

**THE**  
**NMR**  
**NEWSLETTER**

**No. 440**  
**May 1995**

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TABLE 1 DEUTERATED SOLVENTS

| Cat. No. | Description  | Formula                           | Min. Iso.<br>(°C) | Density<br>(g/ml) | MP<br>(°C) | BP<br>(°C) | $n_D^{20} \times 10^6$ @ (°C) |
|----------|--|-----------------------------------|-------------------|-------------------|------------|------------|-------------------------------|
| D-11     | Acetone-d <sub>6</sub>   | CD <sub>3</sub> COCD <sub>3</sub> | 99.8%             | 1.17              | 17         | 58         | 0.551 (32)                    |
| D-120    | Acetone-d <sub>6</sub> + 1% TMS  | CD <sub>3</sub> COCD <sub>3</sub> | 99.8%             | 1.17              | 17         | 58         | 0.551 (32)                    |
| D-13     | Acetone-d <sub>6</sub>   | CD <sub>3</sub> COCD <sub>3</sub> | 99.8%             | 0.81              | 54         | 77         | 0.460 (20)                    |
| D-121    | Acetone-d <sub>6</sub> + 1% TMS  | CD <sub>3</sub> COCD <sub>3</sub> | 99.8%             |                   |            |            |                               |
| D-129    | <b>Cost-conscious quality NMR solvents offered by Wilmad, such as CDCl<sub>3</sub>, are frequently priced lower than more traditional sources. Included in this offering are the most common solvents, like Acetone-d<sub>6</sub>, Benzene-d<sub>6</sub>, D<sub>2</sub>O, and DMSO-d<sub>6</sub>, as well as some of the most unusual solvents for specialty applications, like 1,1,2,2-Tetrachloroethane-d<sub>2</sub>, Octane-d<sub>8</sub>, and Trifluoroacetic Acid-d.</b> |                                   |                   |                   |            |            |                               |
| D-14     | Chloroform-d   | CDCl <sub>3</sub>                 | 99.8%             | 1.50              | -64        | 62         | 0.543 (20)                    |
| D-21     | Chloroform-d   | CDCl <sub>3</sub>                 | 99.8%             | 1.50              | -64        | 62         | 0.511                         |
| D-122    | Chloroform-d   | CDCl <sub>3</sub>                 | 99.8%             | 1.50              | -64        | 62         | 0.511                         |
| D-130    | Chloroform-d   | CDCl <sub>3</sub>                 | 99.8%             | 1.50              | -64        | 62         | 0.511                         |
| D-28     | Chloroform-d   | CDCl <sub>3</sub>                 | 99.8%             | 1.50              | -64        | 62         | 0.740 (20)                    |
| D-31     | Chloroform-d + 1% TMS  | CDCl <sub>3</sub>                 | 99.8%             | 1.50              | -64        | 62         | 0.740 (20)                    |

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| WCV-XL (S-XL)  | 11" X 26"     | HA-100, HA-100A, HA-100D | Gridded-Two Color |
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**FORTHCOMING NMR MEETINGS**

- International School of Biological Magnetic Resonance, 2nd Course: Dynamics and the Problem of Recognition in Biological Macromolecules, Erice, Trapani, Sicily, Italy, **May 19 - 30, 1995** (*Note the new dates.*); Contact: Prof. O. Jardetzky, Stanford Magnetic Resonance Laboratory, Stanford University, Stanford, CA 94305-5055; Phone: (415) 723-6270; Fax: (415) 723-2253; or, Prof. J.-L. Lefèvre, ESBS, CNRS-UPR9003, Univ. Louis Pasteur, Blvd. Sébastien Brant, F67400 Illkirch Graffenstaden, France; Phone: (+33) 88-655269; Fax: (+33) 88-655343; See Newsletter 438, 54.
- Summer School on "Isotope Effects as Tools in Basic and Environmental Research", Roskilde, Denmark, **June 24 - 28 1995**; Contact: Prof. P. E. Hansen, Fax +45 4675-7721, or Phone +45 4675 7781-2432 or +45 4675-7711, ext. 2432; . See Newsletter 438, 39.
- Workshop on "Structure Determination from NMR", Pittsburgh Supercomputing Center, Pittsburgh, PA, **June 25 - 28 1995**; Contact: N. C. Blankenstein: blankens@psc.edu or (412) 268-4960. See Newsletter 438, 29.
- 12th International Meeting on NMR Spectroscopy, Sponsored by the Royal Society of Chemistry, Manchester, England, **July 2 - 7, 1995**; Contact: Dr. J. F. Gibson or Ms. G. B. Howlett - See Newsletter 415, 5; Phone: (44-71) 437-8656; Fax: (44-71) 437-8883.
- ISMAR 1995, Sydney, NSW, Australia, **July 16-21, 1995**; Contact: Dr. W. A. Bubb, Dept. of Biochem., Univ. of Sydney, Sydney, NSW 2006, Australia. Phone: +61-2-351-4120; Fax: +61-2-351-4726; Email: ismar95@biochem.su.oz.au. See Newsletter 437, 20.
- NMR Symposium at the 37th Rocky Mountain Conference on Analytical Chemistry, Denver Colorado, **July 24-27, 1995**; Contact: Dr. Alexander J. Vega, DuPont Central Research and Development, P.O. Box 80356, Wilmington, DE 19880-0356; Tel. (302) 695-2404; Fax: (302) 695-1664; e-mail: vega@esvax.dnet.dupont.com. See Newsletter 432, 34.
- 3rd Scientific Meeting, Society of Magnetic Resonance, and 12th Meeting European Society for Magnetic Resonance in Medicine and Biology, Nice, France, **August 19 - 25, 1995**; Contact: Society of Magnetic Resonance, 2118 Milvia St., Suite 201, Berkeley, CA 94704; Tel. (510) 841-1899; Fax: (510) 841-2340.
- Western Biotech Conference, San Diego, CA, October 18 - 21, 1995; Contact: Western Biotech Conf. Registr'n., c/o Tom Lobl, Tanabe Research, 4540 Towne Centre Court, San Diego, CA 92121; Tel. (619) 622-7035; Fax: (619) 622-7080; E-mail: tlobl@cerf.net.
- 37th ENC (Experimental NMR Conference), Asilomar Conference Center, Pacific Grove, California, **March 17 - 22, 1996/sic**; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87501; (505) 989-4735; Fax: (505) 989-1073.
- 38th ENC (Experimental NMR Conference), Orlando, FL, **March 23 - 27, 1997/sic**; Contact: ENC, 1201 Don Diego Avenue, Santa Fe, NM 87501; (505) 989-4735; Fax: (505) 989-1073.

Additional listings of meetings, etc., are invited.



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April 11, 1995  
(received 4/17/95)

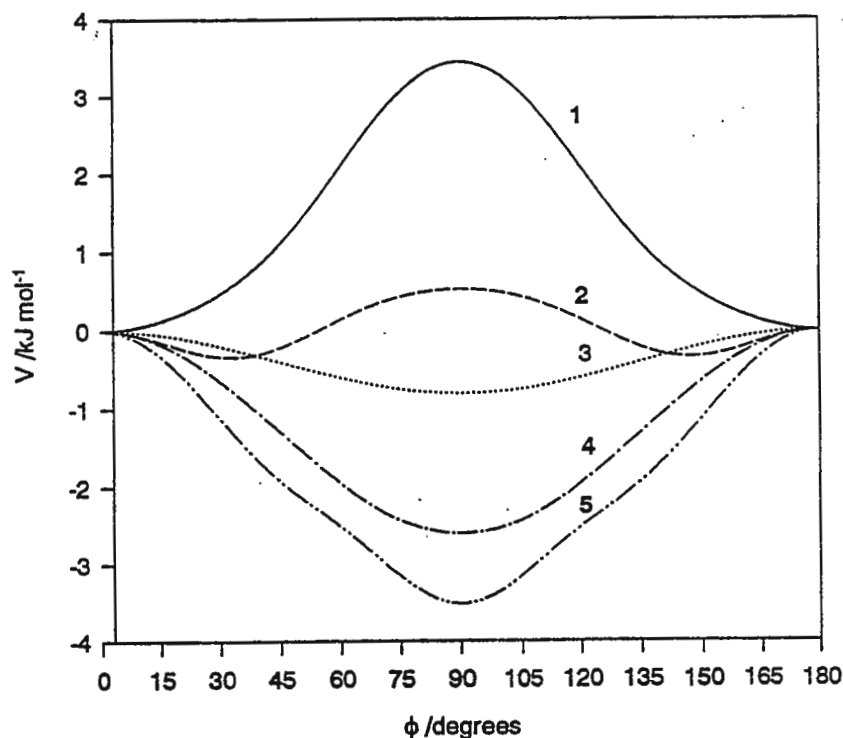
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Dear Barry,

Can one directly derive small ( $\sim kT$ ) internal rotational potentials for a molecule in solution from long-range coupling constants? The answer is yes. Using benzyl fluoride,  $C_6H_5CH_2F$ , as an example, measure all  $^2J(H,F)$ ,  $^3J(H,H)$  and  $^3J(C,F)$  with high precision (shim until you get linewidths of ca 0.03 Hz). Establish the  $\phi$  dependence ( $\phi=0$  corresponds to the C—F bond in the aromatic plane) of as many  $^nJ$  ( $n \neq 0$ , !) as you can: the potential is solvent dependent. Compute, at as high a level of the MO model as you can afford,  $V(\phi)$  for the free molecule:  $\phi$  is always zero at the minimum, as it turns out. Use a quantum/continuum method (in this case, Rinaldi and Pappalardo, SCRF PAC, QCPE 622) to compute the solvent dependence of  $V(\phi)$ .



The figure (drawn by Scott Kroeker) conflates theory and experiment. Curve 1 gives the theory for the free molecule, curve 2 (theory for  $CS_2$  solution), curve 5 (theory for acetone- $d_6$ ), curve 3 (experiment for  $CS_2$ ) and curve 4 (experiment for acetone- $d_6$ ). You can change the phase of the potential by means of solvents, it's clear. You can also do that by means of substituents, as Rob Schurko (who is now learning solid state nmr in Rod Wasylshen's group) showed in his M.Sc. thesis. Conclusion: each benzyl fluoride derivative has a unique internal rotational potential in a given solvent. The details will be available in Can. J. Chem. in a few months. They include some post-Hartree-Fock structures which may be useful to molecular spectroscopists who are willing to tackle the molecule in the gas phase - the magnitude of the potential seems about right for them.

With best wishes,

Ted Schaefer

/ca





# DIGITAL QUADRATURE DETECTION



## *THE NEXT STEP IN DIGITAL NMR*

Over the years, NMR research and development has been focused on the elimination of artifacts in 1D, 2D and 3D NMR. Today typical artifacts can be eliminated by phase cycling and other averaging techniques. However these methods increase the experiment time.

Now, Bruker introduces a breakthrough technology for the *AVANCE* series, called **Digital Quadrature Detection (DQD™)**. With DQD™, the technological leadership position of the *AVANCE* series is extended even further by providing virtually artifact free spectra. DQD™ offers the elegant elimination of low-frequency artifacts, such as DC offset and drifts, flicker noise, 50/60 Hz interference and quadrature imperfections inherent in all traditional NMR receivers. It obtains these benefits without the need for time-consuming phase-cycling and without loss in signal.

Figure 1 shows a single-scan of the dynamic range sample of water, methanol, acetonitrile and t-butanol with a proton ratio of 10,000:100:10:1 acquired with a "traditional" receiver. Noticeable are water and methanol *quad images* at <0.1%, as well as "0 Hz spike" (from slight DC offset) with associated *flicker noise* (inherent in all semiconductor devices). Figure 2 shows the complete elimination of these artifacts using a single-scan DQD™ acquisition on the *AVANCE*.

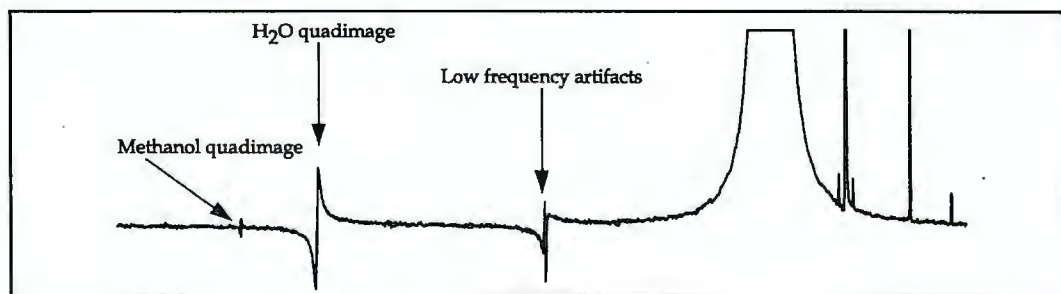


Figure 1: Artifacts from "traditional" receiver.

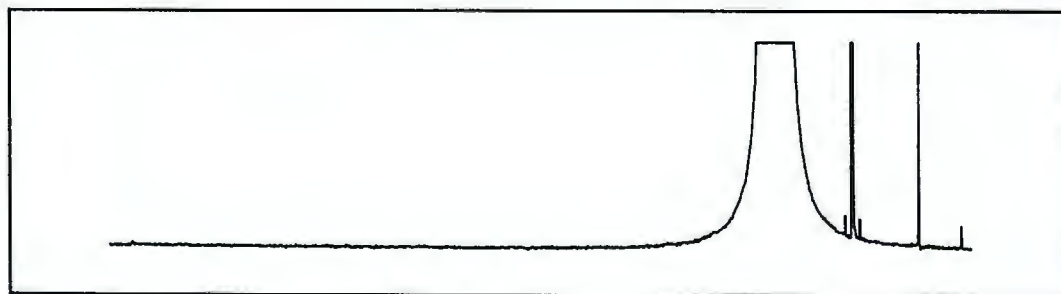


Figure 2: Artifact free spectrum with DQD™.



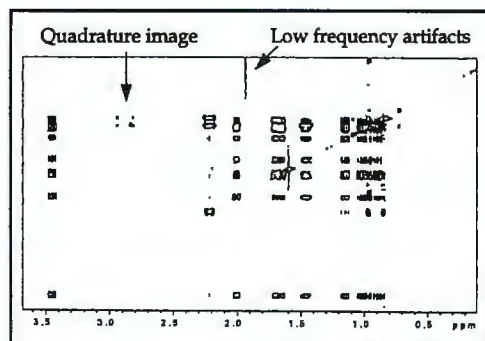
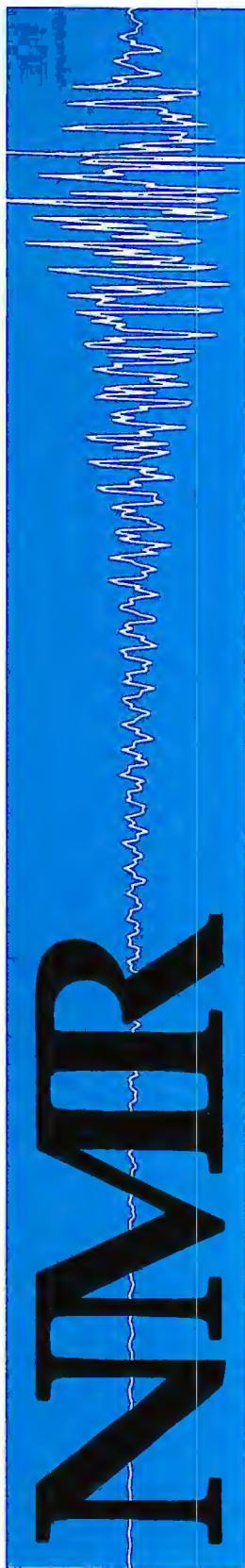


Figure 3: One-scan/ $t_1$  increment. 15 minutes

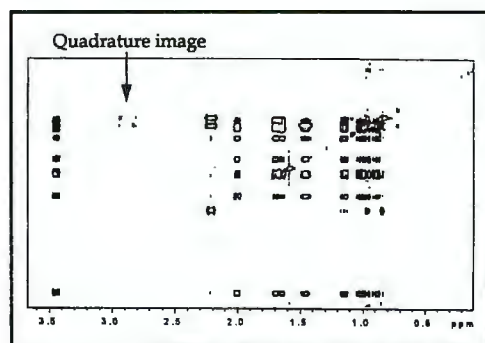


Figure 4: Two-scan/ $t_1$  increment. 30 minutes

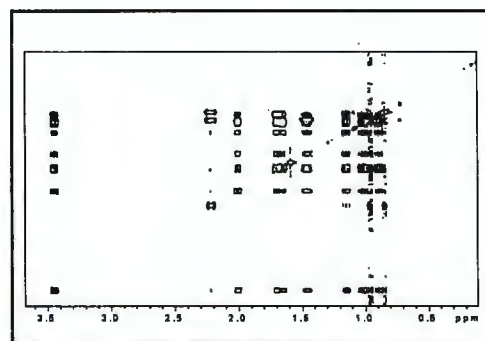


Figure 5: 4-scan CYCLOPS. 60 minutes

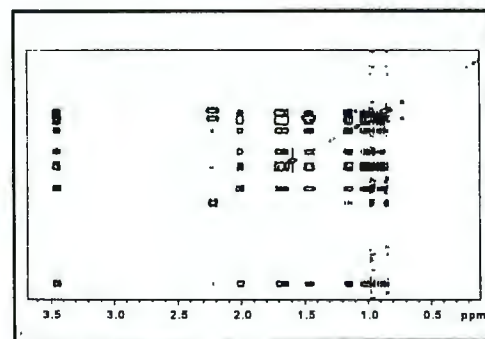


Figure 6: **DQD™** one-scan acquisition.  
One-scan/ $t_1$  increment. 15 minutes

The advantages that **DQD™** provide are best realized in 2D NMR experiments. Figures 3, 4 and 5 show TOCSY spectra of menthol acquired with traditional receiver technology. The data in Figure 3 uses one-scan per increment leading to quad images and low frequency artifacts. As the number of scan per increment are increased to 4 for CYCLOPS, these artifacts are eliminated eventually resulting in an artifact free spectrum as shown in Figure 5.

**DQD™** can achieve the same level of artifact free results using a single-scan per increment (Figure 6), reducing the total acquisition time by 75% when compared to the standard CYCLOPS phase cycling routine.

## THE NEXT STEP IN DIGITAL NMR

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PROF. RAY DUPREE

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(received 4/5/95)

30th March 1995

## Polyenoic Acids - Healthy Fare for the NMR Analyst

Dear Barry,

I wrote some months ago about how we could reliably calculate the  $^{13}\text{C}$  NMR shift separations for monoene and monoyne long-chain acids, alcohols and esters. Our theory will appear soon in *J. Chem. Soc. Perkin Trans. 2*. It uses  $\sigma$ -inductive interactions passing down the polymethylene chain, rather than dipole fields acting through space, and we give it some theoretical backing. The analytical implications are obvious.

We have now applied the same theory to non-conjugated polyenoic esters. We only need *one* additional parameter, essentially the inductive effect of one double bond on another, to explain all the shift differences we have been able to trace in the literature. Even better fits are found when simple allowances are made for carbons near the ends of chains, and for the way that  $-\text{CH}=\text{CH}-$  attenuates the relay of charge by rather less than  $-\text{CH}_2-\text{CH}_2-$ . The Table below lists some results. The inductive effect of the double bond arises mainly from the polarity of its nearer  $sp^3-sp^2$  bond, and is much bigger than one could have in any through-space theory.

**CH=CH shift differences in *cis* polyenoic acids and esters. Calculated values are in brackets.**

| 18:2( <i>n,m</i> )                         | ( <i>n</i> +1)- <i>n</i> | ( <i>m</i> +1)- <i>m</i> | 18:2( <i>n,m</i> )       | ( <i>n</i> +1)- <i>n</i> | ( <i>m</i> +1)- <i>m</i> |
|--|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| <i>n</i> =5, <i>m</i> =12                  | 3.00 (2.18)              | 0.21 (0.27)              | <i>n</i> =2, <i>m</i> =6 |                          | 3.0 (2.97)               |
| 6,12                                       | 1.28 (0.98)              | 0.37 (0.43)              | 3,7                      | 11.7 (11.3)              | 2.2 (2.19)               |
| 7,12                                       | 0.21 (0.11)              | 0.76 (0.71)              | 4,8                      | 3.1 (3.07)               | 1.7 (1.74)               |
| 8,12                                       | -0.64 (-0.72)            | 1.22 (1.21)              | 5,9                      | 1.65 (1.24)              | 1.6 (1.48)               |
| 9,12                                       | -1.77 (-1.79)            | 2.12 (2.10)              | 6,10                     | 0.2 (0.20)               | 1.4 (1.34)               |
| 6,9  | -0.55 (-0.68)            | 2.52 (2.37)              | 7,11                     | -0.45 (-0.39)            | 1.35 (1.26)              |
| 6,10                                       | 0.41 (0.20)              | 1.43 (1.34)              | 8,12                     | -0.75 (-0.72)            | 1.25 (1.21)              |
| 6,11                                       | 0.94 (0.70)              | 0.79 (0.76)              | 9,13                     | -0.95 (-0.91)            | 1.15 (1.19)              |
| 7,13                                       | 0.54 (0.40)              | 0.37 (0.40)              | 10,14                    | -1.05 (-1.01)            | 0.75 (0.84)              |
| 11,14                                      | -2.06 (-1.96)            | 2.06 (1.73)              |                          |                          |                          |
| A:3( <i>n,m,o</i> )                        | ( <i>n</i> +1)- <i>n</i> | ( <i>m</i> +1)- <i>m</i> | ( <i>o</i> +1)- <i>o</i> |                          |                          |
| 18: <i>n</i> =6, <i>m</i> =9, <i>o</i> =12 | -1.22 (-1.18)            | 0.32 (0.33)              | 2.68 (2.62)              |                          |                          |
| 18:9,12,15                                 | -2.23 (-2.29)            | 0.00 (0.06)              | 4.60 (4.79)              |                          |                          |
| 19:7,10,13                                 | -1.90 (-1.77)            | 0.20 (0.19)              | 2.69 (2.58)              |                          |                          |
| 20:8,11,14                                 | -2.20 (-2.10)            | 0.12 (0.11)              | 2.72 (2.56)              |                          |                          |
| 20:11,14,17                                | -2.41 (-2.46)            | 0.00 (0.02)              | 4.55 (4.78)              |                          |                          |
| A:4( <i>n,m,o,p</i> )                      | ( <i>n</i> +1)- <i>n</i> | ( <i>m</i> +1)- <i>m</i> | ( <i>o</i> +1)- <i>o</i> | ( <i>p</i> +1)- <i>p</i> |                          |
| 20:5,8,11,14                               | 0.00 (-0.26)             | 0.00 (0.09)              | 0.68 (0.64)              | 2.88 (2.69)              |                          |
| 22:7,10,13,16                              | -1.99 (-1.89)            | -0.30 (-0.31)            | 0.58 (0.54)              | 2.86 (2.67)              |                          |
| A:5( <i>n,m,o,p,q</i> )                    | ( <i>n</i> +1)- <i>n</i> | ( <i>m</i> +1)- <i>m</i> | ( <i>o</i> +1)- <i>o</i> | ( <i>p</i> +1)- <i>p</i> | ( <i>q</i> +1)- <i>q</i> |
| 20:5,8,11,14,17                            | -0.29 (-0.29)            | 0.01 (-0.03)             | 0.18 (0.14)              | 0.69 (0.65)              | 5.02 (4.94)              |
| 22:7,10,13,16,19                           | -1.82 (-1.92)            | -0.34 (-0.43)            | 0.00 (0.05)              | 0.68 (0.63)              | 4.98 (4.93)              |

We find the inductive effect of the double bond (*cis* or *trans*) to be about 31% of that from -OH. Our method also works for poly-yne, where the corresponding factor is 60%. The attenuation of the inductive effect, imposed by an intervening methylene pair is  $\times 0.32$ , by  $\text{CH}=\text{CH}$  is  $\times 0.43$  and by  $\text{C}\equiv\text{C}$  is only  $\times 0.57$ . Our theory also makes sense of shifts in hydroxylated chains and even, to some extent, of the variations in carbonyl shift. Thus it has considerable analytical versatility.

Very best wishes,

Oliver

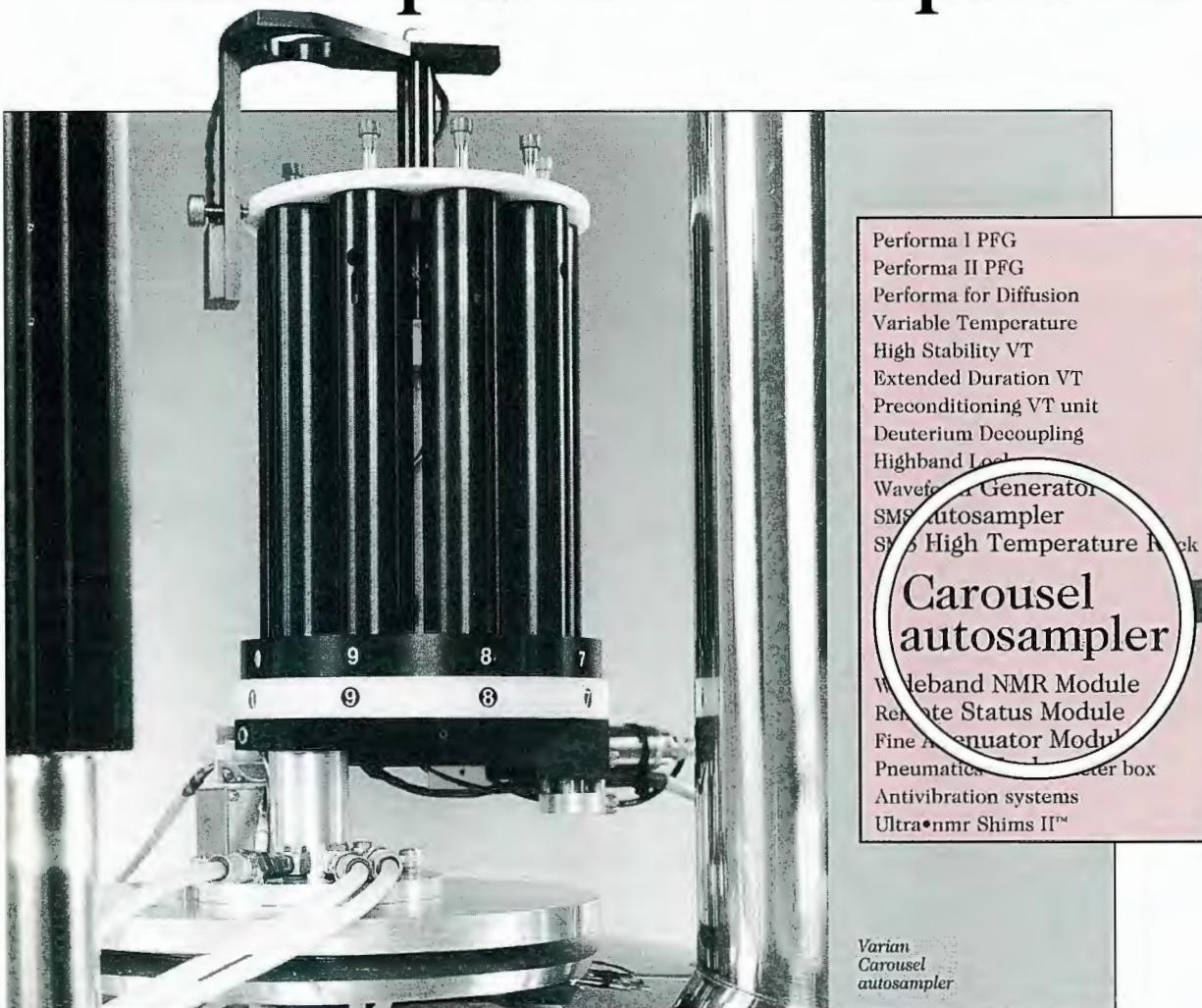
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The new Carousel autosampler from Varian provides a low-cost, reliable automation solution for a wide variety of NMR laboratory settings. The result of yet another joint development project with Zymark Corporation, the recognized leader in laboratory automation, the Carousel increases productivity with the latest state-of-the-art components.

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***The first name in nmr...***



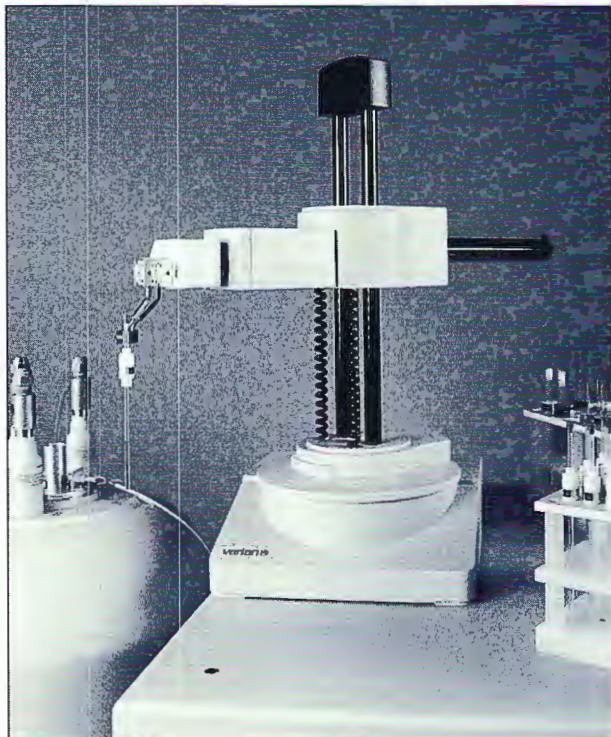
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Self-calibration of autosampler.....  
Tactile sensing gripper.....  
Integrated with NMR software.....  
Available from 200 to 600 MHz.....  
50 or 100 sample racks.....  
Built-in flexibility.....

#### Benefits

Fast turnaround of samples; increased productivity.  
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Securely holds sample during transport.  
Same user interface as NMR console.  
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# The University of Georgia

## Complex Carbohydrate Research Center

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March 31, 1995

(received 4/4/95)

Dr. Barry L. Shapiro, Publisher  
The NMR Newsletter  
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Palo Alto, CA 94303

### *Linkage position analysis of oligosaccharides by <sup>1</sup>H-NMR spectroscopy in H<sub>2</sub>O vs. D<sub>2</sub>O*

Dear Dr. Shapiro,

One of the salient features of carbohydrate primary structures is the manifold of linkage positions in which a glycosyl residue may be found attached to the adjacent residue in the chain (e.g., 1→2, 3, 4, 6, etc.). This feature is generally recognized as providing Nature with the potential of storing more information in carbohydrate molecules than, for instance, in peptides; however, deciphering this potential variation poses problems to the carbohydrate analytical scientist of a magnitude far more complex than those typically faced by a peptide sequencer.

Traditionally, glycosyl linkage positions are determined by tedious chemical derivatization (typically, per-*O*-methylation) of the intact oligosaccharide followed by hydrolysis of the glycosidic bonds and identification of the newly unmasked OH-groups in the partially methylated sugars (which is typically achieved by gas chromatography and mass spectrometry) [1]. Over the years, NMR spectroscopy has contributed its fair share of methods that aid in the determination of linkage positions in oligosaccharides. Worth mentioning are methods based on detection of (1) interglycosidic <sup>1</sup>H NOE effects (using NOESY- or ROESY-type experiments), (2) interglycosidic <sup>4</sup>J<sub>HH</sub>-scalar couplings (by COSY optimized for small couplings), and (3) <sup>3</sup>J<sub>CH</sub> scalar couplings across glycosidic bonds (by HMBC-type experiments). In principle, methods (2) and (3) provide the desired information in an unambiguous way; however, method (2) suffers from the drawback of relying on <sup>4</sup>J values often much smaller than 0.5 Hz; method (3) requires the full assignment not only of the <sup>1</sup>H spectrum but also of the <sup>13</sup>C spectrum of the oligosaccharide.

During our NMR studies on sugars in supercooled H<sub>2</sub>O (see *TAMU NMR Newsletter* 430, July 1994, p. 25-26) we came to realize that the comparison of D<sub>2</sub>O and H<sub>2</sub>O spectra of oligosaccharides contains the same information that is accessible through per-*O*-methylation analysis. Aliphatic sugar skeleton protons that show additional *J*-coupling (typically manifest as line-broadening) in H<sub>2</sub>O vs. D<sub>2</sub>O must be scalar coupled to OH. Therefore, linkage position analysis boils down to identification of those aliphatic sugar <sup>1</sup>H-signals that are identical in H<sub>2</sub>O and D<sub>2</sub>O. Their assignment is routinely achieved by TOCSY-type experiments. In Fig. 1, this concept is illustrated for the disaccharide maltose, that is, Glcp-α(1→4)-Glc', occurring in aqueous solution as a mixture of its α- and β-anomers. The linkage position is easily recognized as C4' of the free reducing Glc' residue by comparison of the TOCSY spectra of the individual glycosyl residues in D<sub>2</sub>O and H<sub>2</sub>O.

CCRC Building: 220 Riverbend Road, Athens, Georgia 30602-4712 USA

CCRC Telephone: 706-542-4401 Facsimile: 706-542-4412

\*Located in Life Sciences Bldg.: c/o Biochemistry & Molecular Biology Dept., Life Sciences Bldg., Athens, Georgia 30602-7229 USA

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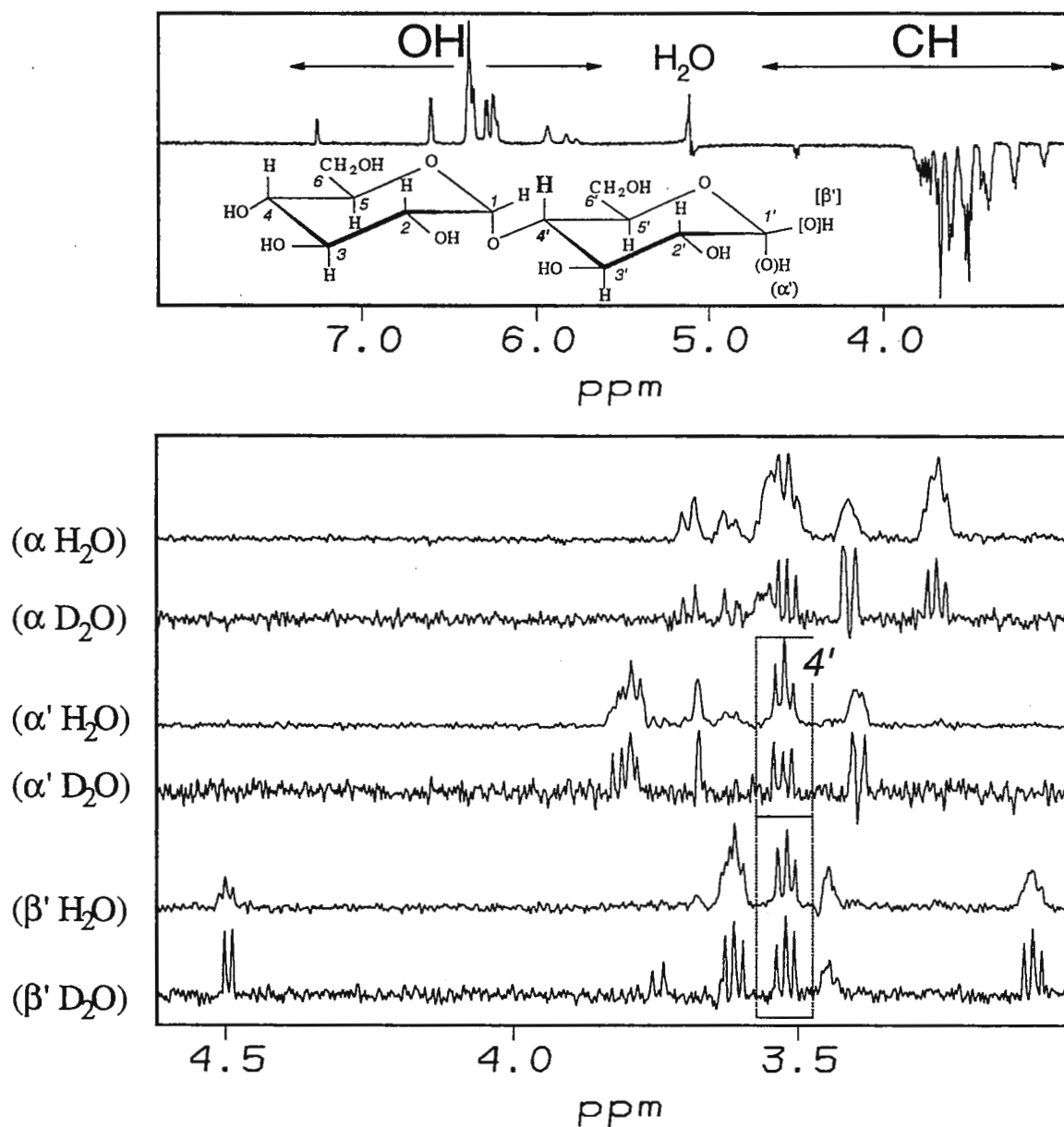


Fig. 1: (top)  $^1\text{H}$  NMR spectrum of maltose in  $\text{H}_2\text{O}$  at  $-15^\circ\text{C}$  and pH 6.3. The spectrum was recorded in 64 scans at 600 MHz, with 1-1 echo water suppression; maltose was dissolved in 50  $\mu\text{l}$   $\text{H}_2\text{O}$  in a 1.5-mm capillary tube at a concentration of  $\sim 20$  mM.

(bottom) 1D TOCSY spectra in  $\text{D}_2\text{O}$  (DIPSI-2, 150 ms mixing time) with selective excitation of  $\text{H1}\alpha$ ,  $\alpha'$  and  $\beta'$  signals, alternated with the corresponding traces through the  $\text{H1}\alpha$ ,  $\alpha'$  and  $\beta'$  proton signals of a 2D TOCSY spectrum in  $\text{H}_2\text{O}$  (MLEV-17, 68 ms mixing time).

[1] W.S. York *et al.*, *Methods Enzymol.* **118** (1985) 3-40.

Sincerely yours,

Shuqun Sheng  
Shuqun Sheng

Herman van Halbeek  
Herman van Halbeek

## 5.0 mm Broadband Triple Resonance Probe



The latest 5.0 mm Broadband Triple Resonance, Magic Angle Spinning PENCIL™ probe from Chemagnetics builds on the features that have become synonymous with the high performance design of the original (H, C, N) triple resonance probe. The patented PENCIL™ spinning module system incorporates such features as self-starting and trouble free spinning, and routine variable temperature operation. This is combined with a unique frequency optimized RF design to offer decoupling powers in excess of 80 kHz.

## Features

## Benefits

|   |  |
|---|--|
| <b>Full Multinuclear Range:</b>           | The X ( $^{75}\text{As}$ - $^{31}\text{P}$ ) and Y ( $^{25}\text{Mg}$ - $^{81}\text{Br}$ ) channels provide a complete range of nuclei combinations for the most demanding of experiments. |
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| <b>PENCIL™ Rotor Design:</b>              | Large sample volume results in decreased experiment time and increased sensitivity.  |
| <b>PENCIL™ Double Bearing Design:</b>     | Smooth, stable spinning, eliminates asymmetric axial oscillation, and allows spinning of the most inhomogeneous samples.   |
| <b>Separation of VT and Spinning gas:</b> | Trouble-free constant spinning speed over complete VT Range ( $-150^{\circ}\text{C}$ to $250^{\circ}\text{C}$ ).   |
| <b>Unique APEX™ II RF Design:</b>         | Allows unprecedented RF performance for reliable reproducible experiments requiring increased decoupler field strengths.   |
| <b>Exclusive VT Stack Design:</b>         | Permits full temperature range to be exploited without compromise of the probe performance.  |

## Typical Specifications

|   |  |
|---|--|
| Probe Outer Diameter                    | 70 mm  |
| Rotor Diameter                          | 5.0 mm   |
| Spinning Speed ( $\text{ZrO}_2$ rotors) | 1-12 kHz   |
| "Y" Channel Frequency Range             | $^{25}\text{Mg}$ - $^{81}\text{Br}$              |
| "X" Channel Frequency Range             | $^{75}\text{As}$ - $^{31}\text{P}$               |
| "H" Channel Frequency Range             | $^{19}\text{F}$ - $^1\text{H}$                   |
| Temperature Range                       | $-150^{\circ}\text{C}$ to $+250^{\circ}\text{C}$ |
| Sample Volume                           | 160 $\mu\text{L}$                                |
| $^1\text{H}$ 90° Pulse Width            | $\leq 3.0 \mu\text{s}$                           |
| $^{13}\text{C}$ 90° Pulse Width (X)     | $\leq 4.0 \mu\text{s}$                           |
| $^{15}\text{N}$ 90° Pulse Width (Y)     | $\leq 7.0 \mu\text{s}$                           |

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# SYRACUSE UNIVERSITY

DEPARTMENT OF CHEMISTRY

Room 1-014 / Center for Science & Technology / Syracuse, New York 13244-4100 / 315-443-2925 / Fax: 315-443-4070

Prof. Bernard L. Shapiro  
Editor/Publisher, NMR Newsletter  
966 Elsinore Court  
Palo Alto, CA 94303

April 5, 1995 (received 4/10/95)

## Re: Time domain filtering in the multidimensional space

Dear Professor Shapiro,

It was very nice to talking to you at ENC, finally I survived the questions, too. It is time to send our next contribution to *The NMR Newsletter*. Should I have forgotten about this, your gentle reminder has knocked on the door. Please, find below a short report on our recent efforts to remove subsets of multidimensional spectra using time domain filter.

Time domain filtering offers a flexible alternative to suppression or extraction in frequency domain, and is becoming more and more popular as software capabilities are enhanced gradually. We have been using this filter in the (should I say, late?) NMRi software for a long time now on two-dimensional spectra, primarily for removing residual solvent signals. Recently we have developed an efficient LP enhanced method (1) to remove in-phase diagonal intensities from spectra, such as 2D-NOE. Diagonal removal can be quite beneficial for homonuclear 3D correlations as well. For example, in a 3D-NOE/NOE spectrum huge body-diagonal intensities introduce high dynamic range, may ruin the 3D base-hyperplane and make both visualization and reliable peak analysis difficult at low intensity levels.

The time domain filter is implemented in a one-dimensional fashion, consequently an (n-1) dimensional object will always be affected in an nD spectrum. From a 3D spectrum special (2D) planes can be extracted conveniently using the time domain filter, for example. If any object of lower dimensionality should be targeted, such as the one-dimensional body-diagonal, a more complex procedure is required; temporary separation of subsets and linear combination of partial results may be necessary. The attached Figure shows a spatial presentation of a large 3D-NOE/NOE spectrum (1GB RRR *z-ant*) of a trisdecamer DNA duplex (*left*) from Prof. Tom James's lab (acquired by Karl D. Bishop) with the body diagonal removed using the time domain filter. An extracted special plane (F2/F3) is also shown (*right*). Full processing took about a day on Sun Sparc2 and SGI Indigo R4000 workstations over the local network with several other users on the net, using *z-ants* (2) in NMRZ. If time is corrected by that needed only for data transfer, the whole process needs only a couple of hours.

This project has been presented in part in Sicily recently (3) (thanks for the organizers, Drs. Filippo Conti and Alberto Spisni for this excellent meeting and opportunity!) and is to be published soon in *Quarterly of Magnetic Resonance in Biology and Medicine*.

Sincerely, with my best regards,

(Filtered to Prof. Kaptein's lab some time ago...)

Chris Spronk

István Pelczer

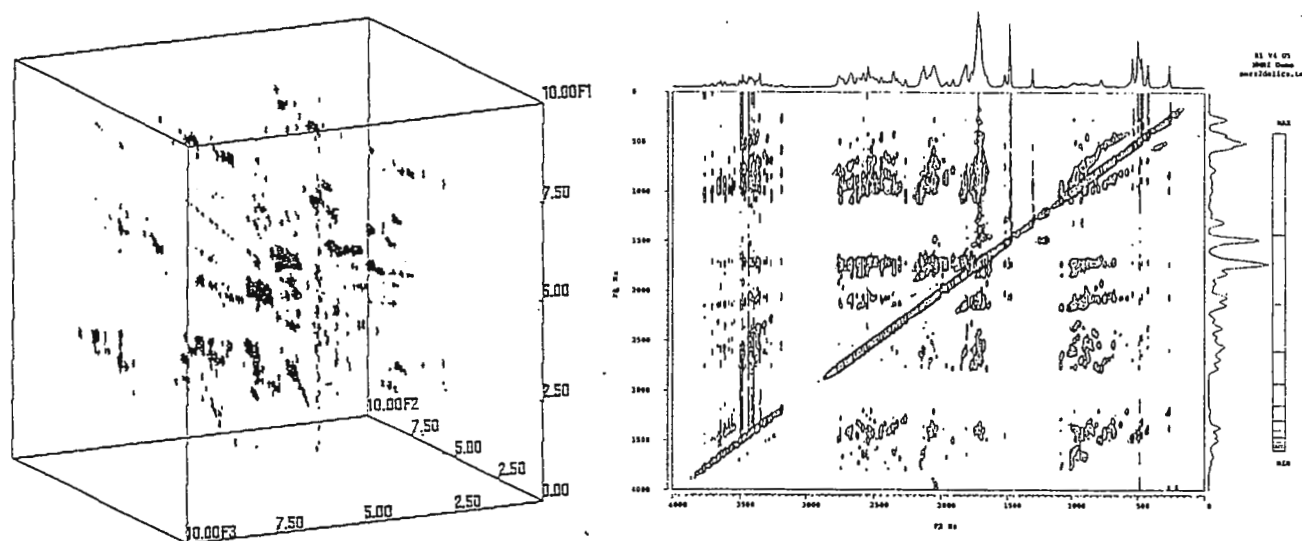


Figure 1.

- (1) Pelczer, I., and Roggenbuck, M. W.; *Clean Homonuclear Correlation Spectra through Combined Time and Frequency Domain Data Processing* Poster at 1993 Eastern Analytical Symposium, Somerset, NJ, USA, Nov. 14-19, 1993, #353 (I. P., M. W. R., and Carter, B. G., to be submitted)
- (2) Pelczer, I., Hoch, J. C., Roggenbuck, M. W., Vaidyanathan, A., Leccarde, M. G. and Borer, P. N.; *Z-ANT Processing; A New Alternative for Multidimensional NMR Data Processing* Poster at 33rd ENC, Pacific Grove, CA, USA, March 29 - April 2, 1992, abstracts: WP 188
- (3) Pelczer, I., Roggenbuck, M. W., Szafranski, M. S., and Spronk, C., *Time Domain Manipulations in Multidimensional NMR Data Processing* Lecture at Advanced School on NMR in Biology and Medicine: "NMR inside biology: from models to *in vivo*", Altavilla Milicia (Palermo), Italy, Sept. 21-30, 1994.

# Model 3445/3446 Amplifiers from AMT

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| Frequency range   | 10-130 MHz   | 10-130 MHz       |
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| CW power (max.)<br>into 50 ohms                           | 200 W  | 100 W            |
| Linearity ( $\pm 1$ dB to 30 dB<br>down from rated power) | 1,500 W  | 800 W            |
| Pulse width   | 20 ms  | 20 ms            |
| Duty cycle  | Up to 10%  | Up to 10%        |
| Amplitude droop   | 5% to 20 ms typ.   | 5% to 20 ms typ. |
| Harmonics   | Second: -25 dBc max.<br>Third: -24 dBc max.  |                  |
| Phase change/output power                                 | 10° to rated power, typ.   |                  |
| Phase error overpulse                                     | 4° to 20 ms duration, typ.   |                  |
| Output noise (blanked)                                    | < 10 dB over thermal   |                  |
| Blanking delay  | < 1 $\mu$ s on/off, TTL signal   |                  |
| Blanking duty cycle                                       | Up to 100%   |                  |
| Protection  | 1. Infinite VSWR at rated power<br>2. Input overdrive<br>3. Over duty cycle/pulse width<br>4. Over temperature |                  |

### Supplemental Characteristics:

|                         |   |                                     |   |
|-------------------------|---|-------------------------------------|---|
| Indicators, front panel | 1. AC power on<br>2. CW mode                                    | 4. Overdrive<br>5. Over pulse width | 6. Over duty cycle<br>7. LCD peak power meter |
| System monitors         | 1. Forward/Reflected RF power<br>2. Over pulse width/duty cycle | 3. DC power supply fault            | 4. Thermal fault                              |
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| AC line voltage         | 208/230 VAC, 10%, 1 $\phi$ , 47-63 Hz                           |                                     |   |
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UCD NMR FACILITY

DAVIS, CALIFORNIA 95616

March 24, 1995

(received 3/25/95)

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

**RE: MRI Sensor for Freeze Damage in Kiwifruit**

Dear Dr. Shapiro:

Here at UC Davis we have been engaged for several years in developing NMR methods, particularly imaging, for non-destructive and non-invasive quality control in agricultural and food products (for example, see Ref. 1). Our latest project, in conjunction with Chris Clark of HortResearch, Hamilton, New Zealand, involves development of an NMR sensor for freeze damage in kiwifruit. Some preliminary data are shown in the Figure below. Figure A presents a spin echo image of two adjacent kiwis, one picked fresh, and one picked, frozen, and thawed. The latter shows clear internal structural changes not evident by visual inspection of the fruit. In addition, images collected with different TE show marked differences between the two fruit in  $T_2$ . Figure B shows a single kiwi with one localized area of freezing clearly detected in the image, again showing the utility of the method for revealing freeze damage even in only a small region of the fruit. These results show promise for development of non-invasive monitoring techniques for freeze damage in kiwis, and other frost-sensitive fruits, by NMR.

Sincerely,

*Jeff de Ropp*  
Jeff de Ropp  
NMR Facility

Chris Clark  
HortResearch  
Hamilton  
New Zealand

Mike McCarthy  
Food Science

Bill Kerr  
Food Science

1. McCarthy, et.al. J. Sci. Food. Agric. 67, pp.13-20 (1995).



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March 23, 1995 (received 3/28/95)

Professor Bernard Shapiro  
TAMU NMR Newsletter  
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U.S.A.

### "Kobe Disaster and Magnets"

Dear Professor Shapiro,

We are destined to live in earthquake country. We can feel over several earthquakes in a year. Big earthquake struck early morning on 17 January, 1995 in the area of Kobe and west Osaka. Over 5500 people have been killed and 250,000 people made homeless by a mere geological event. Kobe earthquake was relatively shallow, and occurred off the main plate boundary on a strike-slip fault. The magnitude of the earthquake was 7.2 on the Richter scale. Max. ground velocities of 30-55 cm/s along the fault zone that ruptured was deduced.

I asked to friends in the area and companies as to damage of NMR equipments. Note that the examination did not cover all equipments.

At least thirteen superconducting magnets were fallen down, and several magnets were furthermore quenched due to the breaking of the magnet stand but they are rechargeable and not damaged. Some displays and/or plotters were slipped down the disk. Other most of equipments have no problems including the homogeneity of a magnet, although there are over a hundred of superconducting NMR in the area. I heard interesting accounts that although a magnet was fallen down, other two magnets were completely living in the same room in a laboratory, and that an EPR system moved about 1 m accompanied with a heavy magnet and are alive. Damage was concentrated on the fault, furthermore depending on the ground condition of a room and a floor of a lab., and the orientation of a magnet.

We cannot consider a permanent counterplan against big earthquake due to its cost, at least we must hold lightly the magnet from a few point of ceiling with ropes for climbing to avoid the falling of a magnet. I have heard recently that new law or regulation for the superconducting magnet was appeared in California. Please let us know about it to the this letter.

Sincerely,

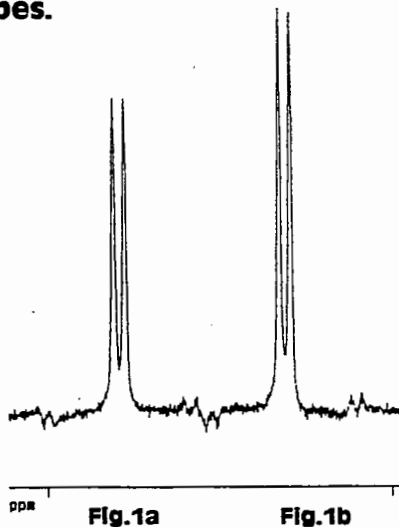


Toshifumi Hiraoki

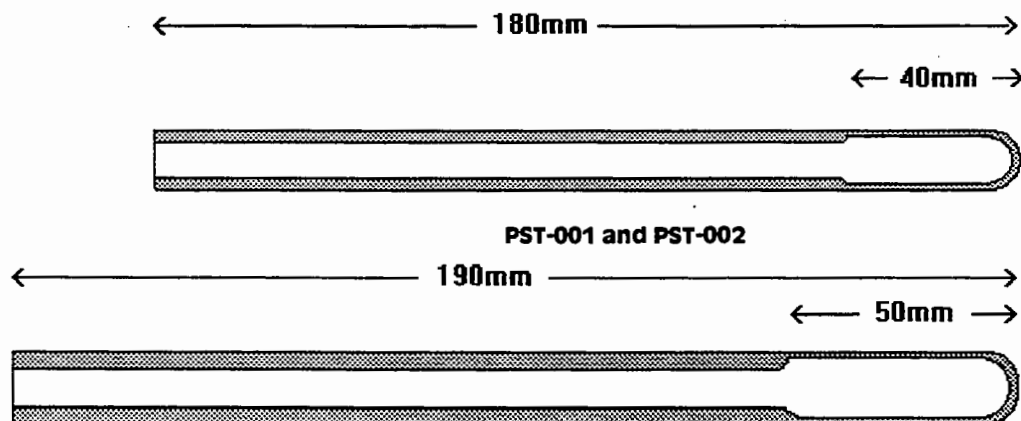


## Specially designed Thin Wall NMR Sample Tube

Shigemi's high precision thin wall NMR sample tube has a unique construction. The wall thickness of this particular tube is reduced only around the position of the detection coil. The result of this new invention allows an increase in the sample volume and higher sensitivity without sacrificing its mechanical strength. Therefore, there is no need for special handling during routine usage of our Shigemi NMR tubes.



The spectra of 20mm sucrose in D<sub>2</sub>O were obtained with a single scan without apodization prior to Fourier transformation on a Bruker AMX-600 spectrometer at 298 K. By using Shigemi high quality 5mm standard tube (Fig.1a) and the Shigemi highly sensitive thin wall 5mm tube (Fig.1b), the spectra confirms a sensitivity enhancement of about 10%.



ST8-001,ST8-002, ST10-001, and ST10-002

| O.D.<br>(mm) | Product<br>Number | Wall<br>(mm) | Concen-<br>tricity/Camber<br>(μ) | OD<br>(mm)         | ID<br>(mm)  | Price Each |         |
|--------------|-------------------|--------------|----------------------------------|--------------------|-------------|------------|---------|
|              |                   |              |                                  |                    |             | 1-99       | 100 +   |
| 5            | PST-001           | 0.21         | 20/ 8                            | 4.96 + 0.00 - 0.01 | 4.54 ± 0.01 | \$15.00    | \$13.50 |
|              | PST-002           | 0.21         | 40/15                            | 4.96 + 0.00 - 0.01 | 4.54 ± 0.01 | \$13.00    | \$12.00 |
| 8            | ST8-001           | 0.25         | 40/ 8                            | 8.00 + 0.00 - 0.01 | 7.52 ± 0.01 | \$31.00    | \$28.00 |
|              | ST8-002           | 0.25         | 50/15                            | 8.00 + 0.00 - 0.01 | 7.52 ± 0.01 | \$27.00    | \$25.00 |
| 10           | ST10-001          | 0.25         | 40/ 8                            | 9.98 + 0.00 - 0.01 | 9.52 ± 0.01 | \$36.00    | \$32.00 |
|              | ST10-002          | 0.25         | 50/15                            | 9.98 + 0.00 - 0.01 | 9.52 ± 0.01 | \$32.00    | \$28.00 |

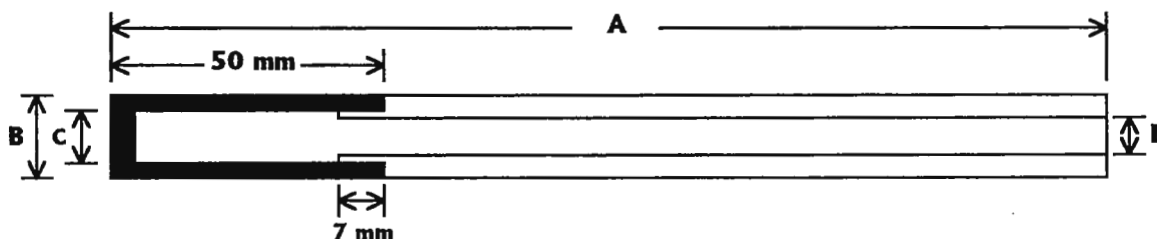
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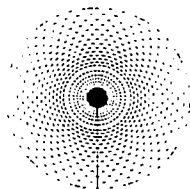


|        | A<br>Length (mm) | B<br>OD (mm)             | C<br>ID (mm)  | D<br>OD (mm) | Camber<br>( $\mu$ ) |
|--------|------------------|--------------------------|---------------|--------------|---------------------|
| Si-005 | 180              | $4.965 + 0$<br>$- 0.005$ | $4.0 \pm 0.1$ | 2.5          | $\pm 0.02$          |
| Si-010 | 190              | $10.0 + 0$<br>$- 0.01$   | $9.0 \pm 0.1$ | 6.5          | $\pm 0.02$          |

| Type   | Diameter | Price for 5 tubes |
|--------|----------|-------------------|
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Dr. Bernard L. Shapiro  
The NMR Newsletter  
966 Elsinore Court  
Palo Alto, CA 94303

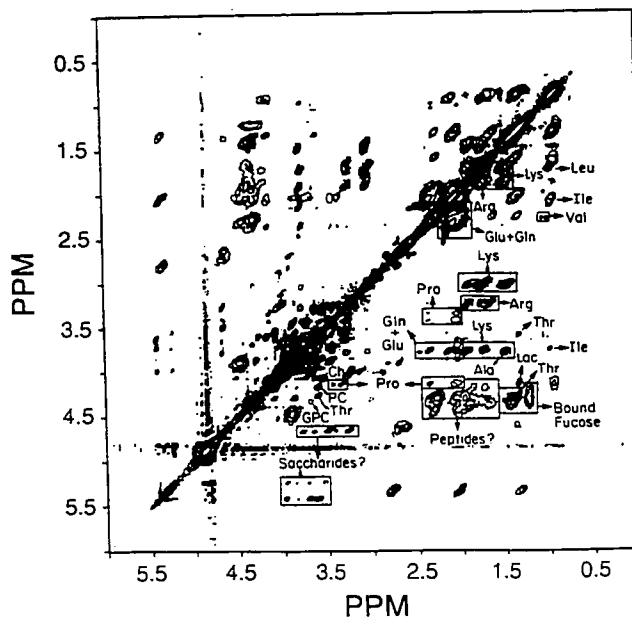
19 April 1995  
(received 4/25/95)

### *Ex Vivo* TOCSY Spectra of Human Smooth Muscle Tumors

Dear Barry,

We have been measuring TOCSY spectra at 600 MHz of samples of human tissue recently, in order to explore *ex-vivo* biochemical analysis of benign human smooth muscle tumor (leiomyoma) and high grade malignant smooth muscle tumor (leiomyosarcoma). A biopsy punch was used to obtain samples 3 mm in diameter and about 20 mm in length. The samples were supported on glass wool in order to center the tissue in the RF coil, and covered with PBS/D<sub>2</sub>O. Of course, the problem with this kind of work is the homogeneity of the magnetic field, or rather, the lack thereof. Those of your readers who think shimming is difficult when dealing with solutions, should try shimming these heterogeneous samples! On good days we can get 10 Hz proton linewidths without too much trouble; on bad days...

An example of the kind of TOCSY spectra we get from benign leiomyoma tissue is shown below:-



Chris

Kerry Souza

Samual Singer

Christopher. J. Turner



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27 March 1995  
(received 4/3/95)

Dear Dr Shapiro

Technological awareness in South Africa

Through colleagues at Zeneca Ag Products in Richmond CA I have been introduced to what is now the *NMR Newsletter*. I would like to congratulate you in producing such a fuss free, yet useful journal and hope that it continues.

I hope this photograph, which was taken by a friend on vacation in Durban (South Africa), may raise a smile amongst your regular readers.



Yours sincerely

Paul Stanley

# SLOW MAGIC ANGLE TURNING IN SOLIDS

Chemical Shift Anisotropy (CSA) is an important indicator of the symmetry around nuclear sites. The CSA gives information about chemical structure, and can be used to determine structural parameters such as molecular conformation and protonation states.

The ideal experiment for obtaining CSA information in solids is a 2D measurement that presents spinning side band CSA patterns in the first dimension, and separates them according to their isotropic chemical shifts in the second dimension. Thus in  $^{13}\text{C}$  spectra containing multiple resonances, the overlapping CSA patterns can be separated.

It is possible to design a 2D experiment that yields such a result, by rotating the sample at very slow speeds and synchronizing the 2D evolution time with the rotation period. Such so-called magic angle "turning" experiments require highly stable spinning at very slow speeds, typically only a few hundred Hz.

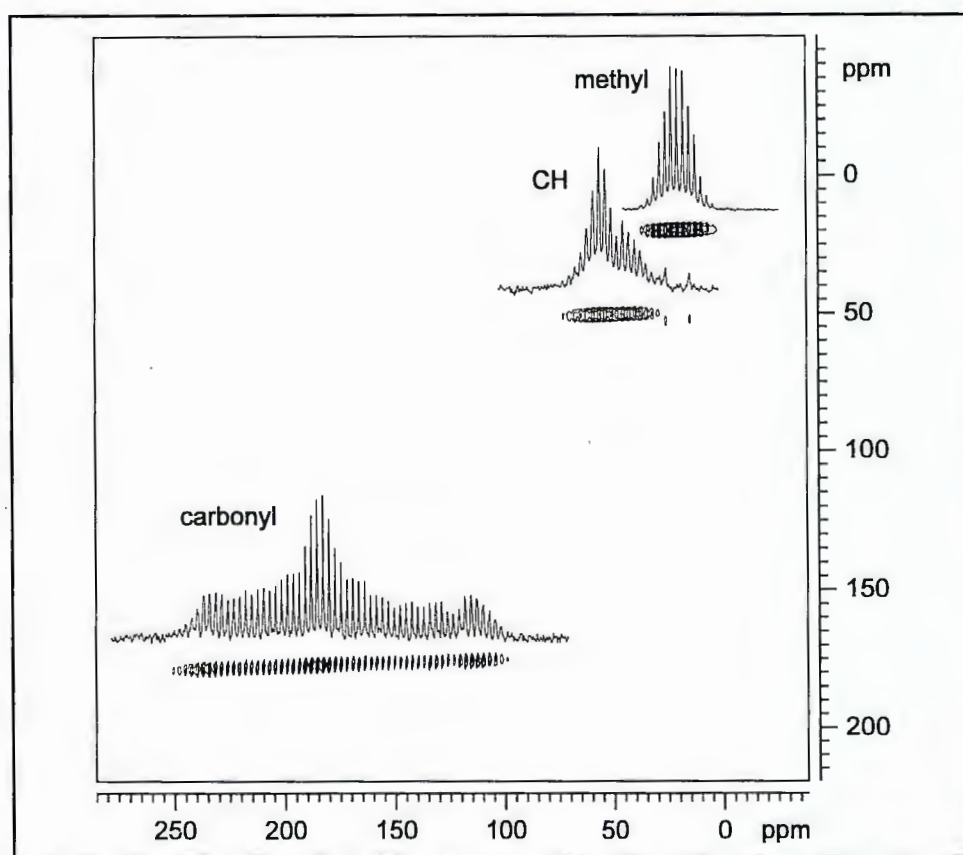
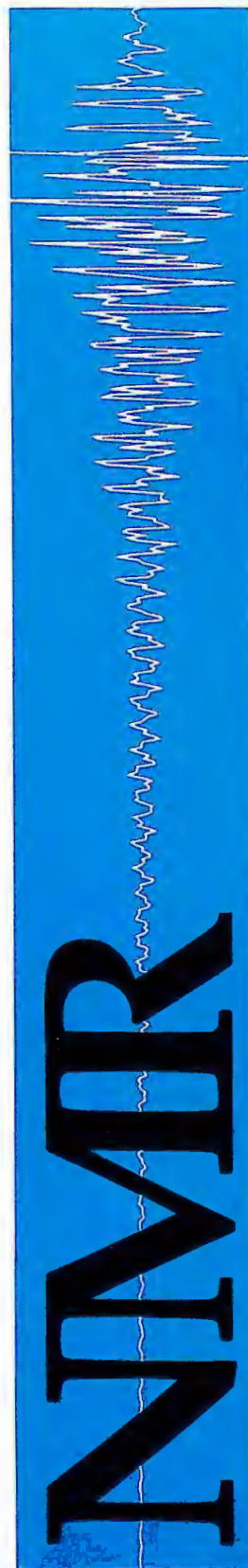


Figure 1: Alanine 2D Magic Angle Turning Spectrum

Figure 1 presents a 2D magic angle turning spectrum of alanine obtained on an *AVANCE* DSX-300 with a 7 mm MAS rotor spinning at 204 Hz. A rotor cap without drive flutes was used to allow better stability at low speeds.



The pulse program used for the experiment is shown in Figure 2<sup>1</sup>. The evolution time consists of a fixed interval ( $T$ ) set equal to the time it takes for the rotor to make several complete rotations (i.e. rotor periods). This interval is divided into six equal sub-intervals and contains five  $180^\circ$  pulses. Instead of varying the total evolution time ( $T$ ), the timing of the pulses within the evolution interval ( $T$ ) is varied according to the variable  $t_1$  shown in the figure.

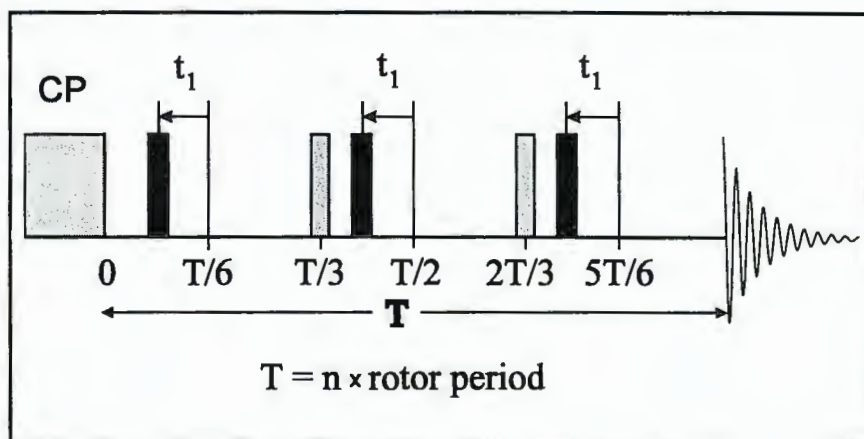


Figure 2: Pulse program for Alanine 2D magic angle turning experiment.

Any Bruker system equipped for CPMAS with the Bruker microprocessor controlled pneumatic unit can perform the magic angle turning experiment shown here. The Bruker microprocessor controlled pneumatic unit is ideal for MAS turning because the microprocessor uses active feedback to regulate the spinning speed, providing a very stable spinning rate. The only special item needed is a Bruker 7 mm rotor cap without flutes (Bruker P/N B200181), which can be ordered from your local Bruker representative.

<sup>1</sup> J.Z. Hu, D.W. Alderman, C. Ye, R.J. Pugmire and D.M. Grant, J.Magn.Res. A 105, 82 (1993)



PROF. DR. F. H. KÖHLER  
ANORGANISCH-CHEMISCHES INSTITUT  
TECHNISCHE UNIVERSITÄT MÜNCHEN

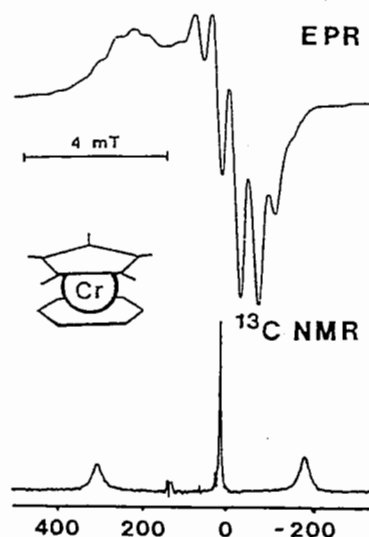
Lichtenbergstr. 4  
D-85747 Garching  
Tel. Nr. (089) 3209-3109  
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March 30, 1995  
(received 4/7/95)

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

**Chromium(I) sandwiches,  
good for NMR and EPR**

Dear Dr. Shapiro,

as you well know compounds having unpaired electrons are a shock for many NMR spectroscopists, for others it's their daily bread. The somewhat experienced people know, that depending on the electron relaxation rate (and a few more time-dependent phenomena), either NMR or EPR spectra may be obtained.



In a recent project we synthesized a series of (mostly substituted) (cyclopentadienyl)chromium(arene) compounds in order to study their electronic structure and their oxidation. It turned out that CpCr(arene) derivatives belong to the few species that yield both NMR and EPR spectra at temperatures that are not extremely different. As an example the Figure shows a solid solution X-band spectrum at 110 K. The same (mean) <sup>1</sup>H hyperfine coupling parameters were obtained by NMR spectroscopy at ambient temperature. More exciting is the fact that <sup>13</sup>C data, which would be extremely difficult to obtain by EPR spectroscopy, are available from the NMR spectra. An example is given in the lower part of the Figure (scale in ppm); the signal assignment from high to low frequency is: CH<sub>3</sub>, five-membered ring, six-membered ring.

A closer look on the electronic structure tells us that, generally, d<sup>5</sup> sandwich molecules should be susceptible to EPR and NMR studies when they have a <sup>2</sup>A<sub>1</sub> ground state whereas a <sup>2</sup>E<sub>2</sub> ground state ties the molecule to NMR spectroscopy. A more thorough reasoning is given in a paper that has been submitted (together with Werner Strauss and Chris Elschenbroich's group) to Inorg. Chem.

With best regards,

*F. H. Köhler*  
(Prof. Dr. F. H. Köhler)

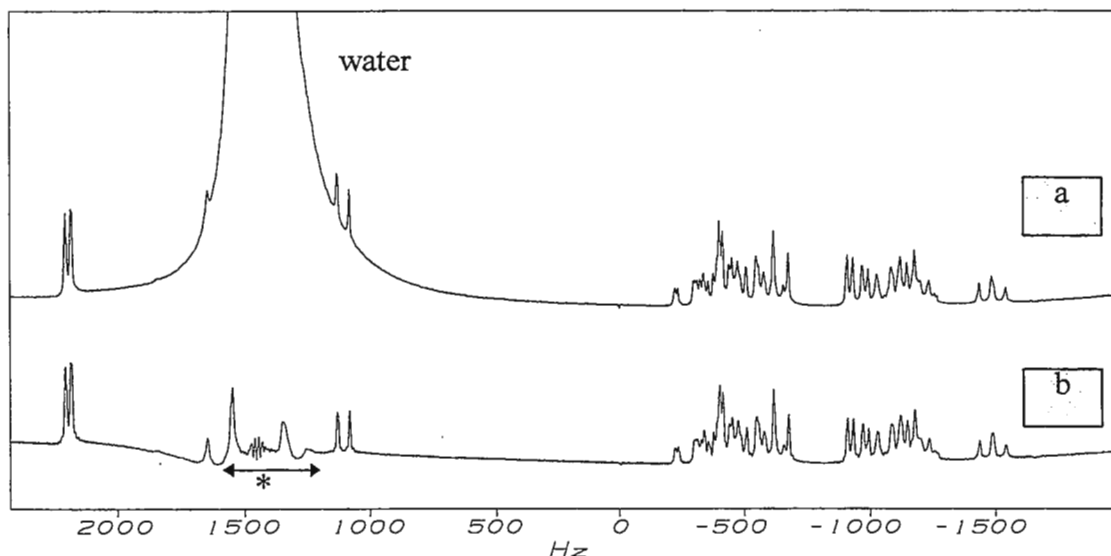
Villeurbanne, 31 March 1995  
(received 4/7/95)Pr. B.L. Shapiro  
The NMR Newsletter  
966 Elsinore Court  
Palo Alto CA 94303 (USA)

## Suppression of huge signals using the Cadzow enhancement procedure

Dear Professor Shapiro,

We have pleasure to inform you that our group has been associated with the CNRS since the 1st January of the present year. One of our topics concerns NMR data processing.

The signal estimator aspect of the Cadzow enhancement procedure [1,2] is attractive and can be used for the estimation of huge unwanted signals. This iterative procedure, based on singular value decomposition of the linear prediction matrix allows to estimate a new signal. The largest singular values correspond to the components having the most important amplitudes. So by keeping only the largest ones in the procedure, at convergence a good estimate of the huge signal is obtained and then subtracted from the raw signal. The amplitudes of the peaks of interest which were masked are not modified. This method can be applied for *in vitro* high resolution spectra to suppress the solvent peak (see figure) as well as for *in vivo* experiments to remove water or fat signals.

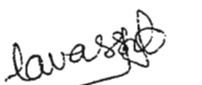


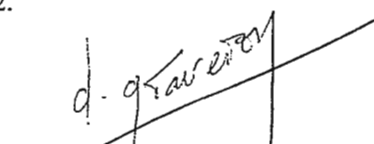
a) 300 MHz spectrum of glucose (400 mM) recorded in  $H_2O$ . b) FT of the signal obtained after subtraction of the estimated water signal using the Cadzow enhancement procedure. \* residual water.

1. Cadzow, J.A., *IEEE Trans. ASSP*, **36**, 49, 1988.
2. Diop, A., Briguët, A. and Graveron-Demilly, D., *Magn. Reson. Med.*, **27**, 318, 1992.

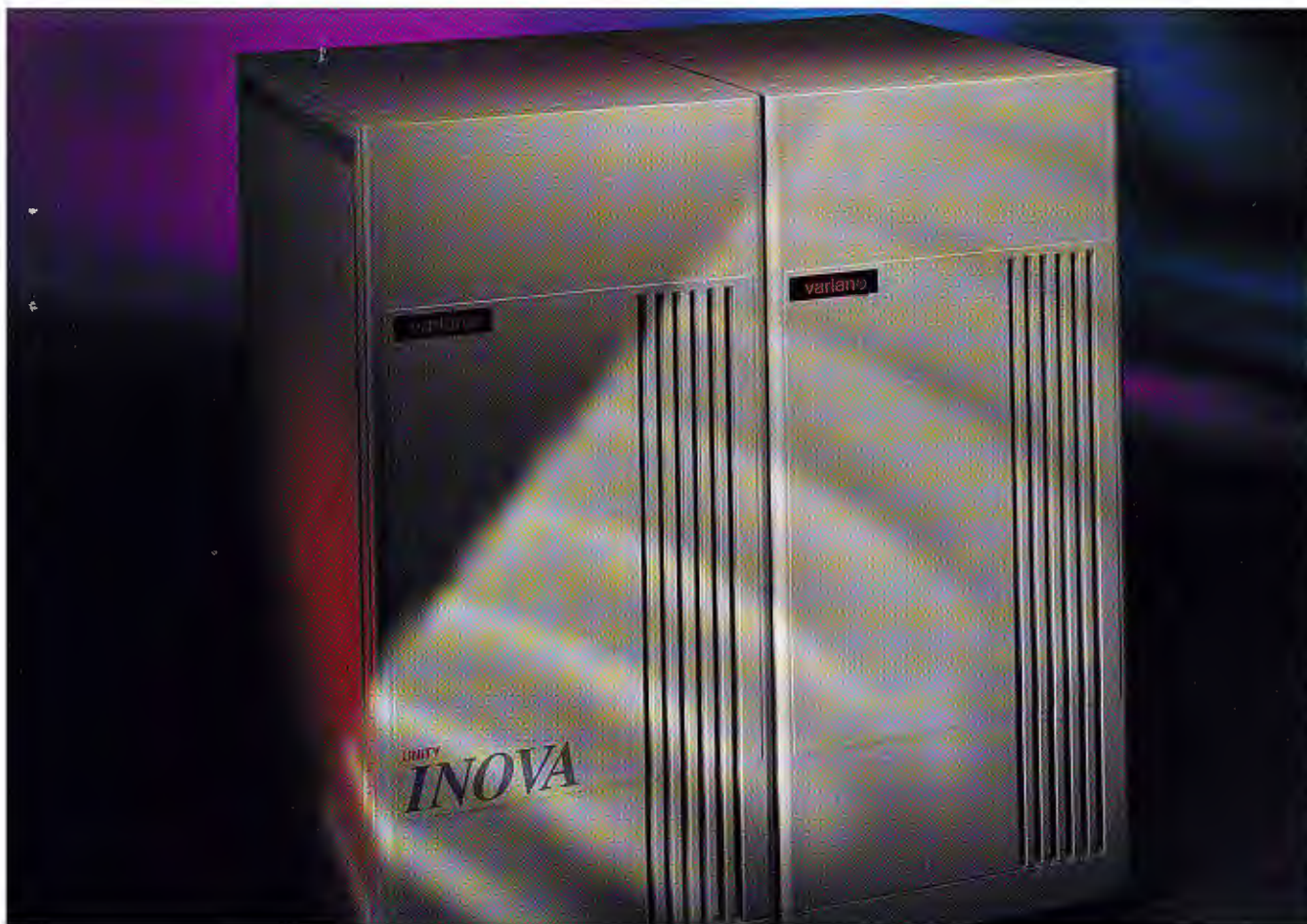
Sincerely yours,

  
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S. CAVASSILA

  
D. GRAVERON-DEMILLY

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Department of Nuclear Magnetic Resonance  
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Prof. Bernard L. Shapiro  
Editor/Publisher, TAMU NMR Newsletter  
966 Elsinore Court  
Palo Alto, CA 94303

March 20, 1995  
(received 3/27/95)

Dear Prof. Shapiro:

RE: Automatic Procedure for Processing Spectra from High Resolution NMR.

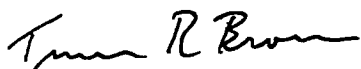
Recently we have developed an automatic procedure for processing spectra from high-resolution NMR experiments. Our goal is to have a tool for easy and rapid display of data from multispectral experiments, acquired on our Bruker Spectrometer. NMR investigation of perfused cells, for example, can result in 30-100 (or more) spectra. The commercial software available in our Department (WINNMR, DISNMR) is sufficient for processing a single spectrum. However, when numerous spectra are to be evaluated and field shifts between spectra have to be corrected by aligning the spectra along a selected resonance, using this software is neither easy, nor fast. For such cases, an automatic procedure for processing and display of large datasets is needed.

In our Department we have extensive experience in handling large multidimensional spectral datasets, resulting from Chemical Shift Imaging (CSI) experiments. We therefore modified the software developed for CSI purposes (data file formatting, implementation Bruker FFT and some changes in the user interface) and have produced a fast, easy method of data processing which requires minimal user input. The procedure consists of three major parts:

- 1. Reading all FIDs in a dataset and summing them.** The summed FID is used to (a) determine the phase parameters and (b) determine the chemical shift regions within which the alignment resonance lies. Figure 1a shows the spectrum obtained after summing the FIDs from a dataset with double peaks for each of the nucleoside triphosphate (NTP) resonances, indicating differences in the field among spectral subgroups, which can occur when NMR data is not collected continuously.
- 2 Processing.** Application of Lorentzian line broadening (by a user specified amount), zerofilling (if desired) and Fourier transformation (Bruker FFT) to each FID in the dataset; phasing and aligning all spectra. Figure 1b shows the sum of the aligned spectra.
- 3. Creating a PostScript of the spectral data.** A variety of options for the display of the data is available. The user can specify the number of spectra to be displayed per page, the layout and the scale. Furthermore, a subset of all spectra as well as spectral region can be selected for display on the screen or on hard copy. For example, Figure 2 presents the spectral region of gNTP in the dataset for Figure 1 before (Fig.2a) and after (Fig.2b) alignment.

Figure 3 shows the result of the described procedure. The entire spectral width of spectra of a dataset obtained during 18 hours of supplement of perfused Rat-2 cells with phosphonium choline is displayed. This procedure significantly speeds up and improves the initial evaluation of large datasets and enables comparison among datasets.

Sincerely,



Truman R. Brown, Ph.D.



Radka Stoyanova, M.S.



Nanci Aiken, Ph.D

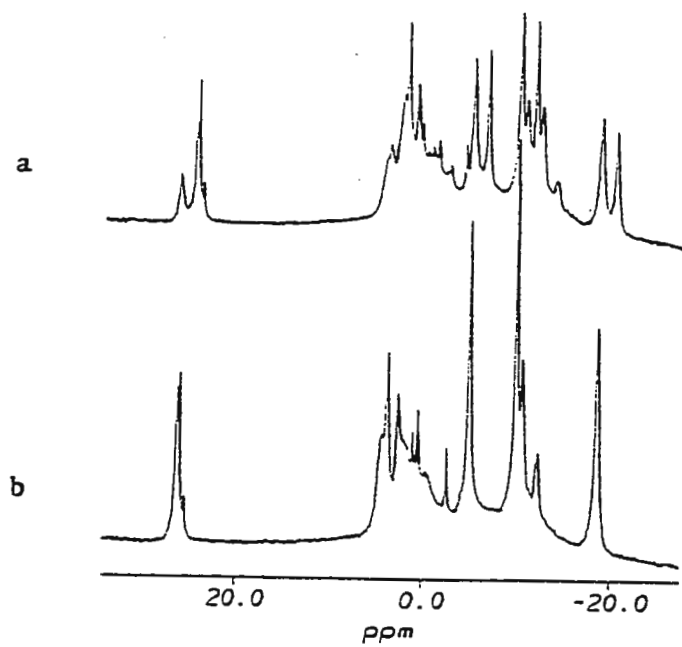


Figure 1

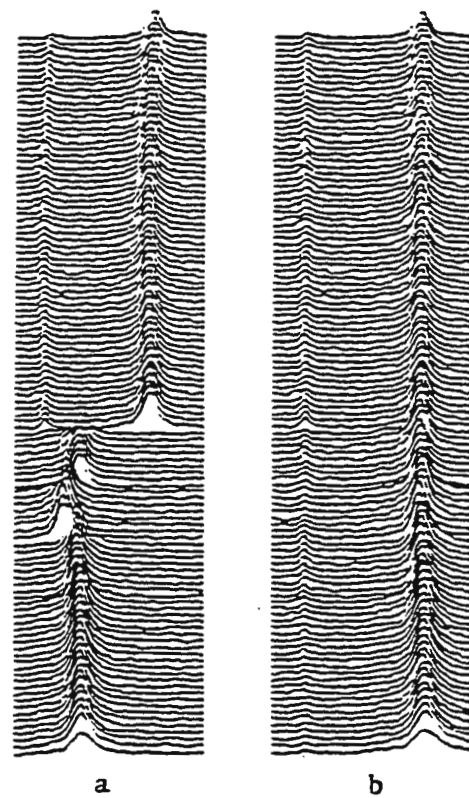


Figure 2

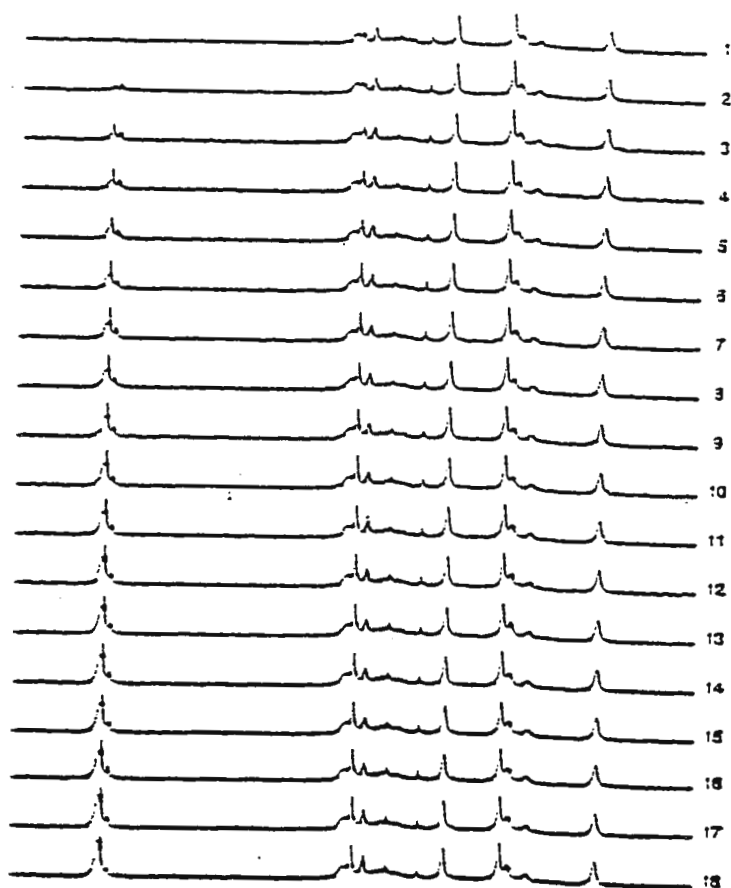
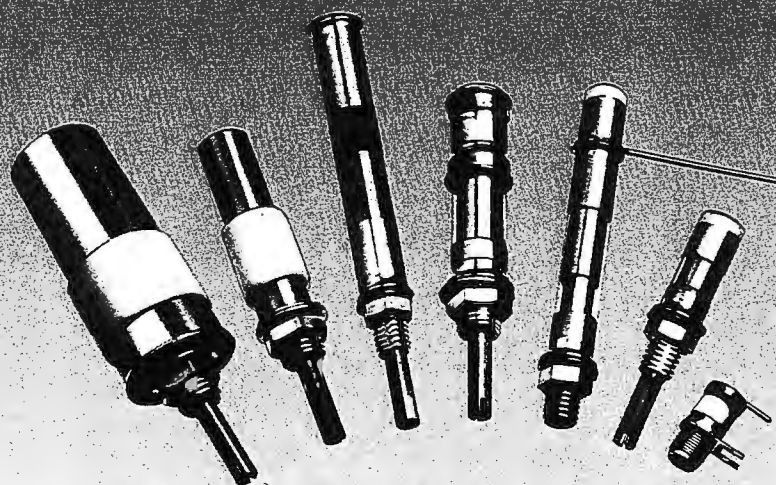


Figure 3



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# Duke University

## NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY CENTER

LEONARD D. SPICER, DIRECTOR  
ANTHONY A. RIBEIRO, MANAGER  
Professor B. L. Shapiro  
The NMR Newsletter  
966 Elsinore Court  
Palo Alto, CA 94303

(919) 684-4327  
(919) 684-6287

April 4, 1995

(received 4/8/95)

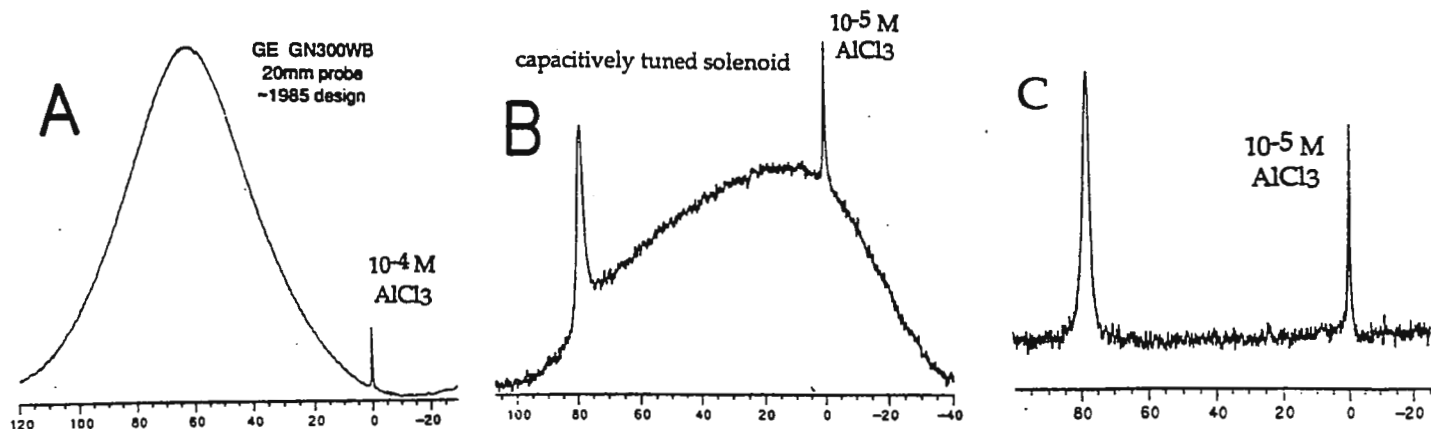
### Background Reduced $^{27}\text{Al}$ Probe

Dear Barry,

Aluminum is the most abundant element in the earth's crust, but its speciation in rivers, lakes, plants, fish etc. is quite dilute, about  $10^{-5}$  to  $10^{-6}$  M. This is about 2 orders of magnitude below the sensitivity of most commercial, multinuclear NMR probes. Also, many vendors supplied NMR probes and tubes use Al-containing glass pieces giving a probe background which can mask the desired signal from the natural sample. Fig. 1A shows the  $^{27}\text{Al}$  NMR spectrum recorded when a  $10^{-4}$  M  $\text{Al}(\text{Cl})_3$  solution is studied using a 20 mm GE GN300WB probe. The probe background centered at 56 ppm dominates the spectrum, while the 0 ppm hexaaqua  $\text{Al}(\text{III})$  signal derived from the  $10^{-4}$  M  $\text{AlCl}_3$  has about 0.2% the intensity of the background. Fig. 1B shows the  $^{27}\text{Al}$  NMR spectrum recorded using a novel, higher sensitivity probe which was constructed using very low Al-containing materials in the probe, coil and sample holder. The spectrum was obtained using  $10^{-5}$  M  $\text{AlCl}_3$  in the outer chamber and an  $8 \times 10^{-4}$  M  $\text{Al}(\text{OD})_4$  reference in the inner chamber of our sample holder. The background is now centered near 30 ppm and is below the level of the  $10^{-5}$  M Al signal. We estimate a factor of 40 reduction in the probe background. At this very low level of background, filtering, delayed acquisition or subtraction methods become effective. Fig. 1C shows the removal of the probe background, revealing well resolved Al resonances that phase with no baseline roll. This probe is being used to routinely record Al NMR spectra from natural samples of mine drainage sites, river water etc.

Sincerely,  
Anthony Ribeiro

Tony



**Address all Newsletter  
correspondence to:**

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

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**Deadline Dates**

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| No. 442 (July)    | 23 June 1995   |
| No. 443 (August)  | 21 July 1995   |
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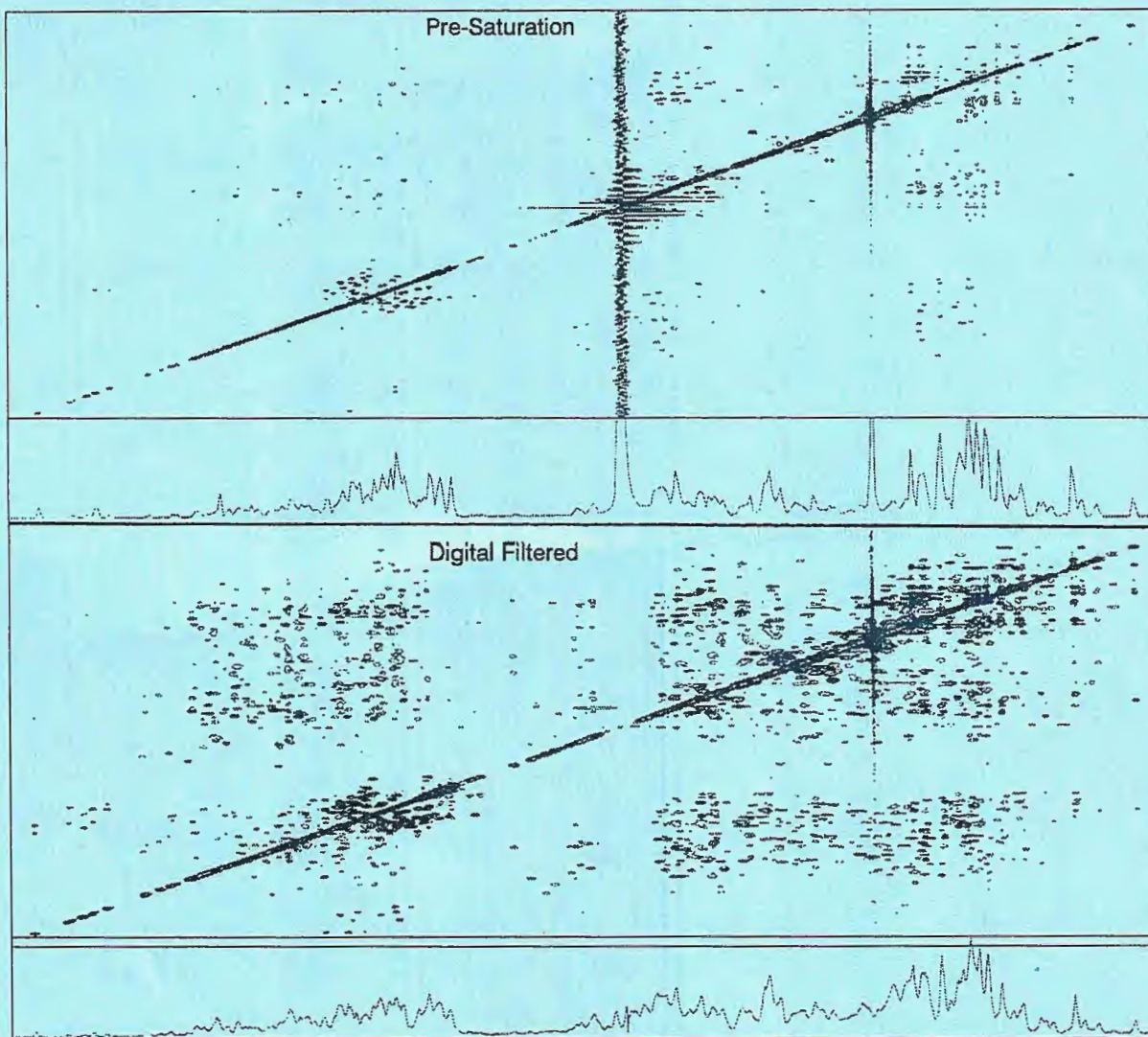
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