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# NUTS

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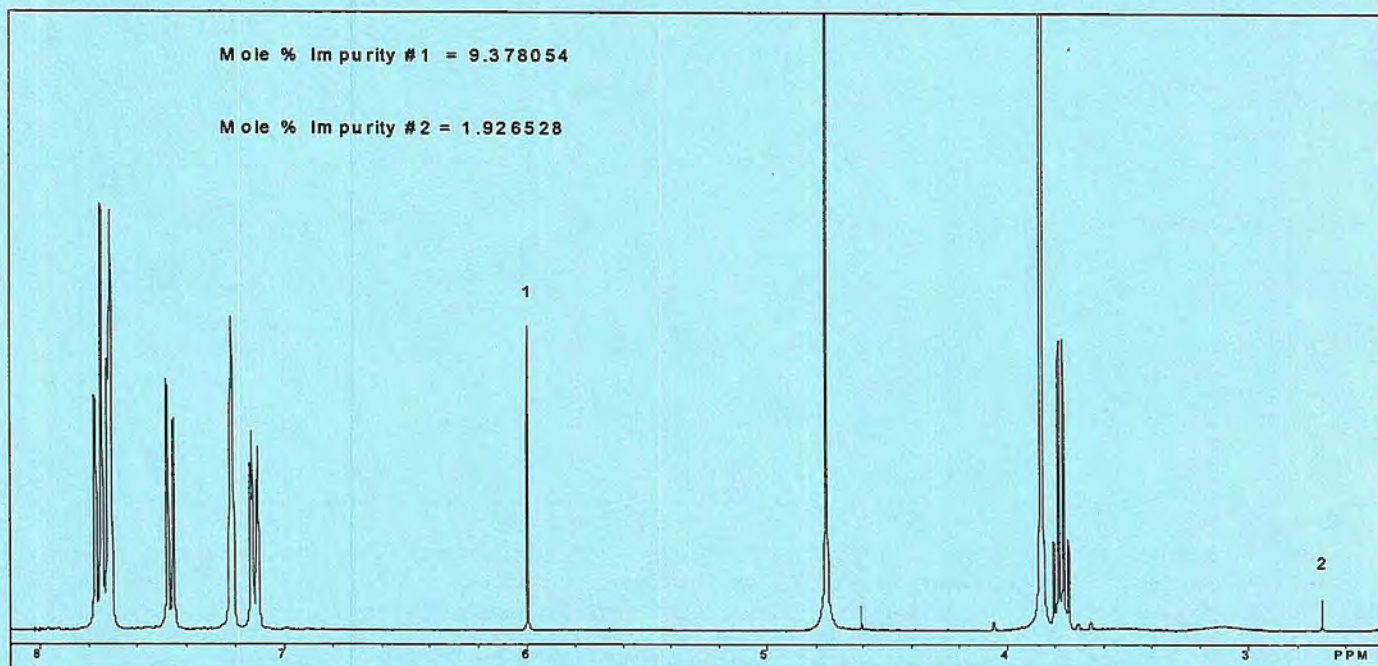
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**FORTHCOMING NMR MEETINGS**

**NMR Spectroscopy of Polymers**, Breckenridge, Colorado, **January 24-27, 1999**; an International Symposium Sponsored by the Division of Polymer Chemistry, American Chemical Society; Organizers: P. T. Inglefield and A. D. English; Registration contact: Neta L. Byerly, Division of Polymer Chemistry, Inc., Virginia Tech, 201 Hancock Hall, M.C. 0257, Blacksburg, VA 24061; 540-231-3029; Fax: 540-231-9452; email: nbyerly@vt.edu.

**7th Annual "Advances in NMR Applications" Symposium**, Omni Rosen Hotel, Orlando, Florida, **February 28, 1999**; Contact: Kathy Bishop, at the Nalorac Corp.; 510-229-3501; kathy.bishop@nalorac.com; See Newsletter 482, 18.

**40th ENC (Experimental NMR Conference)**, Clarion Plaza Hotel, Orlando, Florida, **February 28 - March 5, 1999**, immediately preceding Pittcon in Orlando; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87505; (505) 989-4573; Fax: (505) 989-1073; Email: enc@enc-conference.org.

**Pittcon '99**, Orlando, FL, **March 7-12, 1999** (50th year celebration of the Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy.) Contact: The Pittsburgh Conference, Dept. CFP, 300 Penn Center Blvd., Suite 332, Pittsburgh, PA 15235-5503; 412-825-3220; Fax: 412-825-3224; e-mail: pittconinfo@pittcon.org

**Spin Choreography - a symposium in appreciation of Ray Freeman**, Cambridge, England, **April 8-11, 1999**; web site: <http://mchsg4.ch.man.ac.uk/mcmr/RF.html>; fax: c/o M.H. Levitt +46-8-15 2187; email: mhl@physc.su.se.

**41st ENC (Experimental NMR Conference)**, Asilomar Conference Center, Pacific Grove, CA, **April 9-14, 2000**; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87505; (505) 989-4573; Fax: (505) 989-1073; Email: enc@enc-conference.org.

**Seventh Scientific Meeting and Exhibition of the Intl. Soc. for Magnetic Resonance in Medicine (ISMRM)**, Philadelphia, PA, **May 22 - 28, 1999**; Contact: International Society for Magnetic Resonance in Medicine, 2118 Milvia St., Suite 201, Berkeley, CA 94704.

continued on inside back cover



UNIVERSITY OF VIRGINIA  
DEPARTMENT OF CHEMISTRY  
McCORMICK ROAD  
CHARLOTTESVILLE, VIRGINIA 22901

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

October 29, 1998  
(received 10/30/98)

### Network Printing

Dear Dr. Shapiro:

Multiple user NMR labs typically have several computers and must provide print services from most or all of these. The cost effective way to meet this need is to attach printers to the same network that is used for communication among computers. In our case as in most cases an ethernet-based network is available. Our NMR lab consists of four spectrometers, two are run by Sun workstations and the other two by PowerMacs. Additionally the lab contains two Unix workstations, and several Macintosh and IBM PC compatible computers. The user population is approximately 80. Our printing needs are met by two Hewlett Packard LaserJet printers, a 4M Plus and a 4000N. Each of the printers contains a HP JetDirect print server, a device which allows one to connect the printer directly to the network and complete print jobs from a wide array of computers including Mac, PC, and Unix machines. The JetDirect print servers may be configured directly from the front panel of the printer or remotely by using HP JetAdmin software. Each printer has an ethernet address and can simultaneously handle print jobs from computers using IPX/SPX, AppleTalk, DLC/LLC, and TCP/IP network protocols. We found that the JetDirect print servers and the JetAdmin software were easy to install and set up. Once the JetDirect print servers are set up, installation of the remote printers is as easy as installing a local printer. We have used the LaserJets and JetDirect servers for many months to provide print service for machines using the following operating systems: SunOS, Solaris, MacOS, Win95, and WinNT. IRIX and AIX based systems can also be used if they have a functioning Line Printer Daemon (LPD) or if the Unix server which hosts the network print queue has LPD. In summary, we find that our HP printers with JetDirect servers are a versatile, low maintenance solution for network printing. For more info on HP printers and JetDirect servers see <http://www.hp.com/cgi-bin/peripherals/pandi.pl> and [http://www.hp.com/net\\_printing/jetdirect/index.html](http://www.hp.com/net_printing/jetdirect/index.html), respectively.

Sincerely,

Jeff Ellena



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NMR Operating Frequency (MHz/H)	200			300			400		500		
Field Strength (Tesla)	4.7			7.0			9.4		11.7		
Nominal Room Temperature Bore Access (mm)	54	89	54	89	150	54	89	51	89		
Magnet Type (Standard or shielded)	Standard	Standard	Standard	Standard	Standard	Actively Shielded	Actively Shielded	Actively Shielded	Actively Shielded		
Field Stability (Hz/hour %H)	<2	<2	<3	<3	<15	<8	<10	<10	<10		
Axial 5 Gauss Stray Field Contour (Metres)	1.81	2.65	2.19	2.75	4.2	1.5	1.8	1.8	2.5		
Radial 5 Gauss Stray Field Contour (Metres)	1.42	2.0	1.7	2.2	3.3	1.0	1.3	1.3	1.75		
Cryostat Type	Compact	T3	T3	Compact	T3	T5	T3	T4FB	T4FB	T5FB	
Minimum Helium Refill Interval (Days)	80	235	203	80	235	203	120	183	150	140	
Helium Refill Volume (Litres)	26	79	68	26	79	68	101	62	83	120	
Year Hold Cryostat Option Available	X	✓	✓	X	✓	✓	X	X	X	X	
Nitrogen Refill Interval (Days)	14	14	14	14	14	14	22	14	15	15	14
Minimum Nitrogen Refill Volume (Litres)	32	61	61	32	61	61	135	61	81	81	135
* Minimum Operational Ceiling Height (Metres)	2.69	2.92	2.92	2.69	2.92	2.92	4.16	2.9	3.1	3.1	3.16
System Weight (kg) Including Cryogen's	120	315	391	133	325	399	1050	400	610	625	1200

NMR Operating Frequency (MHz/H)	600		750		800		900	
Field Strength (Tesla)	14.0		17.6		18.8		21.1	
Nominal Room Temperature Bore Access (mm)	51		89		63		63	
Magnet Type (Standard or shielded)	Actively Shielded	Standard	Standard	Standard	(2.2K) Pumped	(2.2K) Pumped	Standard	With Iron Shield
Field Stability (Hz/hour %H)	<10	<12	<15	<15	<15	<15	<15	<15
Axial 5 Gauss Stray Field Contour (Metres)	2.5	5.0	7.6	8.69	6.3	6.3	12.2	8.73
Radial 5 Gauss Stray Field Contour (Metres)	1.75	3.9	6.1	6.89	5.0	5.0	9.7	3.81
Cryostat Type	T5FB	T4FBL	T6	T6L	T7	T7	T8	T8
Minimum Helium Refill Interval (Days)	120	90	60	60	60	60	60	60
Cryostat Helium Refill Volume (Litres)	101	60	187	216	328	328	1200	1200
Minimum Nitrogen Refill Interval (Days)	15	15	14	14	14	14	15	15
Nitrogen Refill Volume (Litres)	136	100	137	162	167	167	1800	1800
* Minimum Operational Ceiling Height (Metres)	3.16	3.4	3.78	3.97	3.97	3.97	8.75	8.75
System Weight (kg) including Cryogen's	1180	1200	3000	4000	4000	4000	18000	18000

## Room Temperature Shim Specifications

Shim Type (Model)	Number of Channels	Dimensions	
		External Diameter (Cryostat Bore Size)	Internal Diameter (NMR Probe Diameter)
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18/89/73	18	89mm	73mm
26/89/73	26	89mm	73mm
28/51/40	28	51mm	40mm
40/51/40	40	51mm	40mm
29/51/45	29	51mm	45mm
36/63/51	36	63mm	51mm

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# OXFORD

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 The NMR Newsletter  
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 USA

October 2, 1998  
 (received 10/8/98)

**Solid state NMR spectroscopic studies of the thiourea inclusion compounds of the two isomers of methyl 4-t-butylcyclohexanecarboxylate**

Dear Dr. Shapiro,

One of us (HvB) was studying thiourea inclusion compounds of cyclohexane derivatives some 30 years ago.<sup>1</sup> A recent publication on an NMR study of carboxylic acid guests in urea<sup>2</sup> gave rise to some nostalgia and promoted us to dig up some of our old thiourea inclusion compounds and to run their <sup>13</sup>C NMR spectra. It appeared that the compounds survived well and the spectra provided us with some new structural information. Here, we report on the <sup>13</sup>C CP-MAS spectra of the thiourea inclusion compounds of the *cis* and *trans* isomers of methyl 4-t-butylcyclohexanecarboxylate (see Figure 1).

It is well known that thiourea forms crystalline inclusion compounds with suitable organic compounds. The host-guest compounds can be described as consisting of hexagonal honeycombs of thiourea surrounding channels with an internal diameter of about 7 Å. Previously, X-ray diffraction (powder) showed that *cis* and *trans* methyl 4-t-butylcyclohexanecarboxylate have a repeat period of 10.7 and 12.3 Å, respectively in the thiourea host.<sup>1</sup> Since this corresponds well with the molecular dimensions of these compounds, it can be concluded that the guest molecules have head-tail stacking in the inclusion compounds.

The <sup>13</sup>C chemical shifts of the esters in the inclusion compounds (see Figure 1) are close to those of the pure esters in a solution of CDCl<sub>3</sub>. This suggests that the chair conformation of the cyclohexane rings of these compounds is preserved upon inclusion in thiourea. Both the C-10 and the C-7 nuclei of the included *trans* ester show two resonances in the <sup>13</sup>C NMR spectra, whereas the resonances for all other nuclei are not split and relatively sharp. Most likely, two different orientations of the guest molecules with respect to each other occur in the thiourea channels.

The line widths of the resonances of the thiourea adduct of the *cis* ester are much larger than those of the *trans* compound, indicating some mobility in the former. The line widths of the C-1, C-2,6, and C-10 are larger than those of the other resonances. This might be explained by exchange between two conformations of the COOCH<sub>3</sub> moiety. It is known that the C=O function of esters groups prefers an eclipsed configuration with neighboring C-C bonds. For the *cis* ester this means that the C=O can be either eclipsed to C1-C2 or to C1-C6.

Sincerely,



Joop A. Peters



Herman van Bekkum

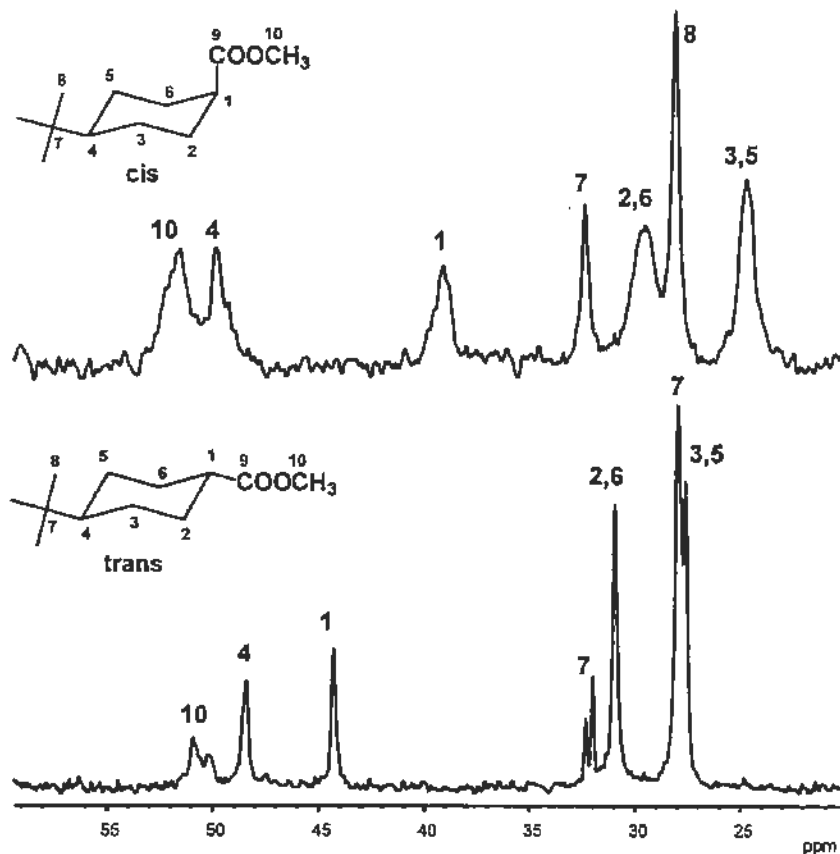


Figure 1.  $^{13}\text{C}$  CP MAS NMR spectra of the thiourea inclusion compounds of *cis* and *trans* methyl 4-*t*-butylcyclohexanecarboxylate. The carbonyl region is not shown.

#### References

- <sup>1</sup> H. van Bekkum, J.H. Palm, P.E. Verkade, and B.M. Wepster, *Recl. Trav. Chim. Pays-Bas* 89 (1970) 913.
- <sup>2</sup> J.E.C. Davies and V.A. Tabner, *J. Incl. Phenom.* 31 (1998).

## Postdoctoral Position Available

I currently have an opening for a postdoctoral scientist in my lab in the Structural, Analytical & Medicinal Chemistry unit at Pharmacia & Upjohn in Kalamazoo, Michigan. The position will involve developing and applying flow NMR techniques to enhance and drive combinatorial chemistry and ligand-binding screening components of drug discovery research. The successful candidate will collaborate with scientists in chemical informatics and in structural, combinatorial and medicinal chemistry. Our facilities include fully-equipped 400, 500 and 600 MHz NMR spectrometers. Applicants should have a recent or soon-to-be-received Ph.D. in chemistry, biochemistry or a related field, with experience in biomolecular NMR spectroscopy. Applications should be sent directly to me at the address below. For more information, please contact:

Dr. Brian J. Stockman  
 Structural, Analytical & Medicinal Chemistry  
 7255-209-007  
 301 Henrietta St.  
 Kalamazoo, MI 49001  
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Dr. B. L. Shapiro  
The NMR Newsletter  
966 Elsinore Court  
Palo Alto, CA 94303

September 30, 1998  
(received 10/17/98)

### Comparison of $^1\text{H}$ , $^{15}\text{N}$ HSQC Spectra for Stromelysin in Free and Bound State

Dear Dr. Shapiro,

Recent studies with the catalytic domain of human stromelysin-1 (SLN) have led us to compare  $^1\text{H}$ ,  $^{15}\text{N}$  HSQC spectra of this protein in the free and bound states. Figure 1 shows (A) the  $^1\text{H}$ ,  $^{15}\text{N}$  HSQC spectrum of the stromelysin-CGS 27023 complex and (B) the  $^1\text{H}$ ,  $^{15}\text{N}$  HSQC spectra of apo-stromelysin-1 overlaid with the spectrum of stromelysin-1 complexed to CGS-27023. Both spectra were acquired in buffer containing 20 mM Tris<sub>d11</sub>, 20 mM CaCl<sub>2</sub>, 0.02% NaN<sub>3</sub>, 90% H<sub>2</sub>O/10% D<sub>2</sub>O, pH 6.8. Chemical shift assignments for the SLN-CGS 27023 complex have been made and the three dimensional structure has been determined (Y.Li, X. Zhang, R. Melton, V. Gannu & N.C. Gonnella, Biochemistry, in press.)

Visual inspection of the overlaid spectra clearly shows significant shifts of amide proton & nitrogen resonances for stromelysin bound to a potent inhibitor (nanomolar range) vs. the uninhibited protein. While many prominent shifts occurred at the binding site (example: Val 163, Leu 164, Ala 165, Leu 222, Tyr 223) other resonances more remote from the immediate binding site also experienced significant chemical shift changes (example: Trp 124, Ala 167, Asp 177, His 179, Thr 187, Arg 231, Ile 242). Hence, although it is expected that inhibitor binding would cause chemical shift changes at the catalytic binding site, we have observed that other areas more remote from the binding site were found to exhibit significant chemical shift changes in the absence of inhibitor.

These results indicate that changes in chemical shifts from  $^1\text{H}$ ,  $^{15}\text{N}$  HSQC spectra may not always unambiguously or exclusively identify the binding site resonances for potent inhibitors. Such considerations need to be taken into account when using HSQC spectra to identify binding site regions especially when the 3-D structure of the protein is not known.

Sincerely,

A handwritten signature in cursive script, reading 'Yu-Chin Li'.

Yu-Chin Li

A handwritten signature in cursive script, reading 'Nina C. Gonnella'.

Nina C. Gonnella

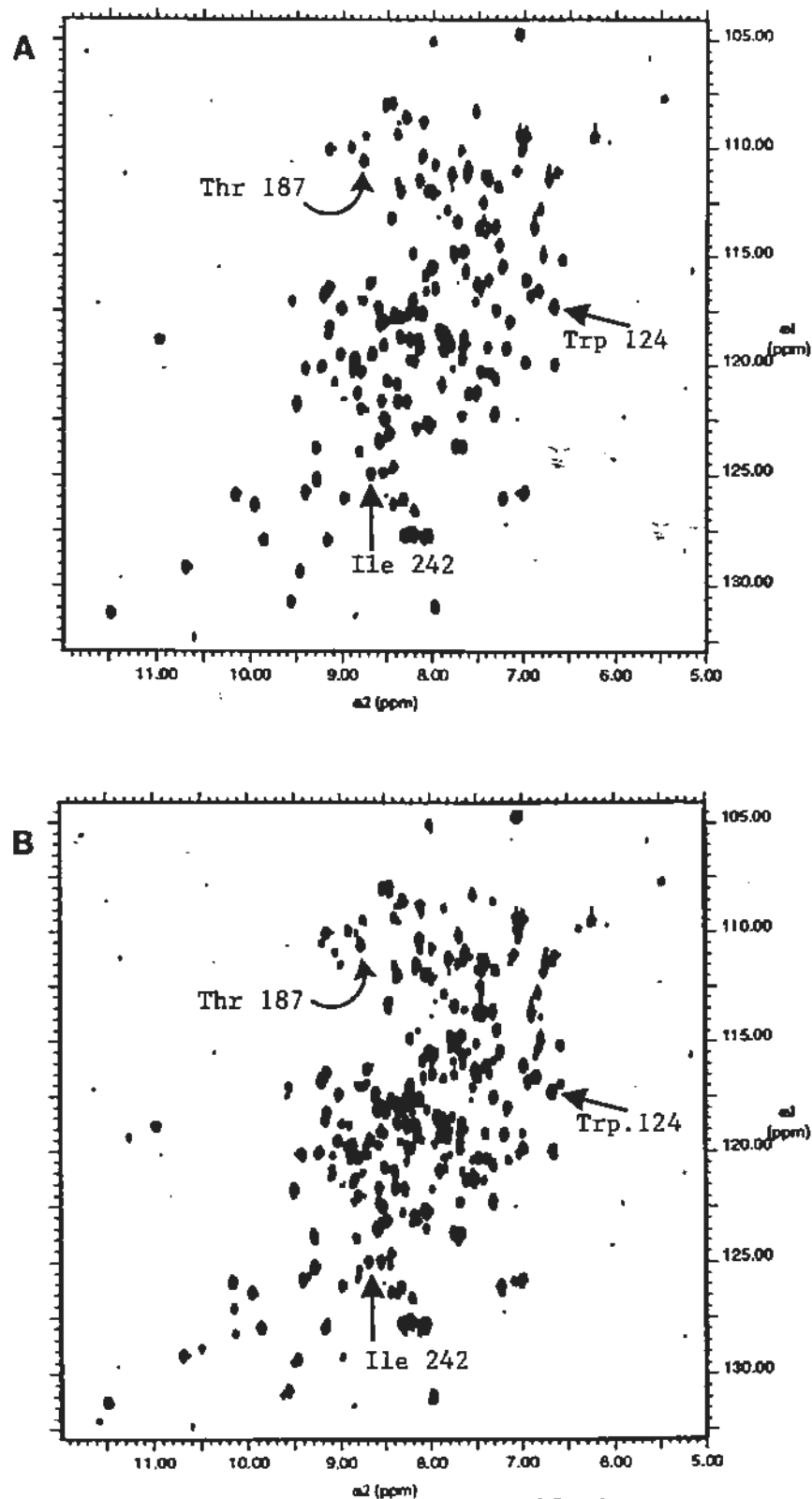


Figure 1. A)  $^{15}\text{N}$ ,  $^1\text{H}$  HSQC of SLN-CGS 27023 complex. B)  $^{15}\text{N}$ ,  $^1\text{H}$  HSQC of SLN-CGS 27023 complex overlaid with HSQC of free SLN. Some resonances remote from the binding site that shift upon inhibitor binding are displayed.





NMR

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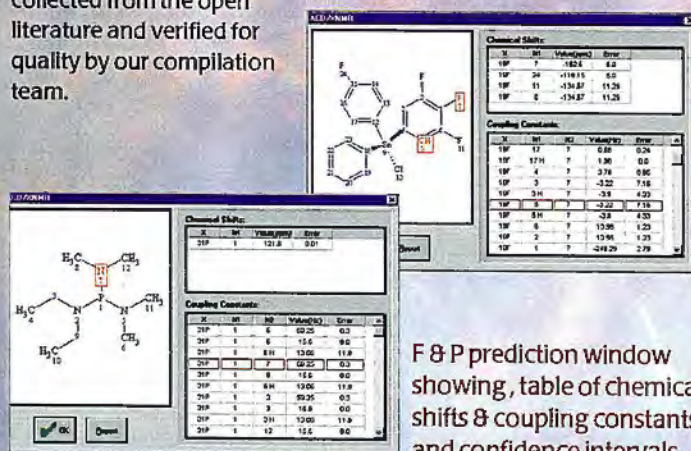
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F & P prediction window showing table of chemical shifts & coupling constants and confidence intervals

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- Manual or automatic numbering of atoms in molecules prior to prediction. Same atomic numbering schemes for all nuclei.
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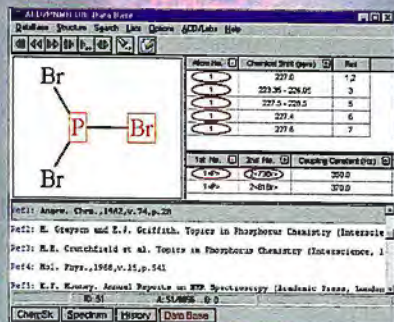
NUCLEUS	# STRUCTURES IN INTERNAL DB	# CHEMICAL SHIFTS	# COUPLING CONSTANTS
<sup>31</sup> P	18,500	23,000	8,600
<sup>19</sup> F	11,400	25,000	15,000

### <sup>19</sup>F / <sup>31</sup>P NMR

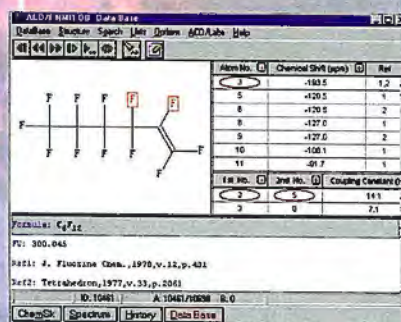
Each database includes original literature references, molecular formula, molecular weight and IUPAC names which can be searched and viewed. All data have been collected from scientific literature and verified for quality by our database team.

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**ACD/NMR DBs allow you to view chemical shifts and coupling constants for known compounds.**



Phosphorus Database window showing chemical shifts, coupling constants, and references



Fluorine Database window showing chemical shifts, coupling constants, and references

See reverse side for contact information





NMR

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UV-Vis

MS

Raman

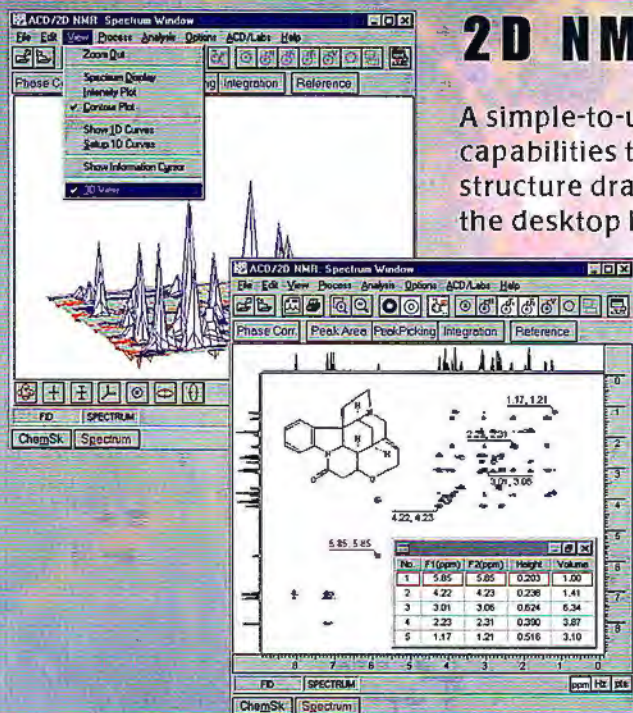
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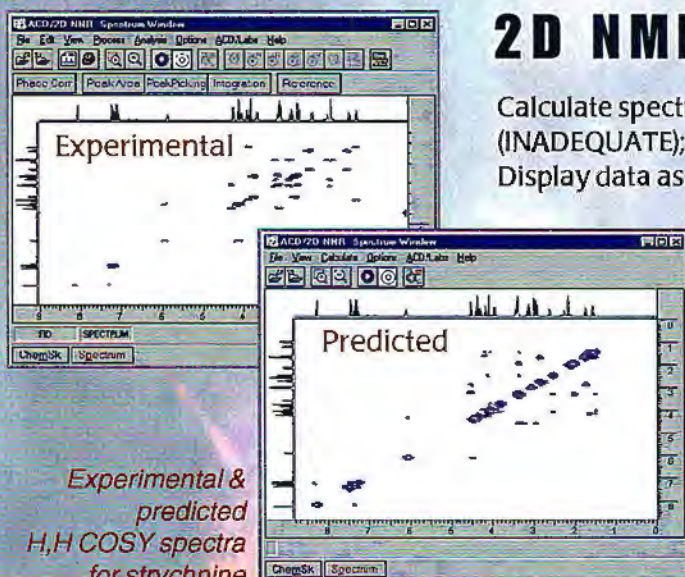
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## **The NMR Newsletter - Book Reviews**

Book Review Editor: István Pelczer, Dept. of Chemistry, Princeton University, Princeton, NJ  
08544

### **"Magnetic Resonance Imaging in Food Science**

by

**Brian Hills**

John Wiley & Sons, Inc., New York, NY 10158; 1998;  
ISBN 0-471-17087-9; 342 pages; \$89.95 (cloth)

In the preface for his book, Brian Hills describes his goals as, "This book should be of value to all food scientists and technologists who seek a better understanding of the present and future role of MRI in their discipline, and conversely, to NMR and MRI specialists who wish to explore the potential of this wonderful technique in the arena of foods." The author has achieved his objectives with this book. Brian has done a fine job of describing the type of information needed for food processing studies and how MRI can provide that information. There is a good balance of basic food processing and engineering information as well as the 'how to use MRI' for obtaining the needed data to complete engineering models.

The book consists of thirteen chapters and a seven-page index. The thirteen chapters are divided into three sections based on distance scale (macroscopic, microscopic and molecular). The definition of what is a microscopic length scale is somewhat arbitrary and Brian uses a voxel with at least one dimension less than 40  $\mu\text{m}$ . MRI studies with larger pixel dimensions are classified as macroscopic.

The initial section on macroscopic length scales begins with an introductory chapter on NMR/MRI. This chapter is written for individuals who have had a previous introduction to the basic theory of NMR. The breadth and impact potential of MRI studies is well covered in this section. The next three chapters deal with macroscopic behavior of food materials during mass transfer, phase changes, temperature measurement, quality and rheological behavior. The last four chapters in this section cover solid-imaging, process control, whole-plant functional imaging, and unconventional techniques.

The book's strength is in the final two sections where Brian has primarily done most of his research. These sections are particularly well written and insightful. The molecular origins of NMR relaxation phenomena are widely misunderstood in food science. Brian's work has greatly improved the understanding of the mechanisms controlling both transverse and longitudinal relaxation in foods. Chapters 12 and 13 should be required reading for researchers using relaxation times to correlate to a 'quality' parameter in a food or agricultural product.

*continued*

The book though is not without some minor problems. Most of the reproduced images are of a slightly lower quality than the original published versions. Several of the references are repeated, for example numbers 124 and 183 are the same. Other references have been missed, such as, the work by L.D. Hall and myself on developing MRI as a viscometer. An additional disappointment with the references is the lack of consistent use of titles. Most references have titles included, which is very useful for the reader. It would also seem more appropriate to use one of Brian's own images of a food product for the cover illustration rather than the image of water around nylon fibers.

The goal of the book is to describe how to incorporate and use MRI to study foods and food processes. The book is not intended as a comprehensive review of food science literature or MRI applications to food science. We are now in a position to use MRI to rigorously test well-developed theoretical models of transport phenomena, which are in the literature. For example, the detailed theoretical and experimental study of drying apples by Crapiste, Whitaker and Rotstein<sup>1</sup> is not mentioned in this book. In their study, they were able to validate their detailed microscopic cellular based mathematical model and by using their model one can calculate the contribution of different pathways for moisture transport (e.g. intercellular spaces, cell-to-cell, or cell wall-to-cell wall). The MRI techniques discussed in this book are precisely the experimental techniques needed to test assumptions in this mathematical model.

<sup>1</sup>Crapiste, G. H, Whitaker, S. & Rotstein, E. (1988). Drying of cellular material – I. A Mass transfer theory. Chem. Engng. Sci., **43**(11), 2919-28.

**Michael J. McCarthy**  
Food Science and Technology  
University of California  
One Shields Avenue  
Davis, CA 95616-8598

mjmccarthy@ucdavis.edu



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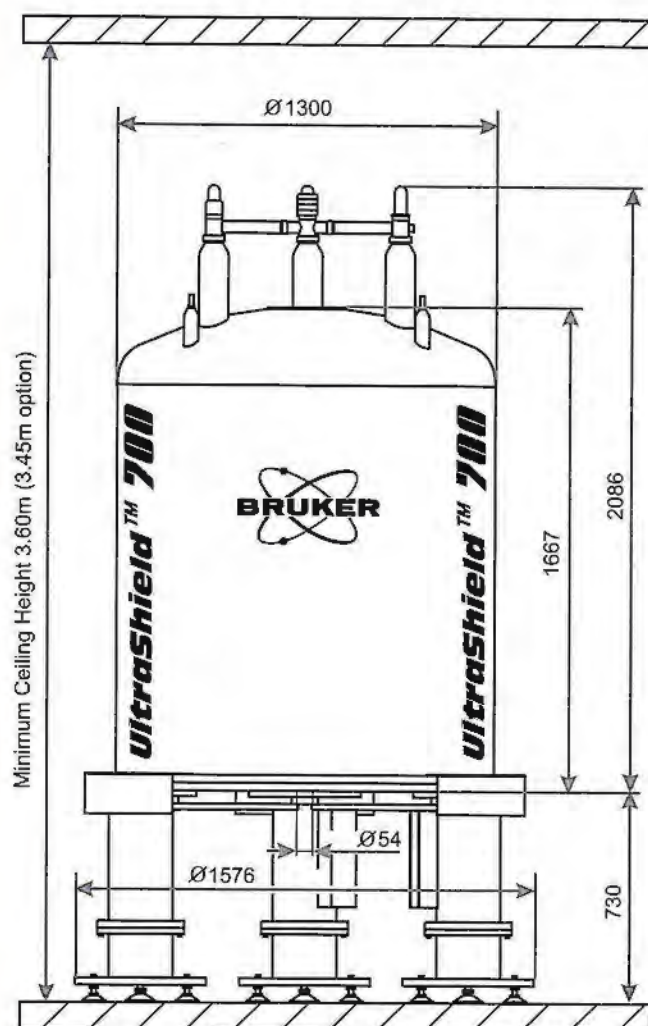
NMR Frequency ( $^1\text{H}$ )	700 MHz
Operating Field	16.45 Tesla
Field Stability (guaranteed value in persistent mode)	< 10.5 Hz/hr
Cryoshims	Z, Z <sup>2</sup> , Z <sup>3</sup> , X, Y XZ, YZ, XY, X <sup>2</sup> -Y <sup>2</sup>
Axial Range with Field Homogeneity better than 10 ppm (w/o RT Shimming)	~ 60 mm
5G Line from the Magnetic Center	
- radial distance	< 2.50 m
- axial distance	< 3.50 m
Resolution at 50% 1% CHCl <sub>3</sub> 5mm spinning	< 0.55 Hz
Lineshape	
1% CHCl <sub>3</sub> 5mm non-spinning at 0.55%	< 7 Hz *
at 0.11%	< 14 Hz *
Spinning Sidebands	< 2%

\* Typical values obtained with the BOSSII™ shim system.

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## Department of Physics

1 October 1998

Dear Dr. Shapiro:

We have been playing with the well-known  $\exp(-bt^3)$  decay of spin echoes. Normally, this arises in the case of spins diffusing through a uniform gradient of magnetic field. Recently, such  $t^3$  decays have been observed in incommensurately distorted *solids*; the interpretation has been given in terms of a diffusing modulation wave, coupling to the spin *via* quadrupole interaction.

All of this bring up the simple question: are there other circumstances in which the spin echo amplitude decays as  $\exp(-bt^3)$ ? Our answer is 'yes'. Specifically, we consider a spin subjected to a slowly *and continuously varying* random field. Provided the random field has an exponential autocorrelation (fairly standard) and one works at times  $t \ll \tau_c$  (the correlation time of the fluctuating field; this is not a standard limit), it turns out that the  $t^3$  echo amplitude decay will occur.

Now, in the old literature Klauder and P. W. Anderson<sup>1</sup> have an analytical expression for both the FID and the echo amplitude for this case. Their expression becomes  $\exp(-bt^3)$  in the limit  $t \ll \tau_c$ .

Now, does this occur in NMR (other than for spins diffusing through a gradient)? For a slowly varying interaction (recall  $t \ll \tau_c$ ) to result in substantial de-phasing, the interaction must be large. And the requirement that the field fluctuate continuously rules out the common examples wherein a given spin interacts with 4 or 8 nearest neighbor spins: when a spin  $S$  flips, there is a discontinuous change in  $S_z$ . So NMR examples will be rare.

But there may be examples in NQR, where the NQR frequency can be substantially modulated by the disorder in the solid. If whatever causes the disorder is mobile, one may find a Gaussian-distributed, continuously varying interaction.

We welcome the thoughts and remarks of the readers.

<sup>1</sup>J. R. Klauder and P. W. Anderson, Phys. Rev. 125, 912 (1962).

Sincerely,



Mark S. Conradi



Andrew F. McDowell  
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Department of Physics  
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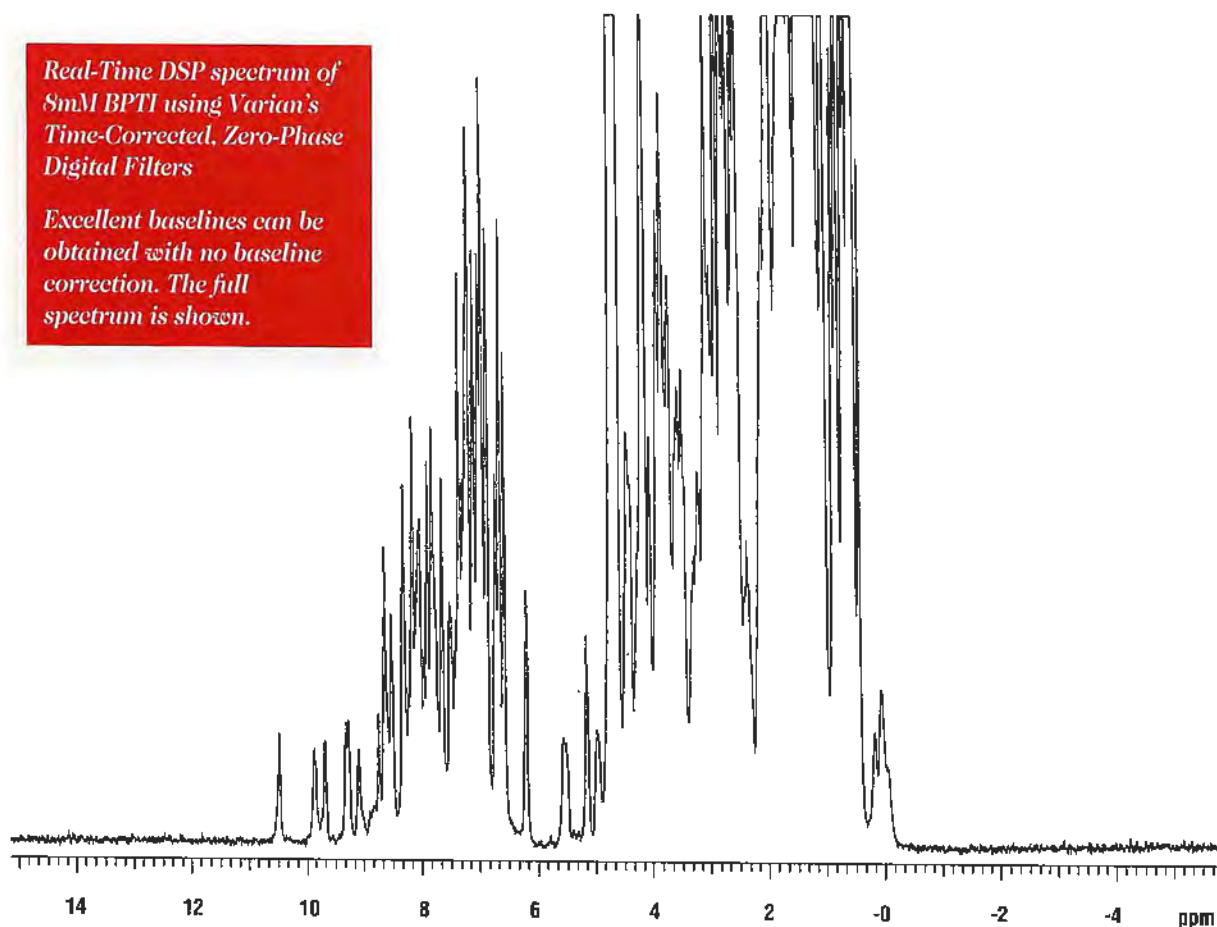
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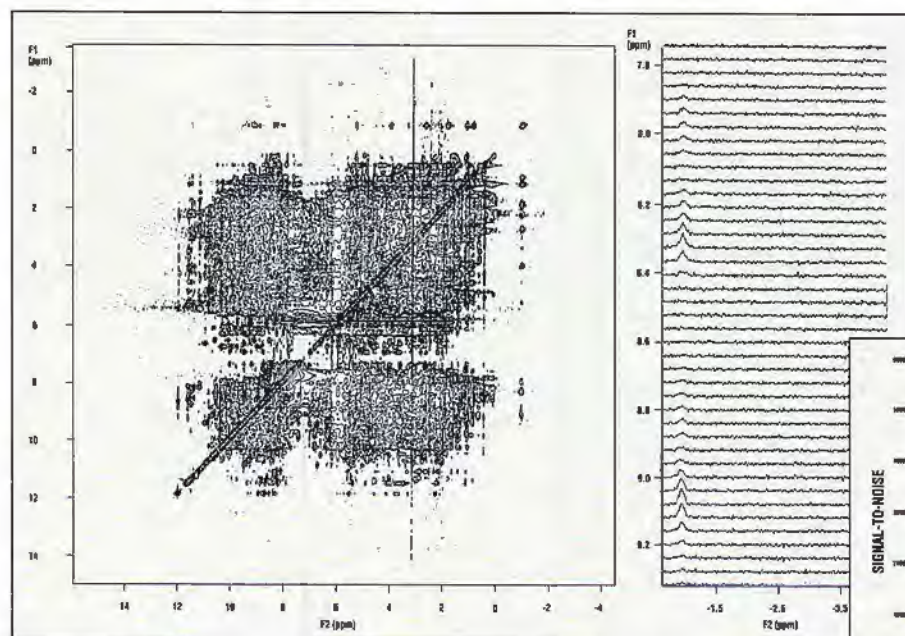
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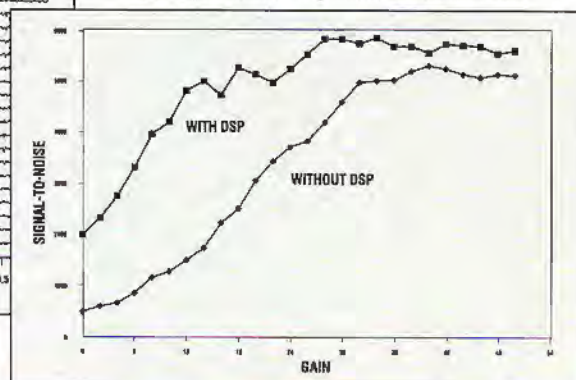


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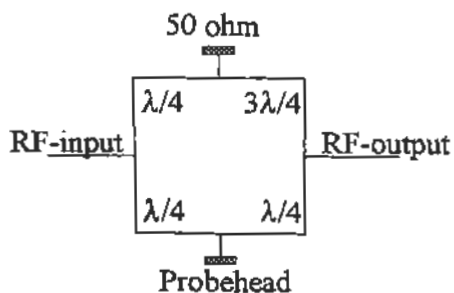
Dr. B.L. Shapiro  
The NMR Newsletter  
966 Elsinore Court  
Palo Alto, CA 94303  
U.S.A

October 5<sup>th</sup> 1998  
(received 10/21/98)

Dear Barry,

On our Varian <sup>Unity</sup>Inova 500 spectrometer we recently changed the cabling between the probe and the magnet leg. Much to our surprise we suddenly experienced changes in our pulse lengths which were quickly traced to a mistuning of our probe. In particular, the N<sup>15</sup> coil of our HCN PFG-probe seemed to be affected, since during execution of the pulse sequence the amplifier shut down. This was the result of too much reflected power from the probe. Upon checking the tuning using a wobbler, it was clear that the probe was seriously mismatched, in spite of the fact that we had tuned and matched it using the tune bridge in the magnet leg, and minimized the reading.

Measurement of the "directional coupler" (Mini Circuits ZFSC-2-2, a splitter combiner used in the tune circuit) showed a directivity of only 20.7 dB at 50.6 MHz, clearly insufficient. The values for <sup>13</sup>C and <sup>1</sup>H were not much better (27.5 and 24.9 dB, respectively). As a result, "tuning to zero" on the display does not yield an optimum tune and match. Moreover, the tune and match become strongly dependent upon the electrical length of the circuit. Hence, our sudden change in behavior when changing the cables. This effect becomes even worse if the standard N<sup>15</sup> filter is used (VSWR = 1.25). Fortunately, there is a simple solution. Using a minimal amount of hardware, we constructed a device, based upon hybrid ring coupling that provides a directivity of >45dB (fig. 1). The major components



are four pieces of coaxial cable (RG174) with the given electrical lengths. When the probe impedance matches the 50 ohm reference, the "upper" and "lower" RF cancels exactly on the RF-output connector. This device can be used in the normal tune-up setup of our console, i.e. we simply use the console RF and detection circuit. Tune and match now proved to be indistinguishable from the result obtained using a wobbler. The only drawback is the fact that the box is selective for a specific frequency and therefore has to be constructed for every nucleus of interest.

Fig.1: dedicated N<sup>15</sup> tunebox.

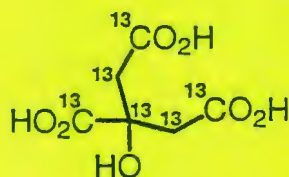
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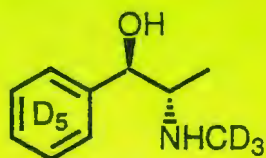
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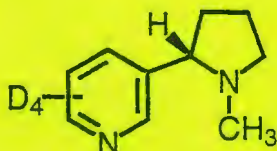




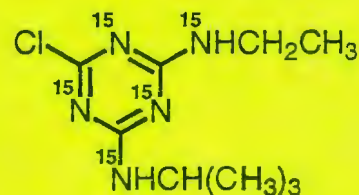
Citric Acid- $^{13}\text{C}_6$



(1R, 2S)-(-)-Ephedrin- $\text{d}_8$



S-(-)-Nicotine-2,4,5,6- $\text{d}_4$



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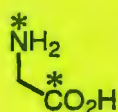
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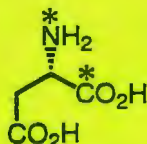
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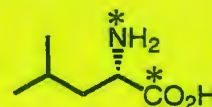
**Glycine-1-<sup>13</sup>C, <sup>15</sup>N**

>99 atom % <sup>13</sup>C  
>99 atom % <sup>15</sup>N



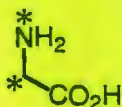
**L-Aspartic Acid-1-<sup>13</sup>C, <sup>15</sup>N**

>99 atom % <sup>13</sup>C  
>99 atom % <sup>15</sup>N



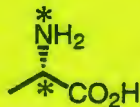
**L-Leucine-1-<sup>13</sup>C, <sup>15</sup>N**

>99 atom % <sup>13</sup>C  
>99 atom % <sup>15</sup>N



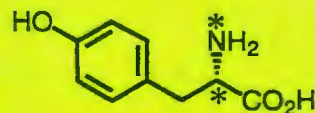
**Glycine-2-<sup>13</sup>C, <sup>15</sup>N**

>99 atom % <sup>13</sup>C  
>99 atom % <sup>15</sup>N



**L-Alanine-2-<sup>13</sup>C, <sup>15</sup>N**

>99 atom % <sup>13</sup>C  
>99 atom % <sup>15</sup>N



**L-4-Hydroxyphenylalanine-2-<sup>13</sup>C, <sup>15</sup>N**

>99 atom % <sup>13</sup>C  
>99 atom % <sup>15</sup>N

*The above Amino Acids are a representative sample of double labelled compounds currently available from Isotec. Our chemists regularly synthesize a variety of Carbon-13, Nitrogen-15 double-labelled compounds as well as many other isotopically labelled compounds.*

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F.H.Koehler@lrz.tu-muenchen.de

October 21, 1998  
(received 10/26/98)

### $^{59}\text{Co}$ , $^{13}\text{C}$ Dipolar Coupling

Dear Dr. Shapiro,

some time ago we needed the solid-state  $^{13}\text{C}$  NMR spectrum of a cationic sandwich compound just for referencing purposes. Decamethylcobaltocenium hexafluorophosphate,  $(\text{C}_5\text{Me}_5)_2\text{Co}^+\text{PF}_6^-$ , seemed to be the compound of choice because of its high symmetry. However, the result was only simple for the methyl groups (signal B in the figure), while the five-membered ring carbons gave a feature near 95 ppm (cf. A in the figure) that contained more information than we were looking for.



The crystal structure revealed that we did not have magnetically different cations in the unit cell, and a spectrum at higher field confirmed that the apparent signal splitting was due to the dipolar interaction of the  $I = 7/2$  and 100%-abundant nucleus  $^{59}\text{Co}$  and  $^{13}\text{C}$ .

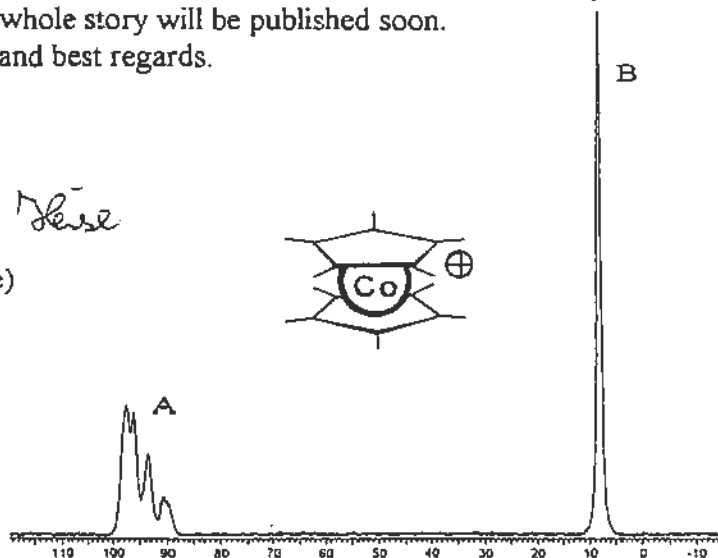
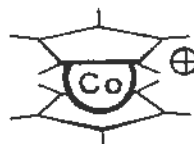
There are now many papers which illustrate the effect of quadrupolar nuclei on the spectrum of  $I = 1/2$  nuclei, and the topic has been reviewed (Harris, R. K.; Olivieri, A. C. *Progr. NMR Spectrosc.* 1992, 24, 435). But we are not aware of a clear-cut example of the pair  $^{59}\text{Co}$ ,  $^{13}\text{C}$ .

From perturbation theory you would expect eight transitions. However, the analysis of part A of the spectrum by drawing corresponding stick patterns was not successful, because some of the experimentally found transitions virtually merge and the intensities of the pattern components are strange. Meanwhile Eric Brouwer of Robin Harris' lab at Durham has performed a more sophisticated simulation, and the whole story will be published soon.

Thank you for the pink reminder and best regards.

Sincerely yours,

   
(Frank H. Köhler) (Henrike Heise)





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5 mm	535-PP-7	500	7 in	0.015"	0.0005"	0.00025"	15.15	+100	12.85
5 mm	535-PP-8	500	8 in	0.015"	0.0005"	0.00025"	16.65	+100	14.15
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5 mm	507-PP-8	360	8 in	0.015"	0.0020"	0.0010"	7.75	+100	6.60
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Dr. B.L. Shapiro  
*The NMR Newsletter*  
966 Elsinore Court  
Palo Alto, CA 94303

October 19, 1998  
(received 10/24/98)

Dear Barry,

### Pulsed NMR Sample Tubes

Absolute pulsed NMR experiments (i.e., signal intensity  $\propto$  sample weight) require clean introduction of the sample into the active volume of the probe. This is a simple operation for normal solutions in the large diameter (18mm) absolute probe on the Bruker NMS 120 spectrometer. However, many of our samples have high viscosities (100's of centipoises) and cannot be transferred with Pasteur pipettes. Moreover, the small diameter 10mm probe must be used for variable temperature experiments (including room temperature) or when short deadtimes are required.

Frank Bosco from New Era has worked with our laboratory to design a specialty tube for pulsed NMR experiments on viscous samples (figure 1). The tube incorporates two key design features.

The body was shortened to allow introduction of the sample into the bottom of the tube using standard length syringe needles. This is essential for absolute NMR experiments in a 10mm VT probe that has a small active coil volume (~10mm height). The neck of the tube was made from standard wall tubing with a precision i.d. Because the wall thickness is substantial, tube breakage is avoided when inserting the fluted plug. The precision bore ensures a secure seal to preserve sample integrity over an extended period of time. The plug was made in our machine shop from 10mm o.d. PTFE round stock that matched the standard tube diameter to provide smooth insertion and removal over the microswitch that the instrument uses to trigger the acquisition.

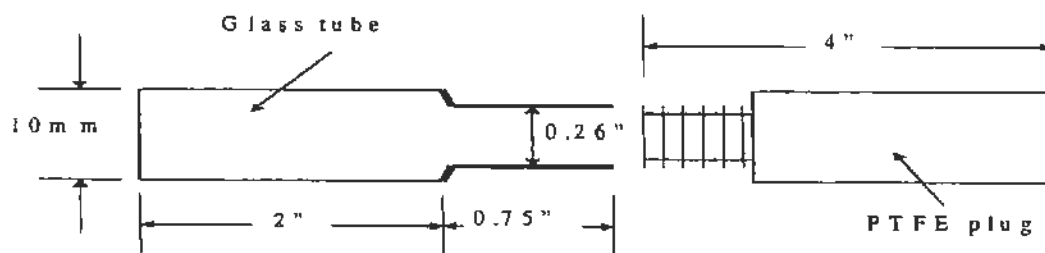


Figure 1

*Mark*

Mark Sullivan  
Msullivan@herc.com

PS: Please credit this contribution to Tom Neiss' subscription.

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  - Principles of NMR and dynamics
- Protein dynamics and reactions • The energy landscape of proteins

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  - Simulating protein and nucleic acid molecular dynamics
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**Contact:** Dr. Tim Saarinen, Ph.D., x 209





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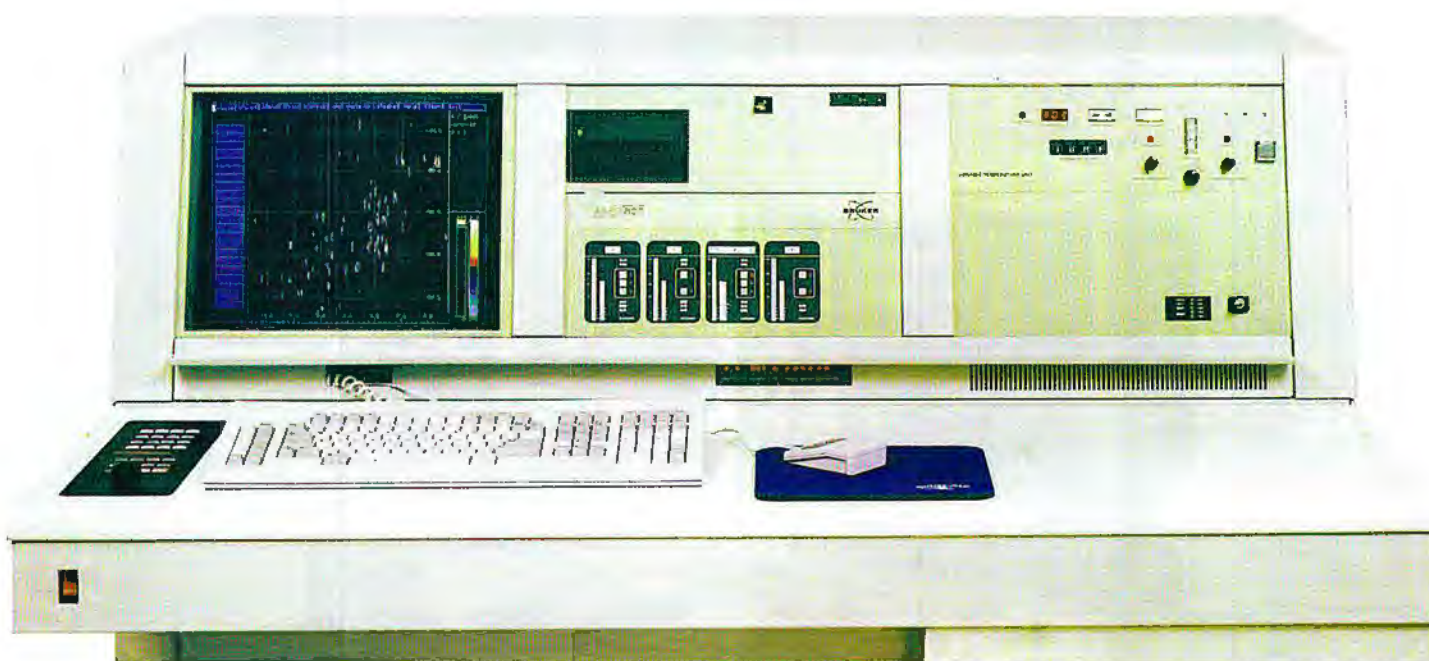




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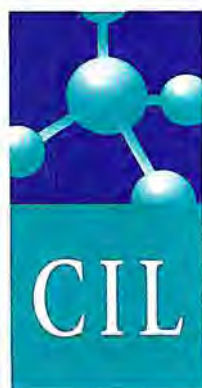
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CNLM-4358	L-Methionine-N-FMOC ( $\text{U-}^{13}\text{C}_5$ , 98%+; $^{15}\text{N}$ , 96-99%)	Request Price
CNLM-4362	L-Phenylalanine-N-FMOC ( $\text{U-}^{13}\text{C}_9$ , 98%+; $^{15}\text{N}$ , 96-99%)	0.1 g \$450 0.25 g \$900
CNLM-4347	L-Proline-N-FMOC ( $\text{U-}^{13}\text{C}_5$ , 98%+; $^{15}\text{N}$ , 96-99%)	0.1 g \$450 0.25 g \$900
CNLM-4349	L-Tyrosine-N-FMOC, O-t-Butyl Ether ( $\text{U-}^{13}\text{C}_9$ , 98%+; $^{15}\text{N}$ , 96-99%)	0.1 g \$990 0.25 g \$1900
CNLM-4348	L-Valine-N-FMOC ( $\text{U-}^{13}\text{C}_5$ , 98%+; $^{15}\text{N}$ , 96-99%)	0.1 g \$450 0.25 g \$800

### MODIFIED NUCLEICS

DLM-4391	5,6-Dihydrothymine (5, 6, 6- $\text{D}_3$ , methyl- $\text{D}_3$ , 95%+)	50 mg \$780
CNLM-4392	5-Hydroxycytosine ( $2\text{-}^{13}\text{C}$ , 99%; $1,3\text{-}^{15}\text{N}_2$ , 98%)	25 mg \$950 50 mg \$1575
CNLM-4393	5-Hydroxyuracil ( $^{13}\text{C}_4$ , 99%; $^{15}\text{N}_2$ , 98%)	5 mg \$895 10 mg \$1495

### ADDITIONAL PRODUCTS

ULM-4482	6-Fluoro-L-Tryptophan (unlabeled)	Request Price
DLM-4481	6-Fluoro-L-Tryptophan (ring- $\text{D}_4$ , 96-98%)	Request Price



## Cambridge Isotope Laboratories, Inc.

50 Frontage Road, Andover, MA 01810-5413 USA  
 PH: 800.322.1174 PH: 978.749.8000  
 FAX: 978.749.2768 E-MAIL: [cilsales@isotope.com](mailto:cilsales@isotope.com)  
 URL: <http://www.isotope.com>



## Postdoctoral Positions at Argonne

I will have two openings at the postdoctoral level in my laboratory in the Chemistry Division beginning October 1, 1998. The positions will involve research in NMR. Specific projects include developing new solid-state methods for chemical-shift MRI of materials, PFG spin-diffusion of gaseous probes in porous systems, MRI of solvent ingress into heterogeneous polymeric materials, and dipolar recoupling measurements to study self-associating peptides.

The successful candidate should have a recent Ph.D. (within three years) in Chemistry, or closely related field, with some experience in hardware and software development, and with experience in solid-state NMR or MRI and their application to structure elucidation.

The Chemistry Division has state-of-the-art NMR facilities, including two new fully equipped Bruker DMX 500 and Bruker DSX-200/100 systems with a full complement of solids, liquids and imaging capabilities, a home-built Tecmag 400 imaging/spectroscopy system, a GE Omega 300, and Varian INOVA 300 spectrometer, and several IBM R-6000 and Silicon Graphics workstations for advanced data processing, calculation and data refinement.

For further information contact:

Robert E. Botto  
Chemistry Division  
Argonne National Laboratory  
9700 S. Cass Ave.  
Argonne, IL 60439  
Ph: (708)252-3524 FAX: (708)252-9288  
e-mail: robert\_botto@qmgate.anl.gov



Sandia  
National  
Laboratories

### POSTDOCTORAL POSITION – NMR SPECTROSCOPY

Sandia National Laboratories (SNL), operated by Lockheed Martin for the Department of Energy, located in Albuquerque, NM has an immediate opening for a postdoctoral position in solid state NMR spectroscopy. The position will involve NMR investigations and characterization of a variety of materials including glasses, ceramics, polymers and hybrid materials. A major portion of the research will include the implementation of heteronuclear and multinuclear solid state NMR experiments to probe the chemistry and medium range structural order in oxide glasses, but a variety of other materials collaborations are possible. A Ph.D. in chemistry, physics, material chemistry or related field is required. Demonstrated competence in advanced solid state NMR techniques, computational methods and material preparation are preferred. The research will be carried out in close collaboration with SNL research staff members, but the applicant is expected to have demonstrated the ability to perform independent research, along with excellent communication skills. This position will be for one year, and is renewable for up to three years. *The program is open to all qualified U.S. citizens without regard to race, color, age, religion, sex, or national origin.* Interested candidates should send a resume and the names of three references to: **Dr. Todd M. Alam (talam@sandia.gov), Sandia National Laboratories, MS 1407, Org. 1811, Albuquerque, NM 87185-1407.**

## **Another Blast from the Past**

**A quotation from the baroque era of NMR - note the date!**

### **"Nuclear and Electron Spin Magnetic Resonance"**

**by**

**John E. Wertz**

**(Chem. Rev. 55, 829-953 (1955))**

#### **III. CHEMICAL SHIELDING**

**"At a time when physicists were busy comparing magnetogyric ratios of various nuclei and expressing these to seven or more significant figures, several disquieting papers appeared (147, 312, 443). It was reported that in compounds of phosphorus, nitrogen, and fluorine the resonant frequency for a particular nucleus depended on the compound in which it was present. This effect was called the "chemical shift," because physicists could think of no stronger term of damnation for an effect which was making insignificant several digits in their nuclear moment data."**



**Address all Newsletter  
correspondence to:**

Dr. B. L. Shapiro  
The NMR Newsletter  
966 Elsinore Court  
Palo Alto, CA 94303.  
650-493-5971\* - Please call  
only between 8:00 am and  
10:00 pm, Pacific Coast time.

**Deadline Dates**

No. 483 (Dec.) 27 Nov. 1998  
No. 484 (Jan.) 24 Dec. 1998  
No. 485 (Feb.) 22 Jan. 1999  
No. 486 (Mar.) 19 Feb. 1999  
No. 487 (Apr.) 23 May 1999

\* Fax: 650-493-1348, at any hour. Do not use fax for technical contributions to the Newsletter, for the received fax quality is very inadequate.

\* E-mail: shapiro@nmrnewsletter.com



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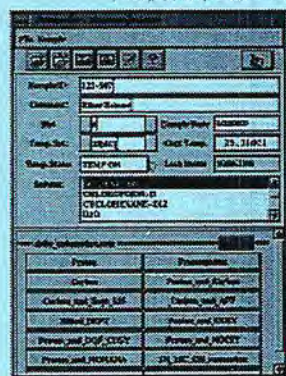
**Forthcoming NMR Meetings**, continued from page 1:

International School of Structural Biology and Magnetic Resonance, 4th Course: Dynamics, Structure and Function of Biological Macromolecules; Erice, Sicily, Italy; **May 25-June 5, 1999**; Contact: Ms. Robin Holbrook, Stanford Magnetic Resonance Laboratory, Stanford University, Stanford, CA 94305-5055; (415) 723-6270; Fax: (415) 723-2253; Email: reh@stanford.edu. See Newsletter 482, 28.

Additional listings of meetings, etc., are invited.



# How To Run JEOL's Eclipse<sup>+</sup> Spectrometer



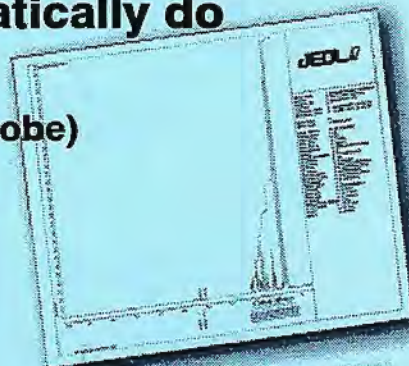
**Step 1: Enter your sample name and the solvent.**

**Step 2: Click the mouse button on the data you want.**

**Step 3: Walk away with your data.**

**JEOL's Eclipse Spectrometer will automatically do everything else for you.**

- ✓ Auto Probe Tuning (with AutoTune Broad Band Probe)
- ✓ Auto-sample Control (with AutoSample Changer)
- ✓ Auto Selection of Spectrometer Conditions
- ✓ Auto Baseline Correction
- ✓ Auto Data Presentation
- ✓ Auto Phase Correction
- ✓ Auto Digital Filtering
- ✓ Auto S/N Monitoring
- ✓ Auto Queue Control
- ✓ Auto Receiver Gain
- ✓ Auto Data Storage
- ✓ Auto Referencing
- ✓ Auto Processing
- ✓ Auto Peak Picks
- ✓ Auto Integration
- ✓ Auto Plotting
- ✓ Auto Shim
- ✓ Auto Lock



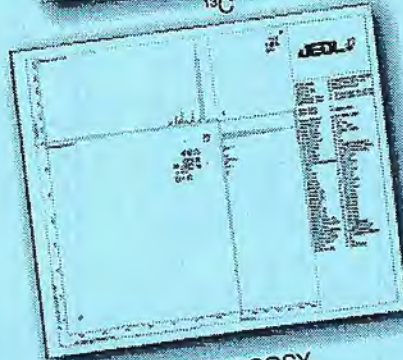
<sup>1</sup>H



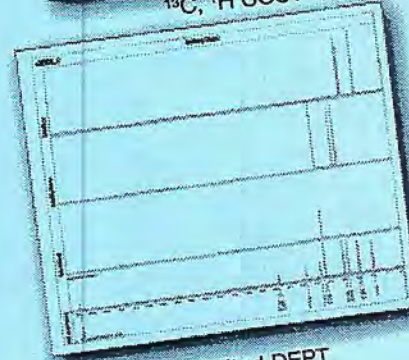
<sup>13</sup>C



<sup>13</sup>C, <sup>1</sup>H COSY



<sup>1</sup>H, <sup>1</sup>H COSY



Edited DEPT

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