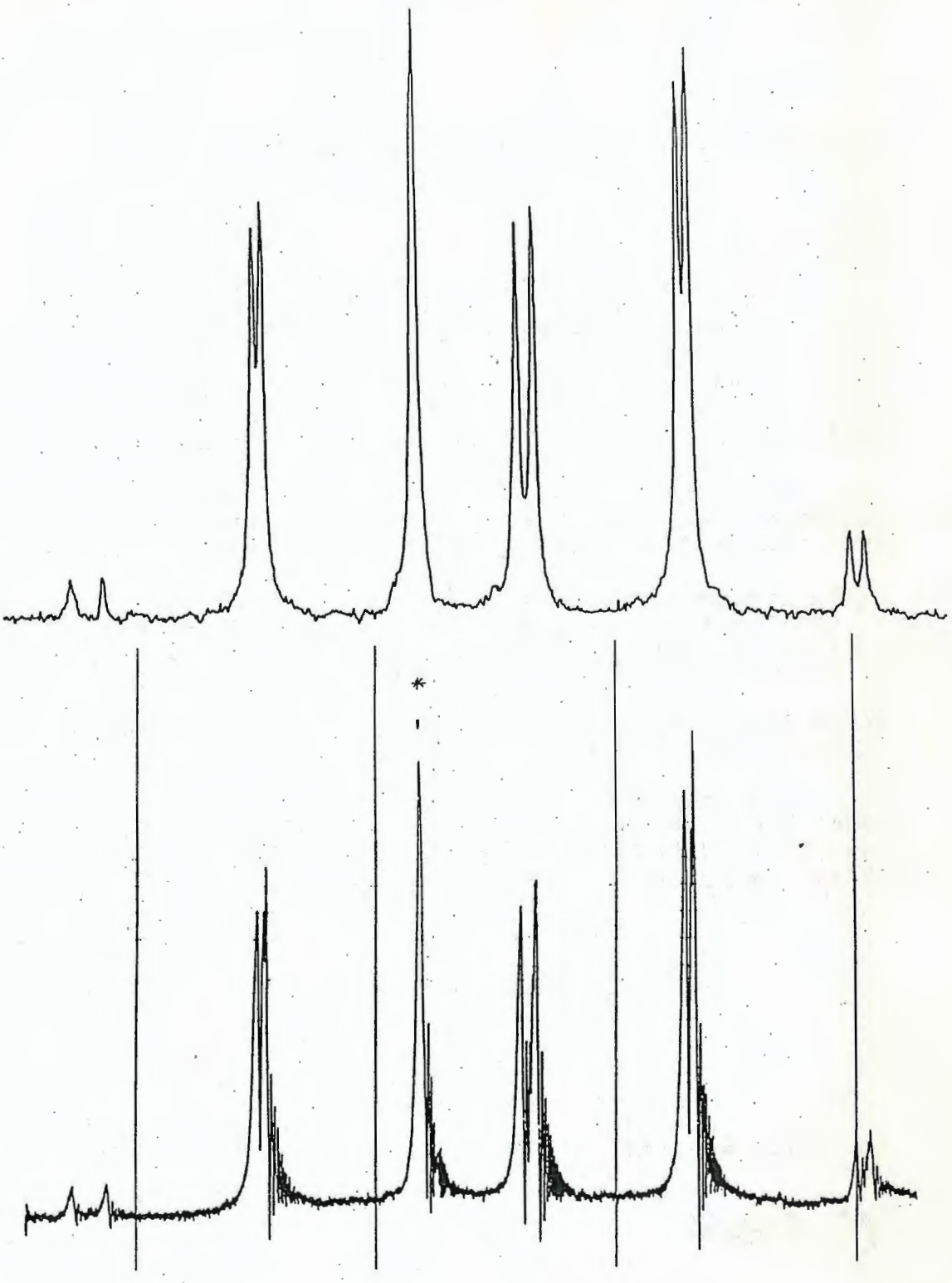
(continued from page 4)



INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS
CZECHOSLOVAK ACADEMY OF SCIENCE
165 02 PRAHA 6 - SUCHDOL

Professor Bernard L. Shapiro
Texas A&M University
College Station, Texas 77843

August 1, 1985

Title: N - peak (echo) detection on old XL - 200

Dear Barry:

Perhaps other users of XL - 200 equipped with the old V-77-200 system were also surprised that their HOMCOR spectra did not follow the flip angle dependence described for COSY spectra and that simple introduction of a second D2 delay into the sequence did yield spectra such as shown on Fig. 1 (with dia peaks on the diagonal) and not SECSY spectra.

The cause is that the manufacturer provided HOMCOR pulse sequence (software release H-1Z and earlier versions) which uses P-peak (antiecho) detection. The remedy is simple:

1/ insert phase calculation:
SUB(THREE,OPH,V1); MOD4(V1,V1); ADD(ONE,V1,V1); MOD4(V1,V1);
into the HOMCOR source program (e.g., just after the last GETVAL statement) and

2/ replace the first pulse command (RGPULSE(P1,OPH,ROF1,0.0))
by RGPULSE(P1,V1,ROF1,0.0);

With this phase cycling N-peaks are detected and SECSY spectra can be obtained (change DELAYS D2 into DELAYS D2/2.0 and insert DELAYS D2/2.0 just before END) as shown on Fig. 2 ("dia" peaks on F_1 = 180 Hz = SW/2).

Sincerely yours,

Vratislav Blechta

V Blechta

Jan Schraml

Jan

Homonuclear (1H) correlated spectra of amide of 5-bromo--2-furanecarboxylic acid (in dimethlsulfoxide-d6)

Fig.1

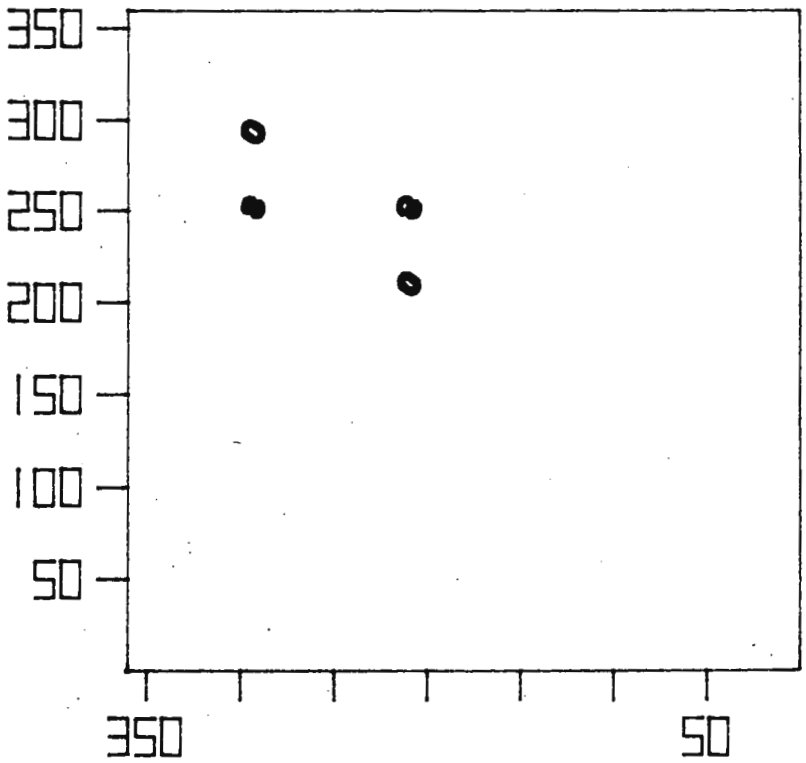
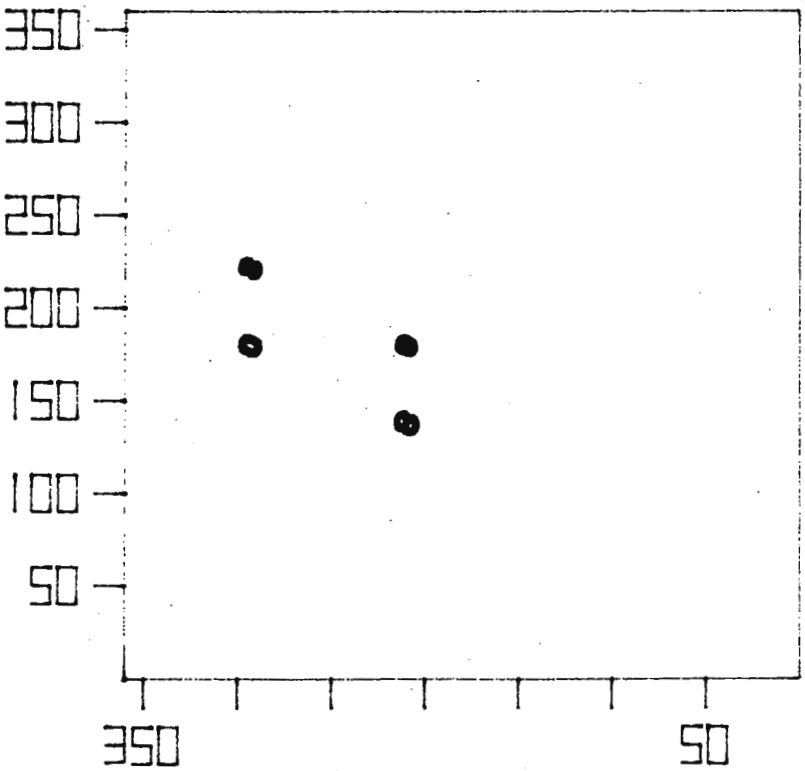


Fig.2



Brandeis University

Graduate Department of Biochemistry
Waltham Massachusetts 02254

August 6, 1985

Professor Bernard L. Shapiro
Department of Chemistry
Texas A & M University
College Station, TX 77843

"REVERSING AN XL-300 FOR GATED HETERONUCLEAR-DECOUPLED COSY AND NOESY"

Dear Barry:

As soon and the new XL-300 appeared, one of us (RHG) eagerly set out to do ^{1}H-(^{13}C) experiments. Unfortunately, the experimental details provided by Varian were insufficient, and only served as a means to down the RF circuitry by blowing dust into a faint-hearted power relay. The reclusive Howard Hill was rumored to have performed such an experiment, and Varian gladly supplied information on reversing an XL-400, which further confused the issue for us.

Led by Sara Kunz, we have succeeded in teaching our XL-300 some new tricks, and wish to pass on the machinations to other TAMUN readers. We use the Varian switchable probe, and set the relays in their normal positions for 13C observation. After cutting the power to the RF components and removing the cables from the observe and decoupler frequency boards, the card for the ^{1}H oscillator is interchanged with the card for broadband frequency generation. The ^{1}H local oscillator output (J3X02) is connected to P3402, and the high-power ^{1}H output (J3X05) is connected directly to the leg of the magnet (obs. transmitter input). A 250 MHz high-pass filter is inserted between the probehead and the ^{1}H quarterwave connection. The offset oscillator (P3406) for the new broadband decoupler board is connected to J3406, and the output of this card is attenuated (6 dB), and filtered with a 300 MHz notch and a home-made 75 MHz filter.

A new ^{1}H transmitter offset is created following the Varian recipe, and the configuration is fixed with a setup command. Proton observation with low-power ^{13}C decoupling mildly perturbs the lock, and a 46 MHz band-pass filter is required for high-power decoupling. The lengths of the ^{1}H and ^{13}C 90^{o} pulses are 17 and 35 usec, respectively.

The standard software for a COSY experiment is easily changed to permit ^{13}C decoupling during acquisition or t_1. The result of a GDCOSY on a solution of (6-^{13}C)uracil are shown in the figure. As will be discussed (Griffey and Redfield, J. Magn. Reson., in press) ^{13}C decoupling on C6 of uracil during t_1 creates signals in the 2D map which are diagnostic for the proton bonded to C6 and its scalar-coupled neighbors. The peaks from the proton at C5, which is unaffected by the ^{13}C decoupling, project as singlets in both dimensions. The cross-peaks from the proton at C6 are asymmetric, and the central signals for the proton are shifted away from the diagonal by $\pm$ J/2 in the t_2

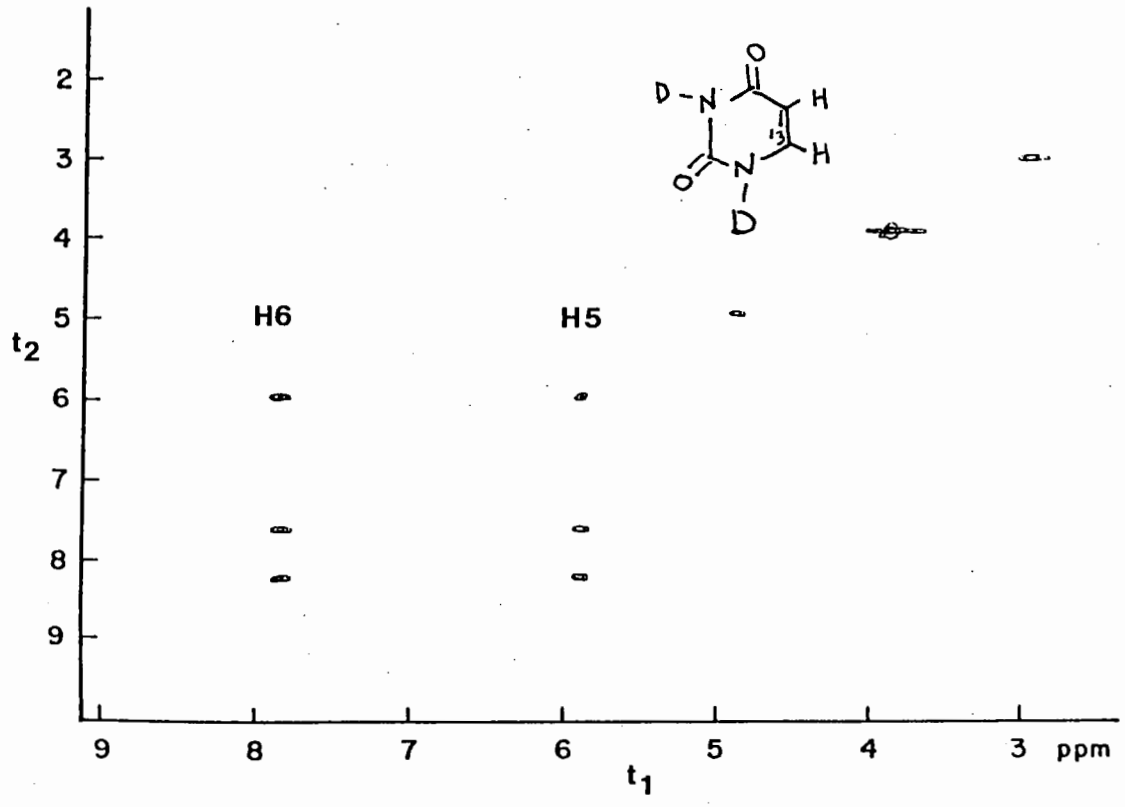
dimension. We have also succeeded in decoupling ^{15}N with a similar configuration of the instrument. We are looking for an "antisymmetrization" routine to remove unwanted cross-peaks from unlabeled protons.

Please credit this letter to the account of Rich Griffey.

Sincerely,

Sara Kunz and Alfred Redfield

Richard H. Griffey
Center for Non-Invasive Diagnosis
University of New Mexico Medical Center
Albuquerque, NM 87131



SYRACUSE UNIVERSITY
NMR and DATA PROCESSING LABORATORY
GEORGE C. LEVY, DIRECTOR (315) 423-4026

DEPARTMENT OF CHEMISTRY, BOWNE HALL, SYRACUSE UNIVERSITY, SYRACUSE, N.Y. 13210

1 August 1985

Prof. B.L. Shapiro
Department of Chemistry
Texas A&M University
College Station, TX 77843

Dear Barry:

^{13}C-nmr of Oligonucleotides

Our new GN-500 has been operating for about two months now and we are really excited about the advantage in sensitivity and resolution it affords. The figure is a ^{13}C spectrum of a DNA octanucleotide obtained in about 5 hours of signal averaging with only 9 mg of the oligomer! We used to get more-or-less equivalent spectra on our WM-360 in about 15 hours with 50 mg of oligomer. Further, the resolution is much better, e.g., we see resolved resonances from all 8 of the C3' carbons in the molecule with measurable ^{13}C-^{31}P couplings for the seven doublets at the left of the expansion. We think that the better resolution also is a function of the bases at the ends of the oligomer. The spectrum shown is of an oligo with only A.T pairs at the ends. Another octamer duplex we studied with terminal G·C pairs has much broader lines -- this duplex probably forms extended end-to-end aggregates. In other work on the GN-500, we have obtained some very nice two-dimensional proton COSY and NOESY spectra on DNA oligomers and small peptides.

Sincerely,

PNBorer

Philip N. Borer
Research Associate Professor
and Operations Director

George C Levy

George C. Levy
Professor and Director

(continued on page 15)

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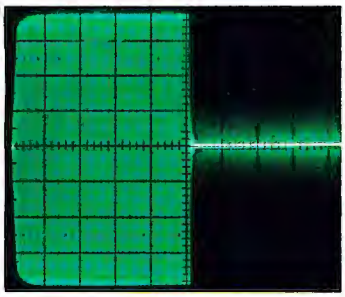
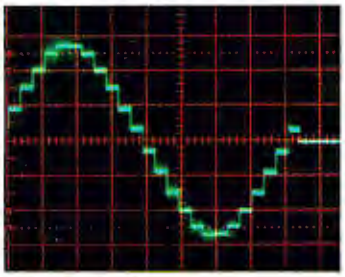
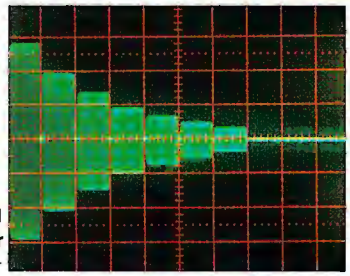




15° phase shift through 360°. ►



Shaped decoupler pulse. ►

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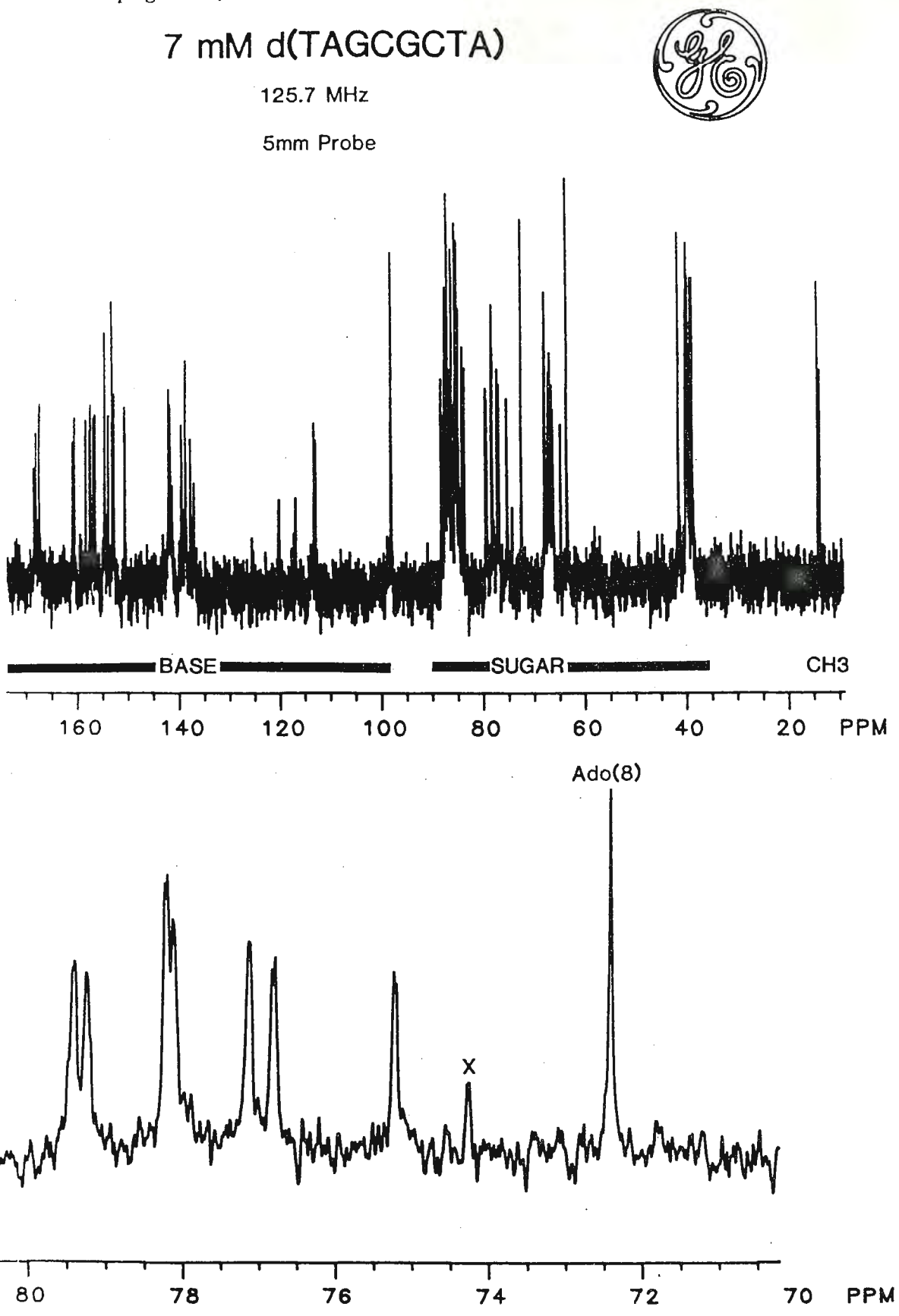
(continued from page 12)



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Dr.B.Shapiro
Department of Chemistry
Texas A and M University
College Station
Texas 77843 - 3255
USA

Váš dopis značky / ze dne | Naše značka 2705 | Vyřizuje / linka | Praha, dne 2.8.1985

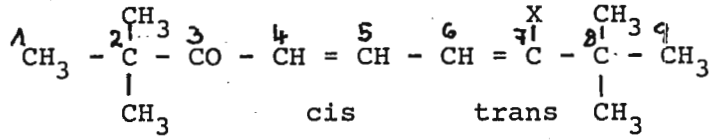
Věc: Limitation of the Simple Additivity Rules for Conjugated Dienones

Dear Prof.Shapiro,

we studied dienone Ia (X=H) to find the configuration of the double bonds. From ^{1}H NMR spectra the vicinal spin--spin coupling constants of protons on sp^2 carbon atoms indicated that one double bond is in cis- and the second one in trans-configuration, respectively. The assignement of signals in both ^{1}H and ^{13}C NMR spectra seemed to be easy by using simple additivity rules and tabulated values of shift increments. This calculation showed the most deshielded proton is H-5.

To verify this assignement we performed ^{1}H-^{13}C shift correlated 2D experiment. We were surprised when we had found the opposite assignement of H-5 and H-6 signals (if the assignement of carbon signals was correct). This contradiction could be explained by the anisotropy of the C=O double bond which can reverse the sign of the relative chemical shifts of protons H-5 and H-6. Very similar results were also reported by Eldvidge and Ralph for methyl 2,4-hexadienoates[1].

Our assignement of signals (see Tab.I) and the determination of the configuration were also supported by the study of the cyanoderivative Ib (X=CN), prepared in the same way. The observed value $^{3}J_{CH}$ (H-6,CN) = 14.1 Hz confirms trans-configuration of both H-6 proton and carbon atom in the cyanogroup.



Please credit this letter to the account of Dr.M.Hájek.

Sincerely yours

Petr Trška

Lit.: 1 J.A.Eldvidge, P.D.Ralph, J.Chem.Soc.B., 1966, 243

Tab.I Chemical shifts of Ia, in $CDCl_3$

	1	2	3	4	5	6	7	8	9
^1H	1,17	-	-	6.21	6.49	7.40	6.10	-	1.08
^{13}C	26.36	43.61	206.06	118.56	144.74	122.76	157.06	33.87	29.07

$^3J_{H,H}$(4-H,5-H) = 11,4 Hz; $^3J_{H,H}$(6-H,7-H) = 15.5 Hz

University
of Strathclyde

Department of Pure and Applied Chemistry

Thomas Graham Building,
295 Cathedral Street, Glasgow G1 1XL Tel: 041-552 4400

9th August, 1985.

Professor Barry Shapiro,
Department of Chemistry,
Texas A and M University,
College Station,
Texas, 77843-3255.
U.S.A.

Effects of Electrical and Magnetic Disturbances on NMR Experiments

Dear Barry,

Your coloured reminders tell me that my subscription is now just about due. Unfortunately there is not much of chemical interest to report, but the recent letter from Drs. Mildvan and Chacko of John Hopkins School of Medicine, reminded me of the trouble we had in the past from various sorts of electrical and magnetic interference.

Let me say at the start that we do not now suffer any significant effects from either sources inside the building or outside, this despite the fact that the present nmr instruments are some 300 ft from the (100 year old, brick-lined) railway tunnel in which the local British Rail suburban line runs. Although there is some vibration from the trains passing which can be felt in the buildings directly above, there is none in our building. Neither is there any electrical or magnetic effect. The railway, however, uses a high voltage (25 Kv) alternating supply, and this is probably much less trouble than the more usual low voltage dc supplies.

In the past however we had a lot of trouble from buses passing in the street perhaps 50 to 70 ft away. Disturbances in the order of a milligauss were found and while these had a profound effect on the instruments we were using at that time, which were Perkin Elmer R10 and R14's, (using unscreened permanent magnets and operated without a lock). We have no trouble in our present equipment (Perkin Elmer R 32 and Bruker WM 250) in which either a permanent magnet type with a barrel shaped yoke or a supercon solenoid are used.

Perhaps the worst effects on the older machines were caused by an electrode boiler used for steam generation. This was owned by another department in the same building as ours. For the benefit of those readers who have never met this sort of abomination, a brief description is in order. The boiler contained an electrolyte of

aqueous sodium carbonate and into this dipped three electrodes connected to the three phases of the mains supply; the steel casing of the boiler was connected to the neutral of the supply and also presumably to the earth (ground) wire. When in operation the boiling of the water caused momentary imbalances in the current taken from the three phases; there also seemed to be some rectification of the AC, the net result was that a DC component was impressed on the phases and the neutral throughout the building, its effect was seen clearly four floors away, and we were unable to compensate it in any way. The magnitude of the disturbances did depend on the state of the electrolyte in the boiler so could be minimized by careful maintenance. Fortunately the department concerned has moved away now. It always amazed me that the device was allowed by the electrical supply people, and if these things are still around they should be avoided at all costs.

Yours sincerely,

Peter Bladon.

Dr. P. Bladon.

Eighth Semi-Annual New Mexico Regional NMR Meeting

The eighth semi-annual New Mexico Regional NMR Meeting will be held at Western New Mexico University in Silver City on the 19th of October. The (out of state) guest speakers will be Lynn Jelinski of AT&T Bell Labs. and Irving Lowe of Pittsburgh. For further information, please contact

Professor Kenneth Ladner
College of Science and Mathematics
Western New Mexico University
Silver City, NM 88061.

NORTHWESTERN UNIVERSITY COLLEGE OF ARTS AND SCIENCES

Department of Chemistry

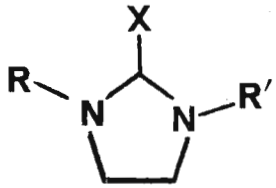
2145 Sheridan Road
Evanston, Illinois 60201

August 14, 1985

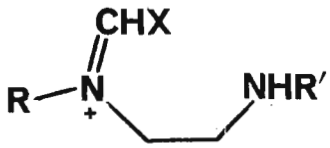
Professor Bernard L. Shapiro
TAMU NMR Newsletter
Department of Chemistry
Texas A &M University
College Station, TX 77843

Dear Barry:

We have been continuing our work on ring-chain tautomerism in 1,3-diazolidines (A and B) in trifluoroacetic acid.



A



B

Our earlier report was only for R = R' = CH_3, and X = H. We now have examined cases for which R ≠ R' and X ≠ H. When R ≠ R' there are two different chain forms, and when X ≠ H there are two different E/Z isomers. We believe we have seen all these types of isomers, in which the substituents are CH_3, CH_3CH_2, or $PhCH_2$. At high temperatures, we see ring-chain tautomerism on the NMR time scale. At low temperatures, we see slowing of NH proton exchange. With such a multiplicity of isomers and processes, the spectra proved to be more complex than we anticipated.

Sincerely,

Joseph B. Lambert

Gen-tai Wang

Title: Ring-chain Tautomerism

JBL:cs

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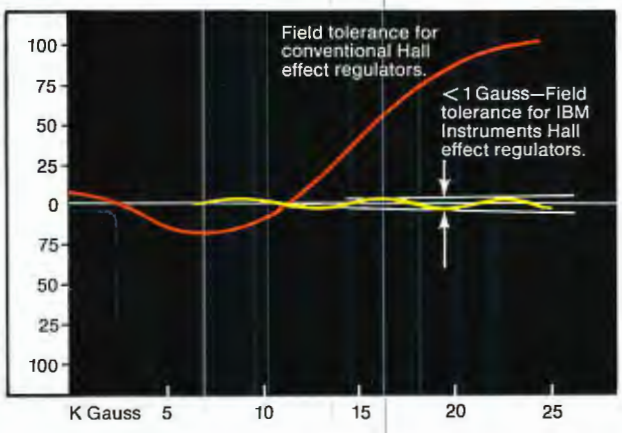

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ע"ש ריימונד ובברלי סאקלר
לכימיה

August 9, 1985

Ref.: 7426

Prof. B.L. Shapiro
Department of Chemistry
Texas A & M University
College Station, Texas 77843
U. S. A.

Dear Barry,

The Discovery of a New Ionophore Using Multinuclear NMR

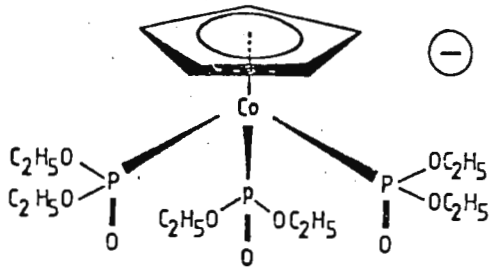

Fig.1

We have been working with an organometallic anion (L^-, Fig. 1) given to us by Prof. Kläui from Aachen-[1,2]. The Cobalt(III) complexes (CoL_2^+) with this ligand and its derivatives comprise the only known class of Cobalt(III) spin crossover compounds [3]. In the course of this study we found that $^{23}Na^+$ relaxation times are dramatically shortened in the presence of L^-. At about the same time Anderegg and Kläui [4] published that the binding constants of alkali metal ions and L^- in methanol have the trend $H^+ > Li^+ > Na^+ > K^+$. The same trend was found by us in aqueous solutions, though with smaller binding constants. Since this anion is lipophilic we thought that it might act as an ionophore for Li^+. As you may know, there is an intensive research for the discovery of Li^+ ionophores mainly because of the importance of Li^+ in the treatment of manic-depressive patients. Since we expect the cations to cross the membrane as uncharged complexes it should be difficult to monitor the transport by potentiometric techniques.

Fortunately, we have an NMR instrument at our disposal! With Gupta's shift reagent $Dy(TPP)_2^{7-}$[5], it is possible to shift $^{23}Na^+$ as well as $^7Li^+$ signals. So here is the experiment:

Unilamelar vesicles were loaded with NaCl and LiCl, the outside salts were replaced by KCl and after the addition of $K_7Dy(TPP)_2$ two signals appear in the spectrum: a large signal of intravesicular $^{23}Na^+$ and a small shifted signal of the residual $^{23}Na^+$ in the outer solution. Switching the spectrometer to $^7Li^+$, we observe the same picture for $^7Li^+$, with an even better resolution (Fig.2, t = 0). Now adding the ionophore and monitoring continuously a series of spectra is obtained (Fig. 2) from which the time course of the transport was calculated and given in Fig. 3. On the same sample very similar plots on a much longer time scale for $^{23}Na^+$ are obtained. So this is how an ionophore is identified and its selectivity for Li^+ and Na^+ is determined, all on a single sample.

Sincerely yours,

H. Shinar Gil Navon

Hadassah Shinar Gil Navon

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2. G. Navon and W. Kläui, Inorg.Chem.,23, 2722 (1984).
3. W. Kläui, J.Chem.Soc., Chem.Commun.,700 (1974).
4. G. Anderegg, W. Kläui, Z. Naturforsch., Teil B, 36, 949 (1981).
5. R.K. Gupta, P. Gupta, J.Magn.Reson., 47,344 (1982).

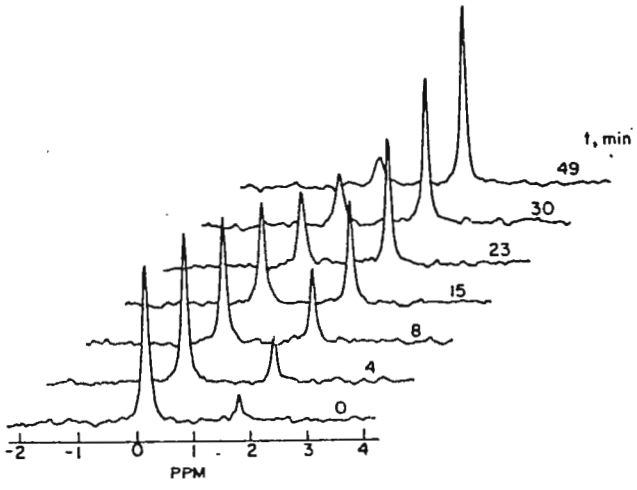

Fig.2

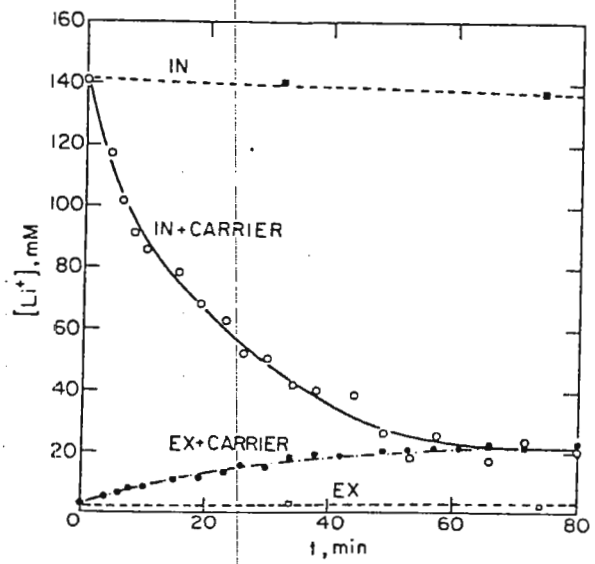

Fig.3

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Public Health Service

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Bethesda, Maryland 20205
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Room : 106
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August 8, 1985

Prof. B. L. Shapiro
Department of Chemistry
Texas A&M University
College Station, Texas 77843

HAWKS

Dear Barry,

In response to the pink sheet, I'm passing along some information about a source of CDC Hawk drives that may be of interest to TAMU Newsletter readers. About nine months ago we began to experience a series of serious problems with an old high-density Diablo disc drive used with our Nicolet 1180 computer. It was clear that the drive was not worth repairing and we tried to replace the Diablo drive with a CDC Hawk drive. Unfortunately, the Hawk's are no longer manufactured by CDC and no longer supplied by Nicolet. However, I received a tip from Nicolet that Hawk drives were available from F-NMR accessories. We found that F-NMR supplies Hawk drives, compatible with 1180 or 1280 data systems, at a fraction of the original price charged by Nicolet. We received shipment of a Hawk drive for our 1180 system about two months ago and it has worked without a problem. Anyone interested in obtaining a Hawk drive should call Mr. Frank Bennis at 312-962-7055.

Sincerely yours,

Dennis A. Torchia

Dennis A. Torchia, Ph.D.
Mineralized Tissue Research Branch
National Institute of Dental Research

Equipment For Sale

The Chemistry Department at the University of South Carolina expects to dispose of certain surplus NMR equipment this fall. A functional CFT-20 NMR spectrometer and various probes, peripherals and support equipment including a spare VDM-620I/L computer (from an XL-100 NMR) will be offered to the highest bidder in a sealed bid auction. For more details concerning the offering or to be included in the mailing list for bid solicitation, please contact Dr. A. R. Garber at (803) 777-2088 or by mail at the Chemistry Department, University of South Carolina, Columbia, SC 29208.

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Westhollow Research Center
P. O. Box 1380
Houston, Texas 77001

August 14, 1985

Professor Bernard L. Shapiro
Department of Chemistry
Texas A&M University
College Station, TX 77843

SUBJECT: THE MAXIMUM ENTROPY METHOD FOR SIGNAL-TO-NOISE ENHANCEMENT

Dear Barry:

I have taken over this subscription to the Texas A&M NMR Newsletter following the retirement of Charlie Reilly, the longtime friend of yours and mine and of many others in the NMR community. Charlie worked for over 30 years in NMR and is now enjoying a well-deserved rest.

Concerning the subject of this letter, most people are perplexed at the idea of using entropy, and maximum entropy at that, to increase the information obtained from a set of data. The problem lies in the fact that entropy is always associated with disorder when it is more properly associated with probability. Hence, the name maximum likelihood method is also used in this context (1). Entropy alone, however, is of little help in obtaining information, but rather entropy subject to constraints is the basis for the method.

To investigate the maximum entropy method (MEM), I wrote a Pascal program for our Bruker Aspect 2000 computer to test the method for sensitivity enhancement. I incorporated the basic ideas in the literature (2), but rather than using the method as an aid in Fourier transforming the data, the program was written to operate on the absorption mode NMR spectrum. Although I am not completely satisfied that this is equivalent to operating on the FID, this method was used because of the simplification in removing the phase parameter from the calculation. As a demonstration a spectrum before and after MEM is shown in the attached figure. The example is a ^{13}C NMR spectrum of 8 mg of unknown material isolated from a reaction mixture and run on a Bruker WH-360. It can be seen from the figure that the signal to noise does improve, and it does so without a loss of resolution. The discrepancies in the peak intensities are presumably due to stopping the calculation before complete convergence; the calculation involves a long and slow iteration procedure, and the Newton-Raphson method which I used may not be adequate to the task. As time allows, I would like to investigate the method further on a larger, faster computer.

(continued on page 29)

WDE185PMP22601

Since its founding in 1960, Bruker has delivered many major contributions to the field of analytical instrumentation.

Here are some highlights:

1963: World's first commercial pulsed NMR spectrometer.

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1968: Introduction of ESR spectrometers.

1969: Introduction of Fourier transform techniques for NMR.

1974: Entrance into FT-IR spectroscopy.

1983: Entrance into NMR Imaging (MRI) and in-vivo spectroscopy.

1984: Introduction of fiberoptics data link for high-speed data transfer and ultra-fast array processors for FT applications in IR and NMR.

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nology. Today we offer an unequalled line of NMR spectrometer systems up to 500 MHz including such recent advances as in-vivo spectroscopy, mini and whole body NMR imaging and real time processing, such as the first fiberoptics data link for high-speed data transfer, and high speed array processors that perform Fourier transformations of 32 kiloword data tables in a few hundred milliseconds.

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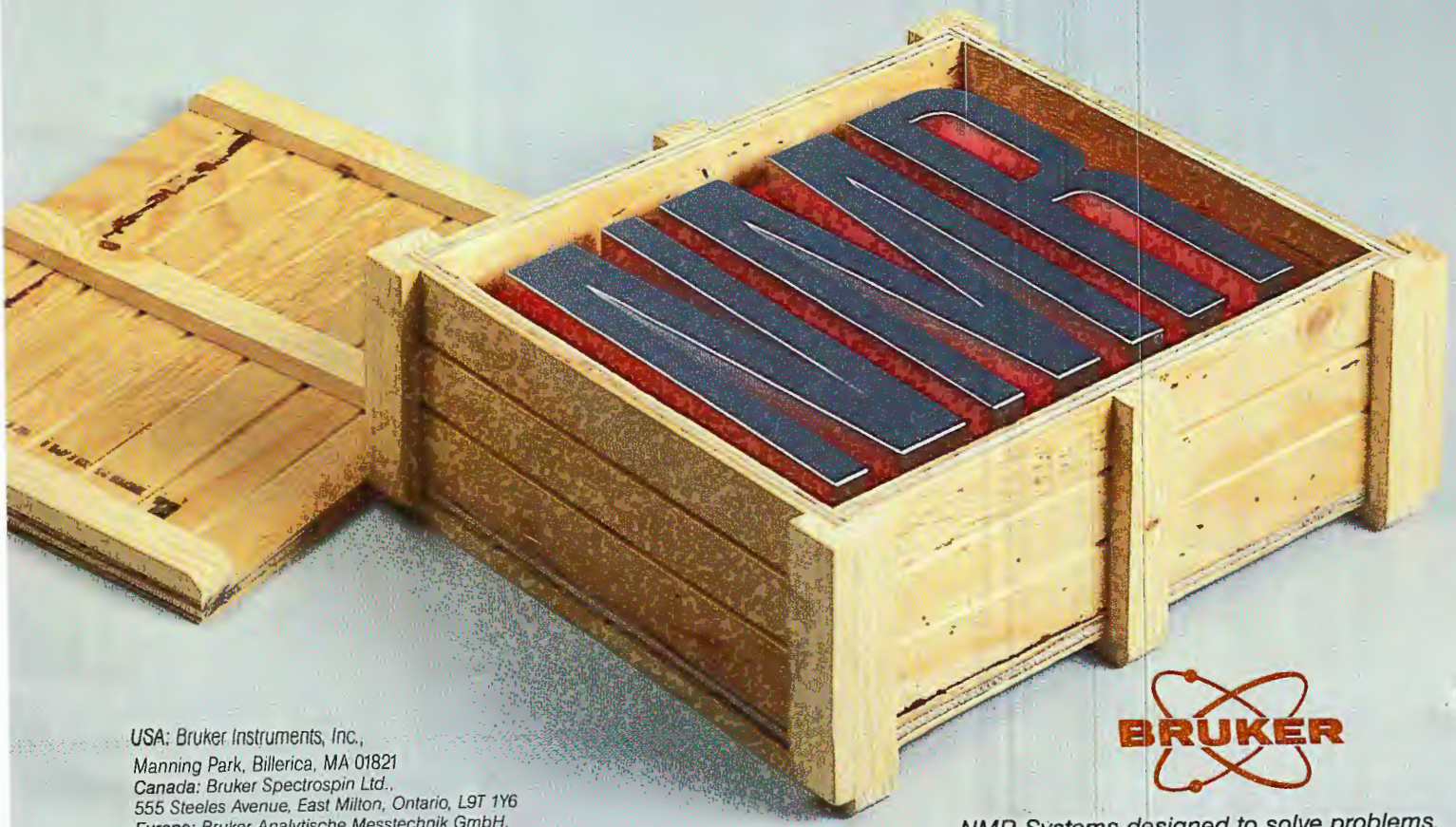

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NMR Systems designed to solve problems.

(continued from page 26)

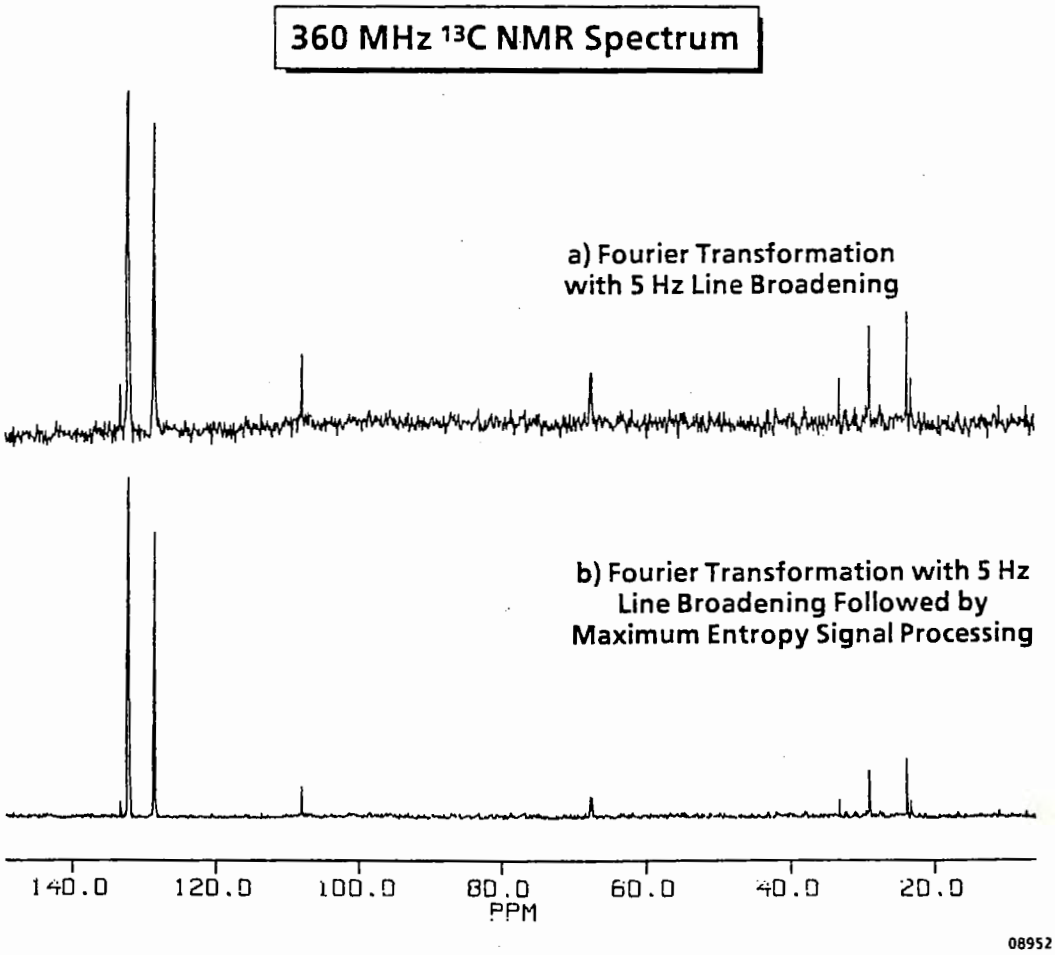
I would also like to acknowledge my friend Randall LaViolette of AT&T-Bell Labs for his assistance with this work.

Sincerely,

Larry L. Sterna
Research Chemist
Analytical Department

1) B. R. Frieden, Deconvolution: with Applications in Spectroscopy (Academic Press, 1984), pp. 227-259.

2) B. R. Frieden, J. Optical Soc. Am. 62, 511 (1972); S. F. Gull and G. J. Daniell, Nature 272, 686 (1978); S. Sibisi, Nature 301, 134 (1983); and S. Sibisi, J. Skilling, R. G. Brereton, E. D. Laue, and J. Staunton, Nature 311, 446 (1984).



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Department of Radiology
717 534-8044

August 16, 1985

Professor Bernard L. Shapiro
Department of Chemistry
Texas A & M University
College Station, Texas 77843

^{23}Na Image in a Live Rabbit;
Positions Available

Dear Professor Shapiro:

In the course of developing David Hoult's rotating frame imaging method (1) and the recently conceived Fourier series imaging technique (2-4) for in vivo NMR, we have recently succeeded in obtaining a one-dimensional spatial image of ^{23}Na in the eye of a live, anesthetized rabbit. The resulting Fourier series image is shown in Figure 1, and clearly depicts sodium in the aqueous humor, lens, and vitreous humor. We are currently measuring ^{23}Na T_1's in the in vivo eye in order to assess the diagnostic capabilities of the method for detecting cataractogenesis, in collaboration with Dr. Joseph W. Sassani of HMC's Division of Ophthalmology.

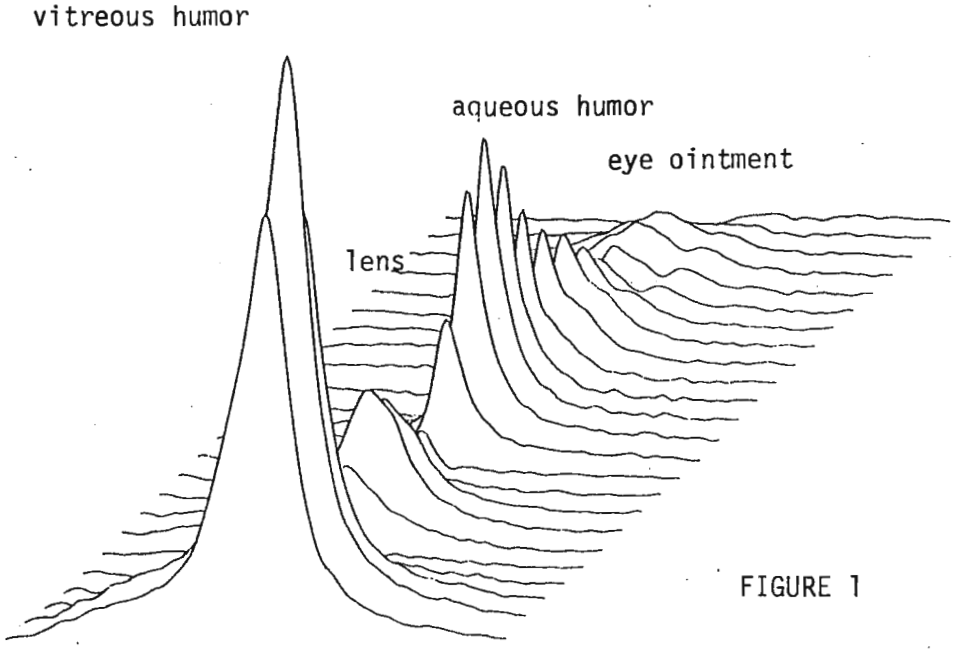

FIGURE 1

We currently have several openings for applicants interested in working in our NMR laboratory. A non-tenure track position is available immediately for an NMR instrumentation specialist. The candidate should have an M.S. or Ph.D. degree with substantial NMR experience. Responsibilities will include day-to-day operation and maintenance of a Bruker AM400WB spectrometer (with some help expected occasionally on a Nicolet 1.9 T 26-cm system), electronics design, construction, and troubleshooting, and instruction of users. Excellent opportunities exist for collaborative research in biophysical and biomedical applications of NMR. Competitive salary with excellent benefits is offered.

Several postdoctoral research positions in the area of in vivo NMR spectroscopy and imaging also exist. Applicants should have a Ph.D. in chemistry, biochemistry, or related field with extensive experience in NMR techniques and instrumentation. Experience in electronics, computer programming, and physiology also helpful. There are excellent collaborative research opportunities in biomedical NMR, primarily of heart, brain, muscle, and kidney. Instrumentation includes a 1.9 T 26-cm bore spectroscopy-imaging system, a Bruker AM400WB, and whole-body 0.15 T and 0.5 T imaging systems (the latter to be upgraded to 2.0T).

Send C.V. and three letters of recommendation to Richard W. Briggs, Ph.D., Departments of Radiology and Biological Chemistry, Pennsylvania State University College of Medicine, M. S. Hershey Medical Center, Hershey, PA 17033. An equal opportunity/affirmative action employer.

References

1. D.I. Hoult, J. Magn. Reson., 33, 183-197 (1979).

2. K.R. Metz and R.W. Briggs, Poster B49, 26th Experimental NMR Conference (ENC), Asilomar, California, April 21-25, 1985.

3. M. Garwood, T. Schleich, G.B. Matson, B.D. Ross, and W.D. Winters, Poster B26, 26th Experimental NMR Conference (ENC), Asilomar, California, April 21-25, 1985.

4. K.R. Metz and R.W. Briggs, J. Magn. Reson., 64, 172-176 (1985).

Sincerely yours,

Richard W. Briggs

Richard W. Briggs, Ph.D.
Assistant Professor of Radiology
and Biological Chemistry

Kenneth R Metz

Kenneth R. Metz, Ph.D.
Research Fellow

RWB/jp

Credit the account of R. W. Briggs.

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DEPARTMENT OF CHEMISTRY
SANTA BARBARA, CALIFORNIA 93106

10 August 1985

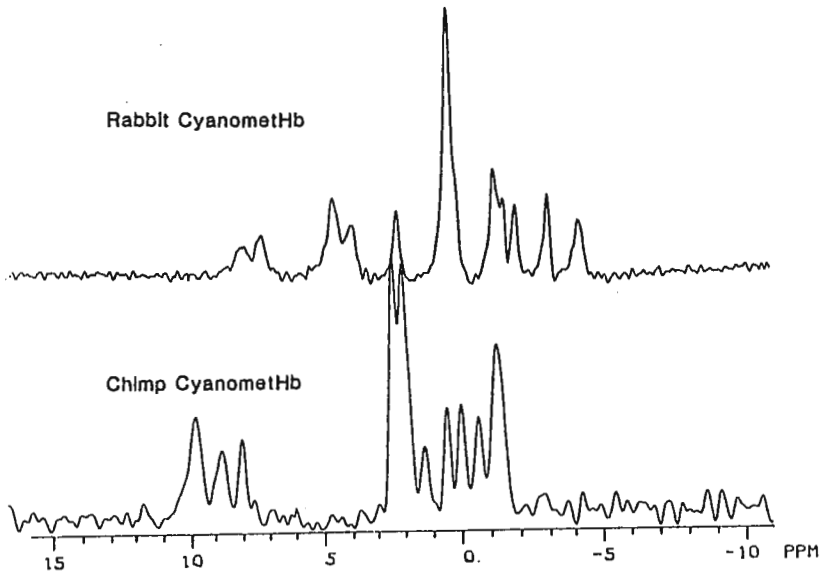
Professor Bernard L. Shapiro
TAMU NMR Newsletter
Texas A & M University
College Station, Texas 77843-3255

Re: Fluorine NMR Studies of Chimpanzee Hemoglobin

Dear Barry,

Despite the advances that have made possible high resolution nmr at high magnetic fields, substantial difficulties still attend the resolution and assignment of proton or carbon-13 nmr signals from proteins or other biologically interesting materials. These problems can often be eased by the introduction of fluorine nuclei; technical requirements for obtaining fluorine nmr spectra of proteins are no more demanding than those for carrying out proton nmr but fluorine spectra from such systems are often much more resolved as a result of the greater dispersion of the fluorine shifts. An example from a rather unusual system is shown below.

Westhead and Boyer have shown that 4-fluorophenylalanine present in the diet of the rabbit becomes incorporated into proteins of muscle, liver and blood [1]. We have previously reported in these pages and elsewhere [2] that the



Fluorine nmr spectra of cyanomethemoglobins, obtained at 282 MHz under conditions similar to those used in Reference 2.

(continued on page 35)

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(continued from page 32)

levels of incorporation are sufficiently high to permit fluorine nmr studies of these proteins. This feeding experiment has now been carried out with an adult female chimpanzee who ingested a primate chow containing about 0.1% by mass of 4-fluorophenylalanine. At the end of the feeding period (68 days) a blood sample was taken (Not a trivial task with a chimpanzee!) and hemoglobin isolated. Amino acid analysis indicated that about 0.2 mole of fluorophe was present per mole of protein. The figure compares the fluorine spectrum of rabbit cyanomethemoglobin [2] with the same form of hemoglobin from the chimp. About 20% of the amino acids present in the rabbit protein are different in the chimpanzee and it is clear that these substitutions alter appreciably the local environments experienced by the fluorophenylalanine reporter groups.

What makes the chimpanzee results interesting is the fact that this hemoglobin is likely identical to human hemoglobin [3]. What we, in effect, have done is to prepare a fluorine-labeled human protein without the necessity of disturbing our human subjects committee! Other forms of the chimpanzee hemoglobin are now under study.

Sincerely,

Tom

M.P. Gamcsik
Postgraduate
Research
Associate

J.T. Gerig
Professor of
Chemistry

[1] Westhead, E.W., & Boyer, P.D. (1961) Biochim. Biophys. Acta **54** 145-156.
[2] Gerig, J.T., Klinkenborg, J.C., & Nieman, R.A. Biochemistry **22** 2076-2987.
[3] Rifkin, D., & Konigsberg, W. (1965) Biochim. Biophys. Acta **104** 457-461.

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August 12, 1985

Professor Barry L. Shapiro
Department of Chemistry
Texas A&M University
College Station, TX 77843

IMPORTANCE OF t_1 WEIGHTING FUNCTION IN LONG-RANGE HETCOR

Dear Barry:

Heteronuclear Chemical Shift Correlation 2D NMR (HETCOR) is a widely-practiced technique, ideally suited to establishment and confirmation of chemical shift assignments. The major use of this experiment is the correlation of bonded nuclei, typically C-13 and H-1. The delays flanking the last two 90 degree pulses are set relative to the J coupling between these nuclei. Long-range correlations between protons and carbons (protonated or non-protonated) can be established by just setting these delays appropriately. This is accomplished in XL systems by setting a value for the parameter JNXH.

Because the long-range J's are an order of magnitude less than one-bond J's, the homonuclear H-H couplings have a more serious effect in the Long-Range HETCOR experiment. The more complex the proton coupling pattern, the more complicated is the transfer of polarization to a remote carbon, since the proton homonuclear couplings spread the proton magnetizations and reduce the available net magnetization for polarization transfer to the carbons. These homonuclear couplings have greater effect the longer they are permitted to be active, and they are active in modulating the proton magnetization during the evolution time and the delays flanking the polarization transfer pair of pulses. Carbon-13's receiving polarization from these protons will have their intensities modulated by the chemical shifts of these protons, but the intensities of these modulations will decay rapidly relative to modulations arising from protons which have a minimum of homonuclear couplings.

These factors have direct relevance to one who is interested in establishing long-range correlations, particularly for unknown structures. A simple example is given in the figure for the case of menthol. The lower part of the figure shows a printer "dump" of the display screen for the interferogram of C-6. These data are from a collection of 128 FID's, with maximum t_1 of 0.160 seconds. As customary, the interferogram is "sine-bell" or "pseudo-echo" weighted to produce a symmetrically shaped product which is then subjected to Fourier transform with respect to t_1 (the evolution time), giving a slice in F1, the proton shift dimension. A major long-range correlation is seen to the methyl protons of C-7. This data could easily be interpreted as indicating only one correlation for C-6.

The same raw data was used to generate the upper half of the figure. In this case the weighting function was set to emphasize modulations which

decay early (these are visible in the interferogram). The transformed data now clearly show the modulations arising from H-5α and H-2β.

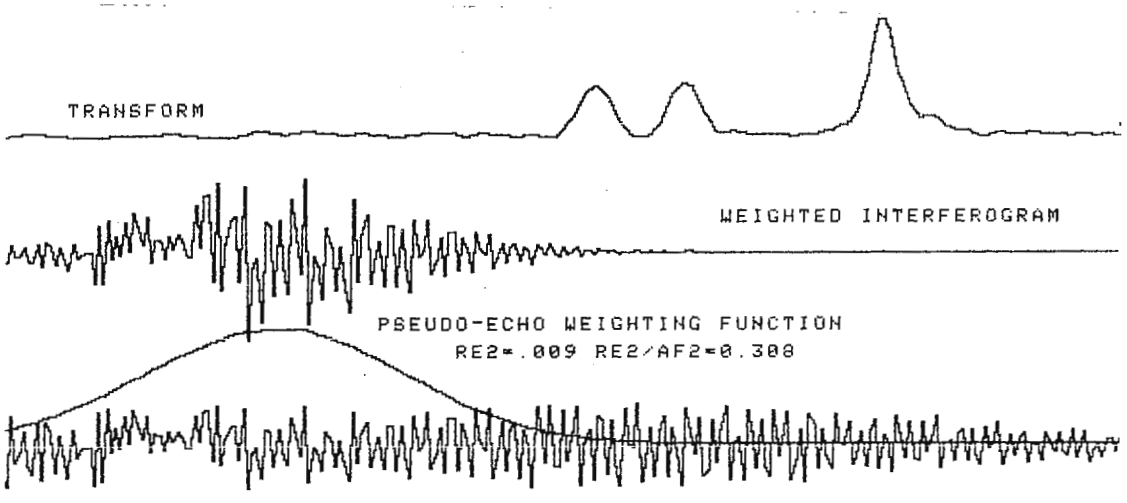
The data demonstrate that one should examine data carefully with respect to the choice of weighting functions in t_1. Information might be there that could easily be ignored!

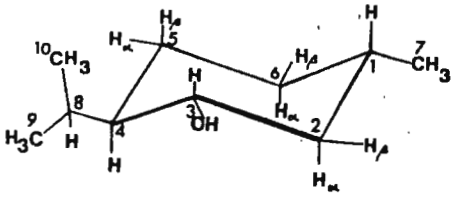
Sincerely yours,

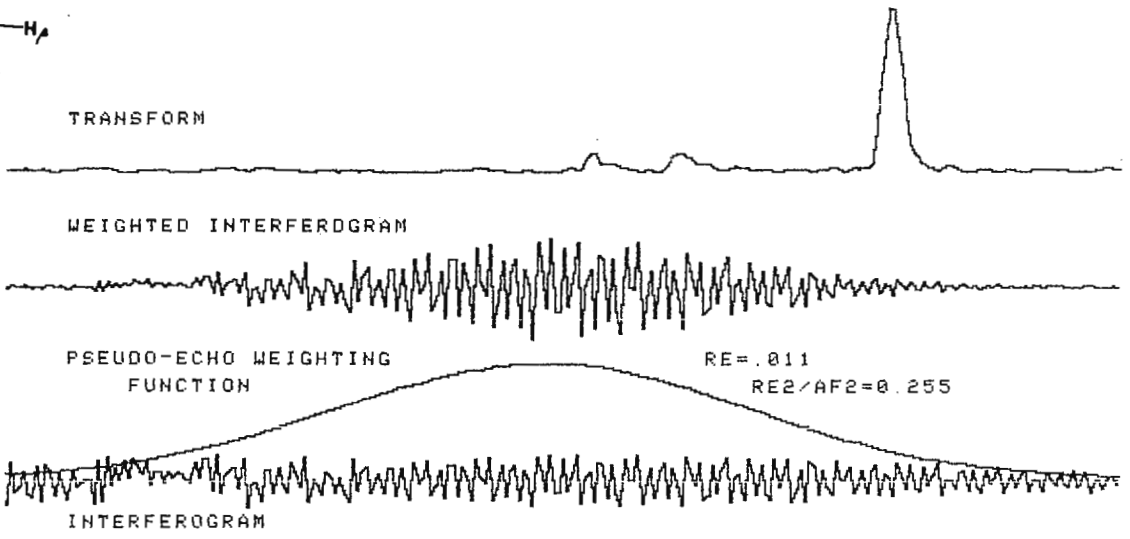
George

George A. Gray
NMR Applications Laboratory

GAG/bry







DEPARTMENT OF HEALTH & HUMAN SERVICES

Public Health Service

National Institutes of Health
National Cancer Institute
Bethesda, Maryland 20205

August 14, 1985

Prof. B. Shapiro
NMR Newsletter
Dept. of Chemistry
Texas A&M University
College Station TX. 77843-3255

Pyrimidine 2D-COSY cross-peaks in tRNA

Dear Barry:

At the last ENC we reported our preliminary observations of the unique cross-peaks due to cytosine C5-C6 protons in 2D-COSY spectra of oligodeoxynucleotides.

We would like to describe some similar observations with tRNA. Ordinarily one would not expect to see cross-peaks from a macromolecule of this size diue to the slow correlation time. But, several such cross-peaks are observed as shown in the figure. These arise from mobile pyrimidines among the 17C and 12U residues present in tRNA(Phe) which may be present in the loop or terminal regions. The fact that the relative internsities of these cross-peaks change with temperature should enable us to correlate these signals with specific residues in the sequence.

Sincerely yours,

Jack S. Cohen, Ph.D., Siddhartha Roy, Ph.D., Babul Borah, Ph.D.
Biophysical Pharmacology Section
Clinical Pharmacology Branch

Figure legend: 2D-COSY spectra of tRNA(Phe) at 400 MHz taken on a Varian XL-400 spectrometer at the temperatures shown. Concentration ca 1mM in 0.01M Pi buffer pH 7, 0.1M NaCl; 256x512 data points.

(continued on page 41)

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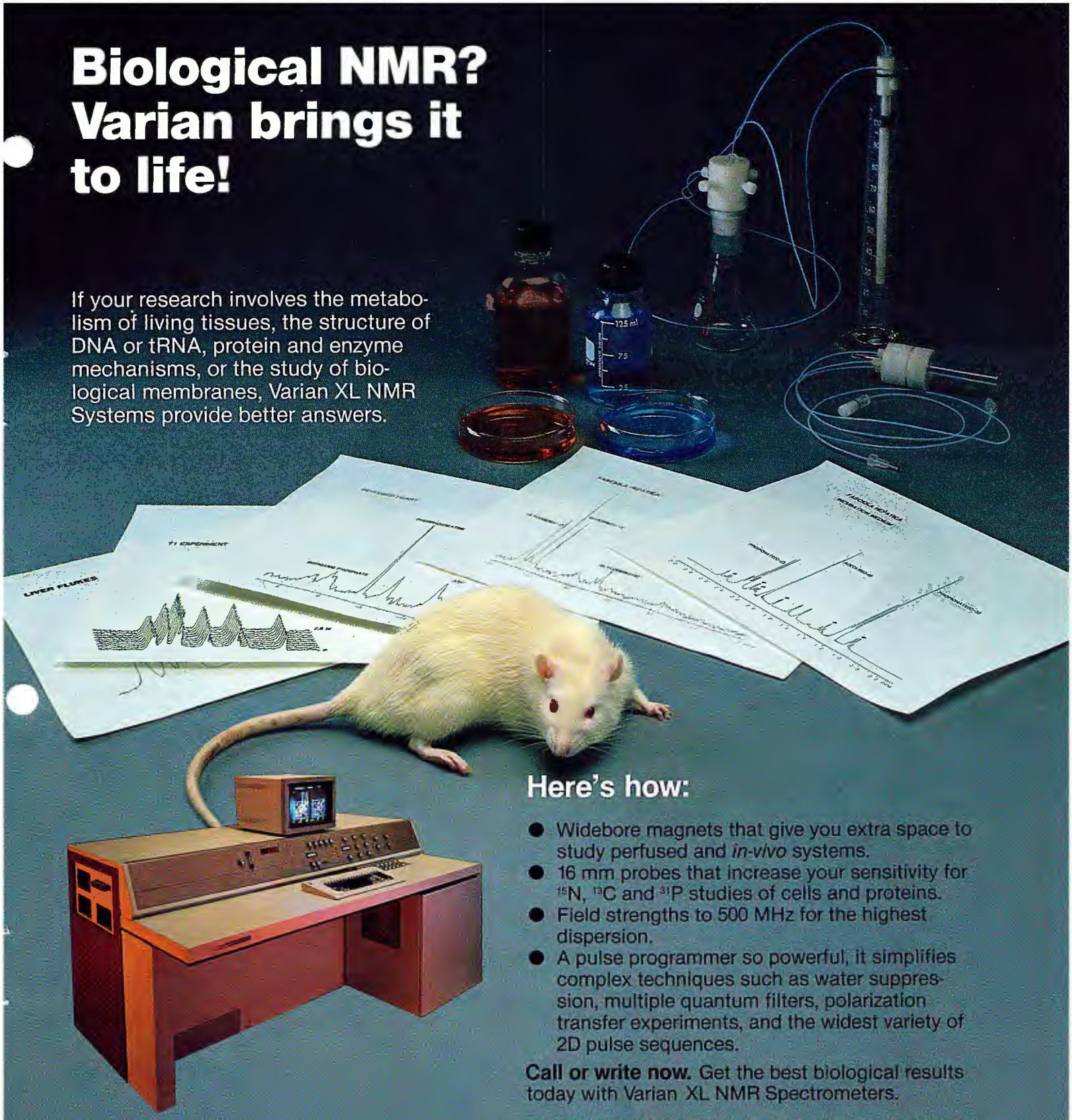

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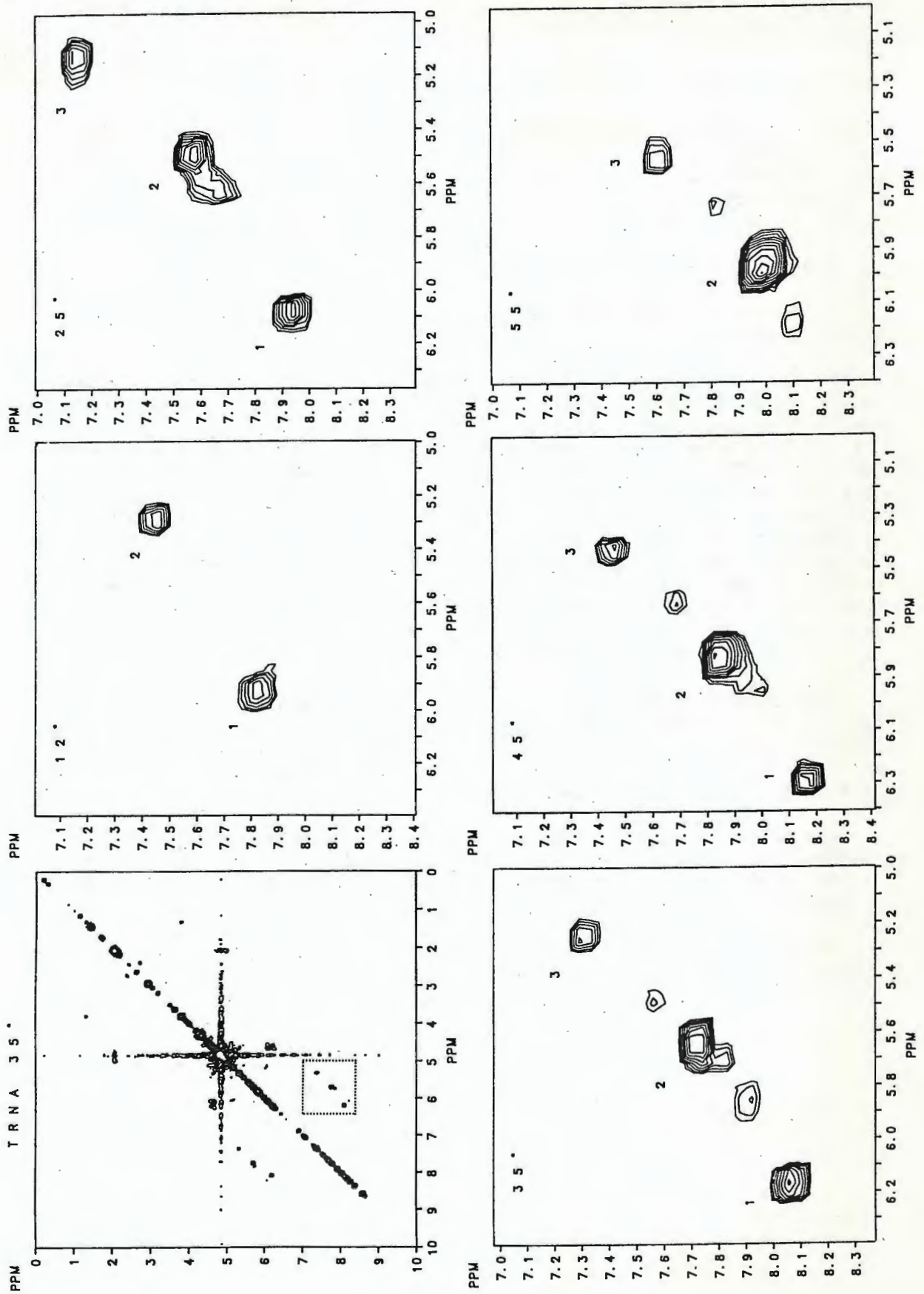

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Professor Bernard L. Shapiro Editor
TAMU Newsletter
Dept. of Chemistry
Texas A&M University
College Station, Texas

19 August 1985

^{29}Si NMR of Ceramics

Dear Prof. Shapiro

I am trying to keep the grim reaper away by sending you this offering for the newsletter.

We have been using magic angle spinning to study a variety of ceramics and one of the results is sufficiently interesting to make the newsletter. This is ^{29}Si resonance in silicon nitride, Si_3N_4. Silicon nitride exists in two crystalline forms, alpha and beta, with the former being formed by heating to 1400° and the latter to 1600°C. Measurements were made on Bruker AM-250 and AM-400 spectrometers at 49.69 and 79.48 MHz respectively and spinning rates of 3.5-4.5 KHz. Alpha samples of high purity were obtained from Ube, Starck, and Sylvania and all showed two peaks at -46.6±0.2 and -48.8±0.2 ppm referenced to TMS. Beta Si_3N_4 was obtained from Dr. D. Messier of the Army Materials and Mechanics Research Center and showed only a single peak that is approximately in the middle of the two alpha peaks. The result is in agreement with structural studies that show two types of silicon atoms in the alpha form and one in the beta.

Considerable difficulty was encountered in obtaining resonances due to the very long T_1 values. The Ube and Starck T_1 values were measured using a 90-τ-90° recovery sequence and values of 558 and 673 seconds respectively were obtained. Such long values are common in spin 1/2 nuclei in ceramics but should be kept in mind when working with new materials.

The SiN_4 tetrahedral chemical shift value is useful because it provides and end point for the series from SiO_xN_{4-x} to SiN_4 that may be present in many silicon containing ceramics. Further studies on this type of ceramic will be reported later.

Thanks are due to Dr. D. Burum and Mr. M. Appel of Bruker for obtaining the spectra.

Sincerely

Amos J. Leffler

with Louis G. Carreiro

Paul L. Sagalyn

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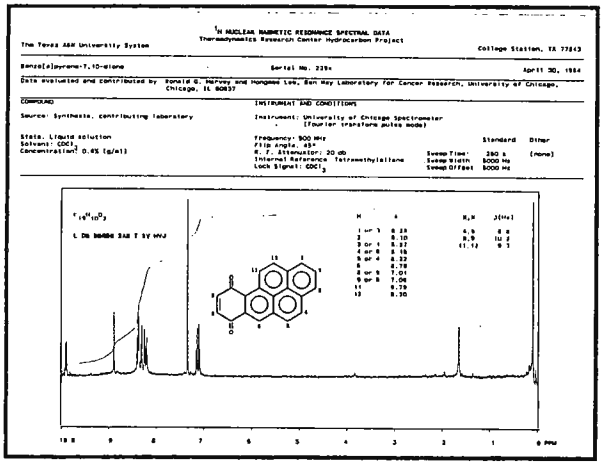

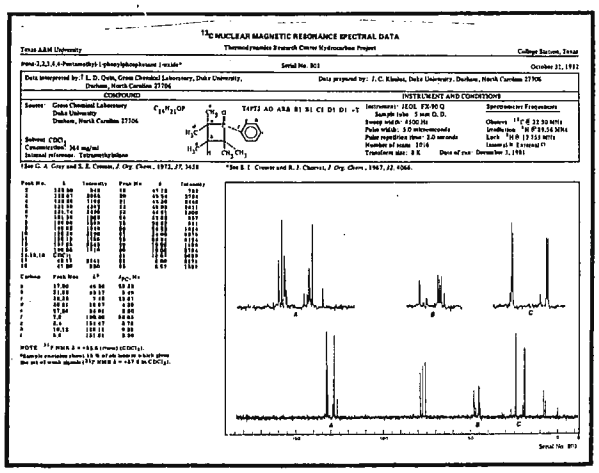

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Attention: K. N. Marsh

CHEMICAL CENTER
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Lund, August 20, 1985

Prof. Bernard L. Shapiro
Dept. of Chemistry
Texas A&M University
College Station, Texas 77843
USA

Post Mortem Metabolism in Meat

Dear Barry,

Scared stiff by your pink remainder notice we hasten to put down a brief report on one of our lines of research.

Since two years we have, in collaboration with the Swedish Meat Research Institute in Kävlinge, outside Lund, studied the post mortem metabolism in meat with NMR. Mainly beef but also pork and meat from lamb at 25°C. For this "post-vivo" NMR project we used the most popular nuclei in this "field", namely phosphorus. We followed ATP, PCr, Pi and pH as the rigor mortis developed. The results were compared with conventional biochemical assays and pH measurements and we found that they agreed quite well (cf. enclosed Figure).

Enthusiastic papers about low power decoupling (WALTZ-16) and water suppression methods convinced us to change nucleus - first to C-13 and later to H-1. These nuclei also gave us access to the lactate and creatine development during the pre rigor period. Excited as we were about the water suppression we included this technique (1331) into the COSY experiment (for short "1331-in-vivo-COSY") with nice but disappointing results.

In our latest experiments we turned "back to our roots", P-31 NMR. We have now concentrated our interest on the temperature and muscle type influence on the post mortem metabolism. Together with conventional methods in "meat research circles" we expect a more complete picture of the tenderizing process than before.

With our best regards

Peter Lundberg Hans Vogel Torbjörn Drakenberg Sture Forsén

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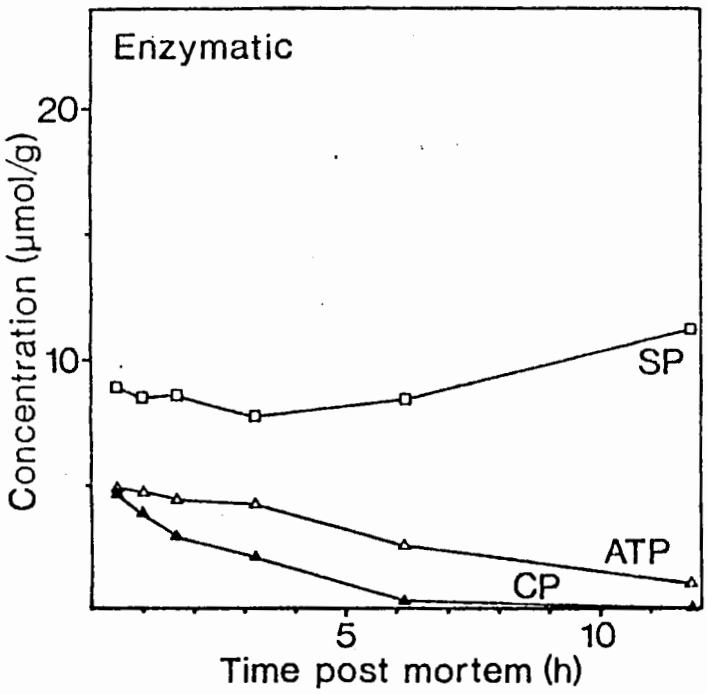

Fig. 1. Biochemical assays of beef (M. longissimus dorsi) during post mortem metabolism. (SP = sugar phosphates, CP = creatine phosphate).

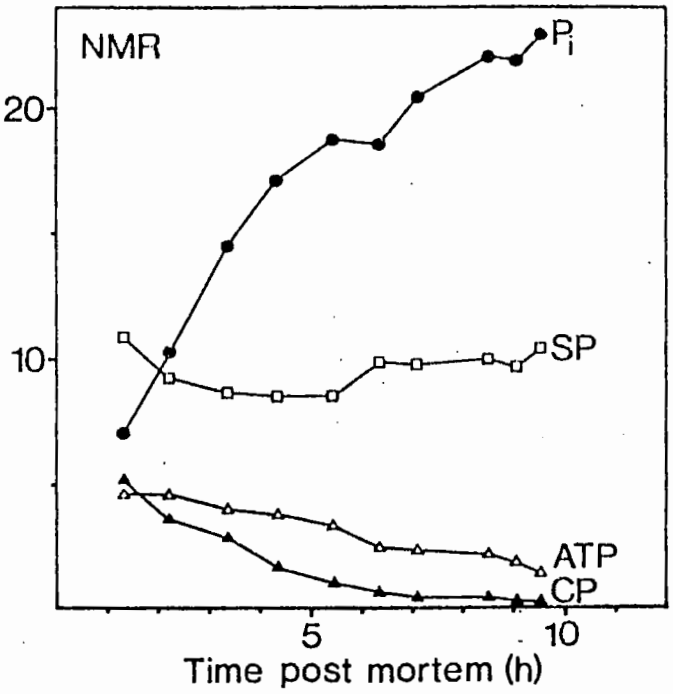

Fig. 2. Corresponding P-31 NMR measurements. (160 scans, 8s. waiting time) solenoidal probe (10 mm).

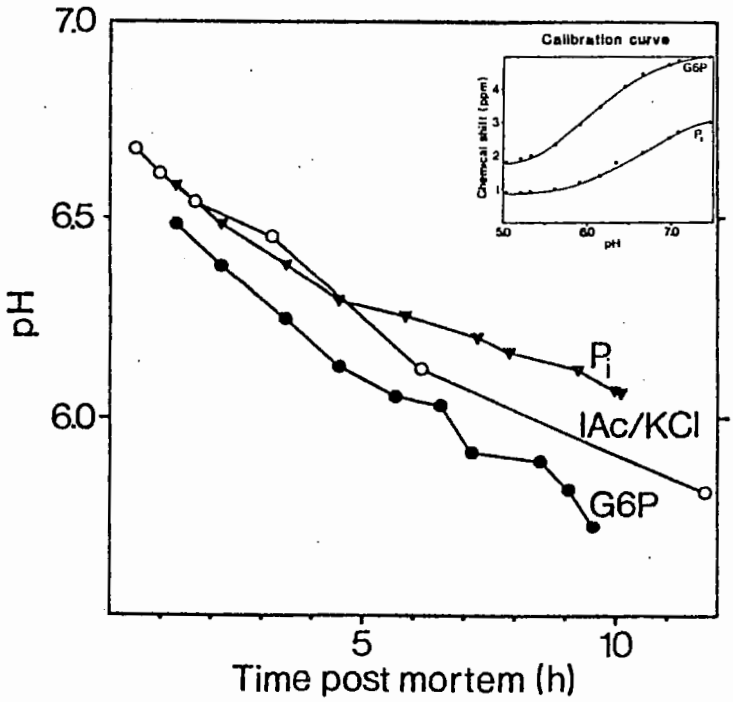

Fig. 3. pH development during the post mortem metabolism. Comparison between P-31 NMR and iodo-acetate measurements.

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EAS SHORT COURSES - Dr. Robert E. Santini, Chairman (317)-494-5230
Dr. Gwendolyn N. Chmurny, Associate Chairman (301)-695-1326

Monday, November 18th, 1985

"1D, 2D, 3D Pulsed NMR of Liquids, Solids and Spaces: A Practical Approach"
Chairman: Dr. John Grutzner

1. "The Selection of NMR Techniques for Problem Solving". Dr. Roy Bible, G.D. Searle & Company, Skokie, IL
2. "Introduction to 2D NMR - A Practical Introduction". Dr. John Grutzner, Purdue University, West Lafayette, IN.
3. "Introduction to Solid State NMR". Dr. Bernie Gerstein, Iowa State University, Ames, IA.
4. "Basic NMR Imaging", Dr. David Foxall, Varian Associates, Palo Alto, CA.

Tuesday, November 19th, 1985

"Inside Your NMR: Introduction to Hardware Aspects of NMR Instrumentation".
Chairman: Dr. Robert Santini

1. "Inside Your NMR". Dr. Robert Santini, Purdue University, West Lafayette, IN.
2. "Optimizing and Trouble Shooting Your NMR using Spectra and Standard Samples". Dr. Gwendolyn N. Chmurny, NCI-Frederick Cancer Research Facility, Frederick, MD.
3. "Essential Electronic Support Equipment". Dr. Robert Dykstra, Fox Chase Cancer Center, Philadelphia, PA.
4. "Getting the Best Results from a Field Service Call". Dr. G. Joseph Ray, Amoco Research Center, Naperville, IL.

Wednesday, November 20th, 1985.

"An Introduction to Laboratory Microcomputers: Hardware and Software".
Chairman: Dr. Stanley N. Deming.

1. "Introduction to Laboratory Microcomputers". Dr. Stanley N. Deming, University of Houston, Houston, TX.

2. "Why You Want to Have a Microcomputer" Mr. Kimber Fogelman, Purdue University, West Lafayette, IN.

3. "Programming Languages for Microcomputers". Dr. Stephen L.Morgan, University of South Carolina, Columbia, SC.

4. "Applications and Computer Interconnections". Dr. Richard L. Deming, California State University, Fullerton, CA .

EAS NMR WORKSHOP - Dr. Amy Abe, Director (616)-323-4814

Tuesday, November 19, 1985 - 2:00 - 5:00pm

"Modern NMR"

1. "Sophisticated NMR Made Easy". Dr. Douglas P. Burum, Bruker Instruments, Inc., Billerica, MA.

2. "New Dimensions in NMR". Dr. Jerry L. Dallas, G.E. NMR Instruments, Freemont, CA.

3. "Advances in Computer Controlled Data Acquisition and Analysis". Dr. Steven L. Patt, Varian Associates, Palo Alto, CA.

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Workshop fees: $25.00 + $25.00 (meeting preregistration fee) $35.00 after October 25, 1985. The workshop is limited to 35 attendees.

The EAS NMR program was advertised in the June 1985 issue of the TAMU NMR Newsletter (No. 321, pp. 17 and 18).

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DEPARTMENT OF CHEMISTRY DAVIS, CALIFORNIA 95616

August 21, 1985

POSTDOCTORAL POSITION - NMR SPECTROSCOPY

A postdoctoral position is available in my research group, starting between Jan 1 and Mar 1, 1986, in the area of high resolution NMR studies of proteins. Our current emphasis is multinuclear approaches to structural and dynamic properties based on specifically isotope labeled heme proteins, utilizing a combination of isotope labeling, steady state and truncated NOEs, as well as several 2D methods. The stipend is $15,000 - 16,000, depending on qualifications. Experience in high resolution NMR methodology is very desirable. The position is for one year, renewable by mutual consent. Our equipment available continues to be among the best (completely multinuclear Nicolet-200, Nicolet-360 with ^{1}H, ^{2}H, ^{13}C, ^{31}P, Nicolet-500 with ^{1}H, ^{2}H, ^{13}C and ^{31}P and Oxford TMR-32 with several nuclei. We are now placing an order for a 7.05 T 150 mm bore horizontal magnet based spectrometer with multinuclear sideways spinning probes). Please send resume and arrange to have forwarded two letters of reference at the earliest convenience to G. N. La Mar, Department of Chemistry, University of California, Davis, California 95616.

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August 15, 1985

Professor Bernard L. Shapiro
Department of Chemistry
Texas A&M University
College Station, TX 77843

C-13 Decoupling on a JEOL

Dear Barry:

Recently there has been much interest in using isotopic substitution (^{15}N or ^{13}C) to permit the selective detection of protons directly bonded to isotopically enriched atoms. Many of these techniques are described or referenced in a recent paper by Griffey et. al. ((1984) Biochemistry 24:817). These techniques should be useful in a variety of biological systems where either the macromolecule or substrate can be enriched with stable isotopes.

Since I recently moved to The University of Texas Health Science Center at Houston, it was necessary to develop these techniques on our JEOL GX-270. A 5 mm 'H probe with broadband decoupling coils located outside of the proton coils was developed for our use by Howard Hutchins at JEOL, Peabody MA. This probe has a 7.5 µsec proton 90° pulse and a 35 µsec carbon 90° pulse. We have been able to successfully perform the pulse sequences shown in Figure 1 on our GX-270. As an example, the spin echo (A) and difference echo (B) spectra of [6-^{13}C]uracil obtained using the pulse sequence in Figure 1B, are shown in Figure 2. The value of τ_a used in this experiment was 2.7 msec. Currently we are using [6-^{13}C]uridine nucleotides to probe for covalent protein-nucleic acid adducts.

We will be glad to provide anyone owning a JEOL with copies of our pulse programs. Please credit this letter to the account of Paul Rosevear.

Sincerely yours,

Paul R. Rosevear, Ph.D.
Assistant Professor

Kamalam Muthukrishnan, Ph.D.

PRR/td

Figure 1

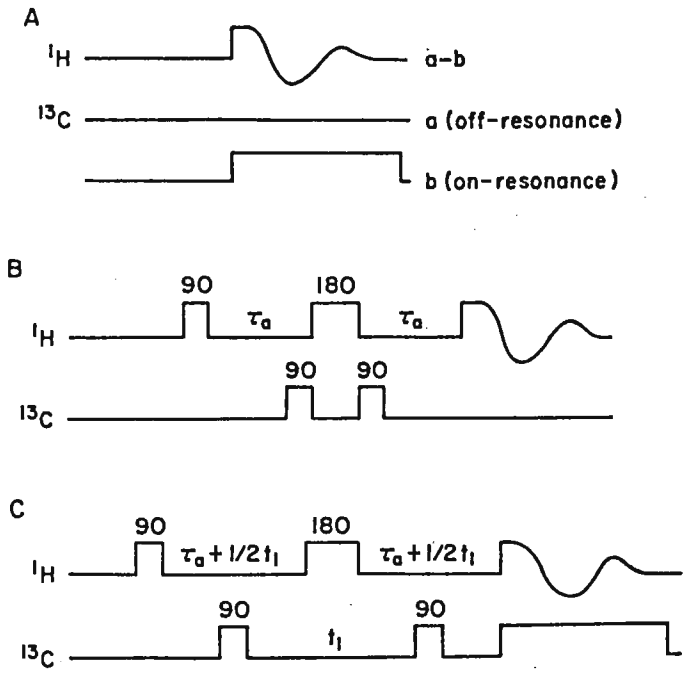
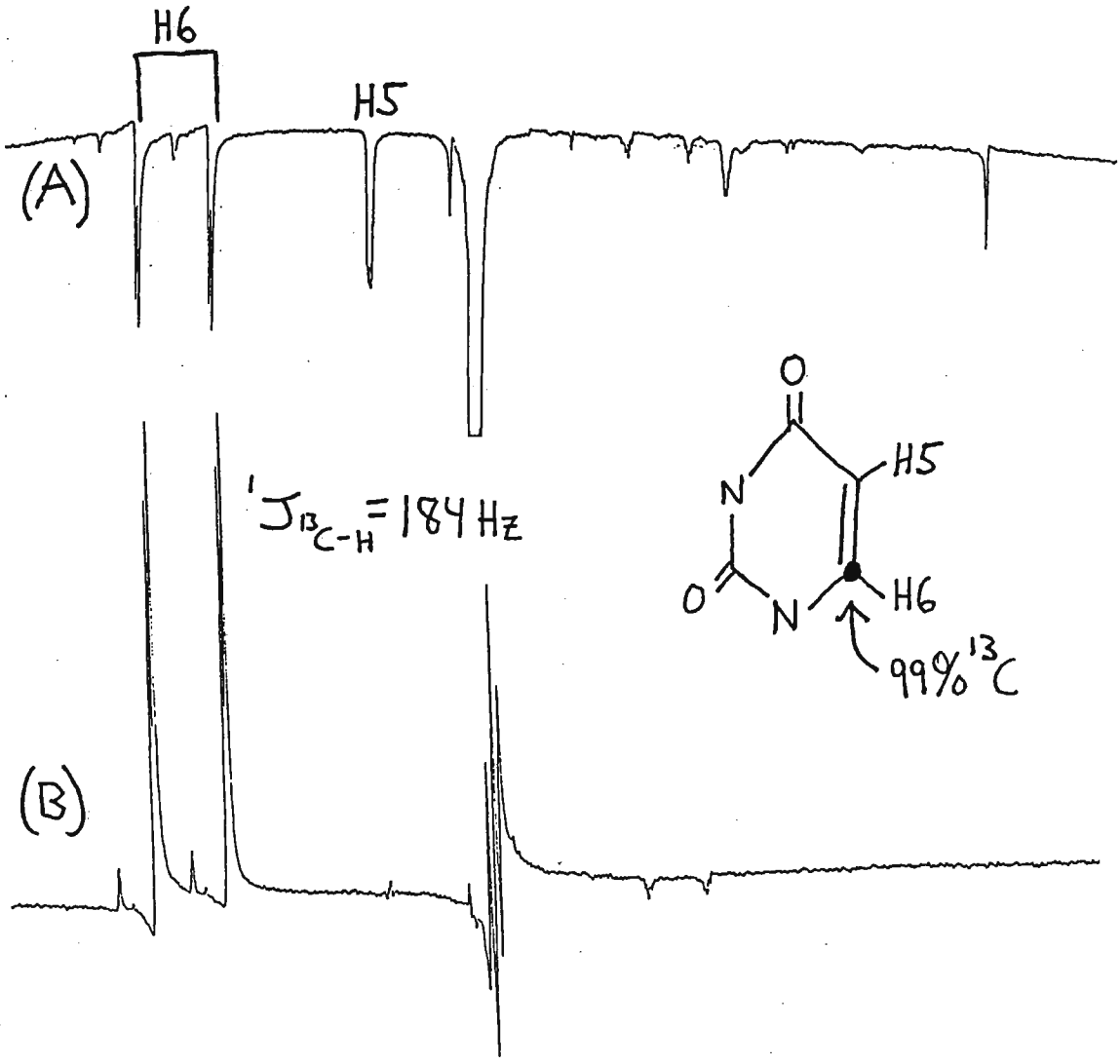
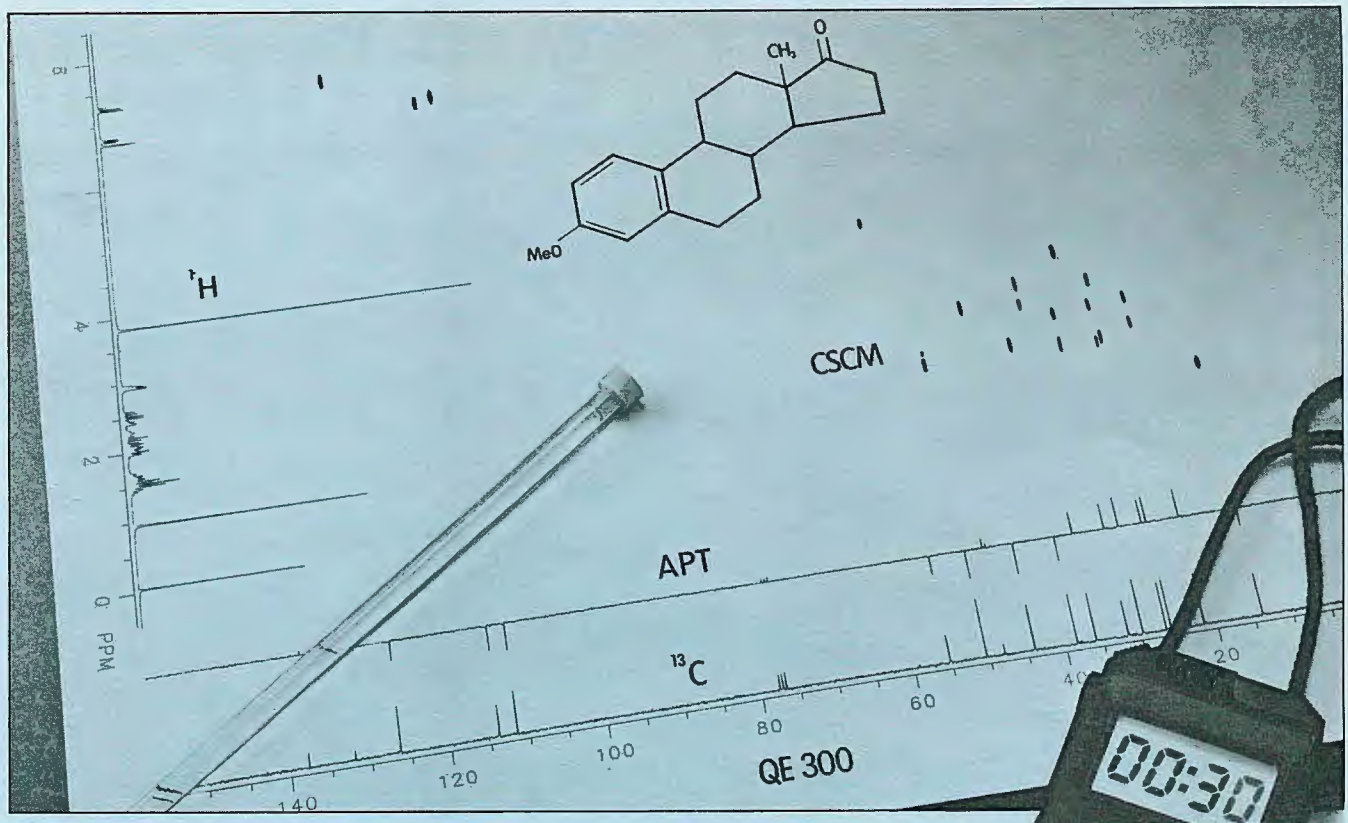


Figure 2





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For many organic molecules, the four experiments presented above will be all you need to determine or confirm molecular structure. For more complex applications, GE/NMR offers an extensive ^{13}C library with outstanding search capability. This library contains data from over 10,000 compounds and is currently being expanded using a QE-300 in operation at the Aldrich Chemical Company.

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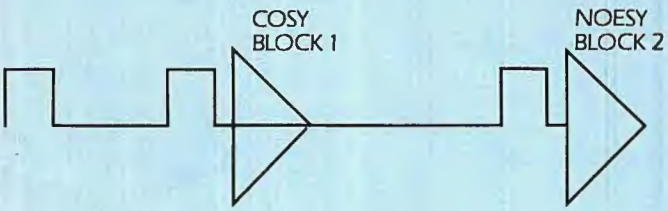
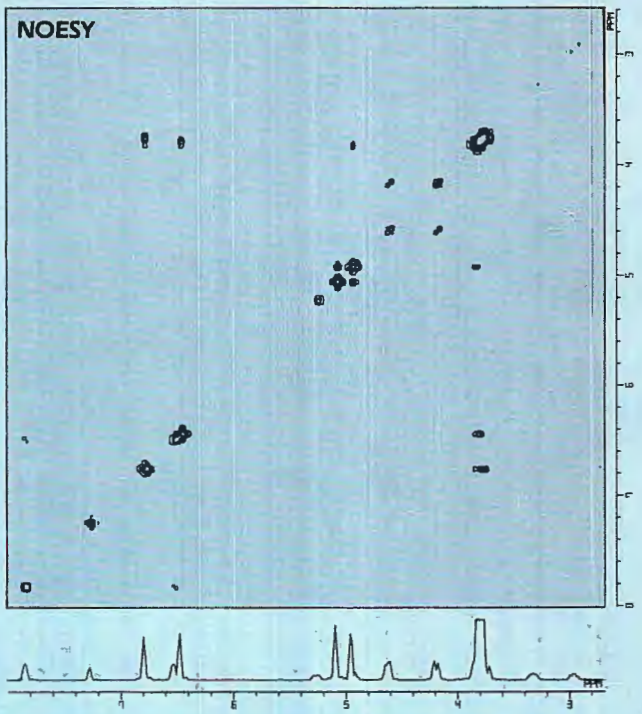
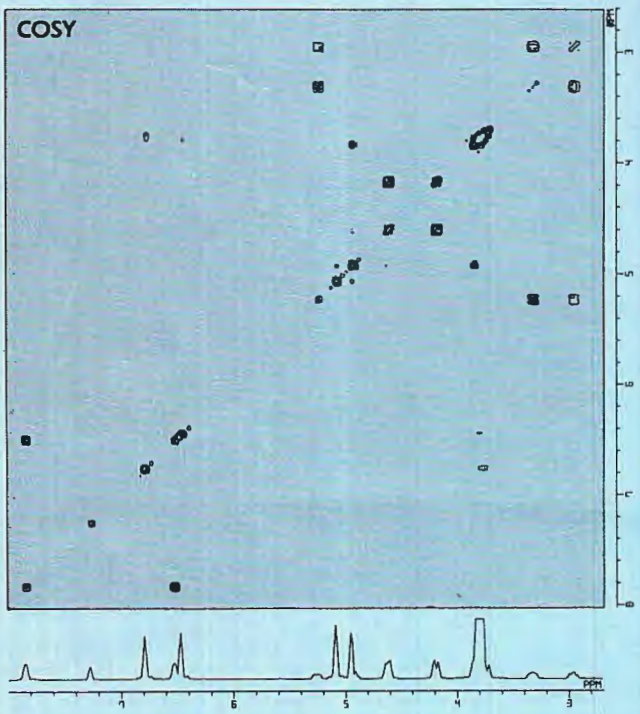
Why do two experiments when one will do?*





- Simultaneous acquisition of COSY and NOESY



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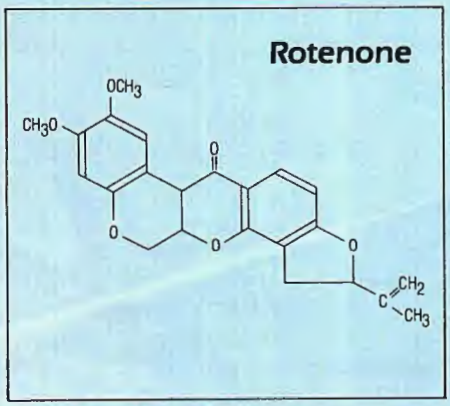
*COCONOSY (Haasnoot, et. al., J. Magn. Reson., 56,343 [1984])



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