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THE NMR NEWSLETTER
NO. 493, OCTOBER 1999
AUTHOR INDEX

Bain, A. D. . . 5
Camb. Health Inst. 24
Coussot, P. . . 23
Dykstra, R. .
Golotvin, S. . 19
Martin, G. E. . 15, 21
Pratum, T. K. . 9
Shaffer, K. . . 23
Stilbs, P. . . 2
Shapiro, B. L. . 25

THE NMR NEWSLETTER
NO. 493, OCTOBER 1999
ADVERTISER INDEX

Advanced Chemistry Development, Inc. . . 13
Avanti Polar Lipids, Inc. . . 17
Bruker Instruments, Inc. . . 7
JEOL . . . . outside back cover
Programmed Test Sources, Inc. . inside front cover
Varian, Inc. . . 3

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FORTHCOMING NMR MEETINGS

NMR Technologies: Development and Applications for Drug Discovery, Baltimore, MD, November 4-5, 1999; Contact: Cambridge Healthtech Institute, 1037 Chestnut St., Newton Upper Falls, MA 02464; cl. 617-630-1300 or (in U.S.) 888-999-6288; Fax. 617-630-1325; e-mail: chi@healthtech.com; www.healthtech.com; See Newsletter 493, 24.


Biennial Meeting of the Australian and New Zealand Society for Magnetic Resonance (ANZMAG2000), Mt. Buller, Victoria, Australia; February 13-17, 2000; Contact: Dr. Jenny Wilson, Victorian College of Pharmacy, Monash University, Parkville, Victoria 3052, Australia; E-mail: anzmag@edda.vcp.monash.edu; vcp.monash.edu.au/chemistry/anzmag2k.

PITTCON 2000, New Orleans, LA, March 12-17, 2000; Contact: The Pittsburgh Conference, 300 Penn Center Blvd., Suite 332, Pittsburgh, PA 15235-5503; Phone: 412-825-3220; Fax: 412-825-3224; Email: expo@pittcon.org.

8th Scientific Meeting and Exhibition, International Society for Magnetic Resonance in Medicine, Denver, CO, April 1-7, 2000; Contact: ISMRM, 2118 Milvia Street, Suite 201, Berkeley, CA 94704. Tel. 510-841-1899; Fax. 510-841-2340; E-mail: info@ismrm.org; http://www.ismrm.org.

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; E-mail: enc@enc-conference.org. Web: enc-conference.org

15th European Experimental NMR Conference, Leipzig, Germany, June, 2000. For information, see http://eenc.uni-leipzig.de.


Royal Society of Chemistry: 15th International Meeting on NMR Spectroscopy, Durham, England, week of July 8-13, 2001; Contact: Mrs. Paula Whelan, The Royal Society of Chemistry, Burlington House, London W1V 0BN, England; +44 0171 440 3316; Email: conferences@rsc.org

Additional listings of meetings, etc., are invited.
Re: CORE for PC and Alpha (OpenVMS and NT) available for download

Dear Barry,

Thank you for your orange Ultimatum. Since March 1999 the CORE (1-3) program (OpenVMS Alpha, 'Intel PC' and 'Alpha (NT) PC' versions) has been freely available from my homepage indicated below. This is presently not a 'windows program', however (it runs in a 'DOS window'). Graphics display through Matlab is supported. Pentium II or III computers show quite reasonable processing times (about twice those of Alpha's with the same clock frequency).

CORE (Component Resolved Spectroscopy) is a useful computational procedure that utilizes all available information in data sets of 'kinetic type', i.e. where component band-shapes stay constant but undergo common and known/testable intensity changes. CORE was originally developed for analyzing multi-component FT-PGSE NMR self-diffusion data in the case of severe spectral overlap, but can often easily be adapted for other problems. The present version of CORE has working interfaces for importing Bruker AMX/DMX type data, and pure ASCII files (like from spreadsheets or Matlab). Through the kind help of Rolf Kyburz of Varian I also have access to Varian data sets, and hope to get time to work on some type of interface for reading those as well. Future CORE versions may include provisions for 'DOSY display' of FT-PGSE results.

Yours Sincerely

Peter Stilbs

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September 9, 1999 (received 9/13/99)

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

WEAK COUPLING IN EXCHANGE, PRO AND CON

Dear Barry:

We are still trying to make chemical exchange lineshape calculations as simple and efficient as we can. Our MEXICO program is progressing (things always take longer than you think), and I hope that by the time this gets published, a new version will be available. However, as we have been developing it, the usual tradeoffs between speed and accuracy start to arise.

A couple of the improvements over Binsch's landmark DNMR3 program are a more exact description of the $T_2$ effects on lines, and the possibility of weak coupling. With $T_2$ properly treated, we can get an essentially exact simulation of the lineshape. However, as with most simulations, the time required for the calculation rises steeply just as the spin systems start to get interesting. Table 1 gives some data obtained on a rather old SGI Indy computer.

<table>
<thead>
<tr>
<th>Table 1: Two-site Non-mutual Exchange, Strong Coupling</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spin System</td>
</tr>
<tr>
<td>---------------</td>
</tr>
<tr>
<td>ABCD</td>
</tr>
<tr>
<td>ABCDE</td>
</tr>
<tr>
<td>ABCDEF</td>
</tr>
</tbody>
</table>

For a strongly coupled ABCD system with two sites, there are 56 transitions in each site, giving a $112 \times 112$ complex matrix to be diagonalized. Factoring on the $F_2$ quantum number breaks the system into blocks, the largest of which is $48 \times 48$. All of this ends up taking about 2.5 seconds. However, standard matrix diagonalization scales as the cube of the size of the matrix. Adding a spin increases the size of the matrix by roughly a factor of 4, so that costs us a factor of 64 in time, as we can see in the table. Doing the matrix manipulations in less standard ways can avoid some of this rather frightening scaling (next year's letter!), but the temptation is to use a weak coupling approximation to reduce the matrix size as well.
Table 2 shows what you can do with weak coupling. The reduction in size comes from the loss of combination transitions, which are almost always negligible. In the table, the spaces between the letters indicate weak coupling, so AB CDE is really an ABXYZ system in proper Pople notation.

<table>
<thead>
<tr>
<th>Spin System</th>
<th>Total</th>
<th>Largest</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABCDE</td>
<td>420</td>
<td>200</td>
<td>56</td>
</tr>
<tr>
<td>ABCDE</td>
<td>160</td>
<td>60</td>
<td>9.1</td>
</tr>
<tr>
<td>ABCDE</td>
<td>364</td>
<td>168</td>
<td>42.5</td>
</tr>
<tr>
<td>AB CDE</td>
<td>340</td>
<td>156</td>
<td>31.1</td>
</tr>
<tr>
<td>AB CDE</td>
<td>264</td>
<td>116</td>
<td>18.1</td>
</tr>
</tbody>
</table>

In fact, the fully weakly coupled system can be treated as a bunch of $2 \times 2$ exchanges, so it can be done quite efficiently.

But remember that weak coupling gives reliable frequencies (usually), but not very good intensities. Line positions are perturbed only to second order, but intensities are perturbed to first order. In spite of the seductive nature of the numbers in Table 2, we usually try to keep all the strong coupling, at least towards the end of a fitting procedure. If you really need the speed, buy a faster computer, or do your matrix manipulations by some method other than Householder.

Yours truly,

Alex D. Bain
Professor of Chemistry
bain@mcmaster.ca
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Attempts to Apply Large Sideband Corrections to CPMAS Spectra
Tom Pratum, Department of Chemistry, University of Washington, pratum@u.washington.edu

Carbon-13 CPMAS NMR is an important tool for the analysis of carbon functional groups in natural organic matter. Tempering the optimism for the use of this technique are quantitation, and S/N problems. The tried and true method for obtaining these spectra is to operate at a low field and moderate spinning rate so as to reduce the possibility of spinning sidebands while not having to spin at a rate such that cross polarization is adversely affected. The recovery of S/N in these low field spectra has been dealt with by increasing the sample size through the use of large volume spinning assemblies (1). For many NMR laboratories, it is not possible to justify acquisition of a separate low field NMR spectrometer with a specialized spinning assembly for solids work, so they have attempted to acquire these data on their existing high field spectrometers; in some cases at fields up to and including 14 Tesla (600 MHz 1H) (see e.g. ref 2). Acquisition of these spectra at such high fields appears to be ill-advised, but occurs nonetheless. In situations where the researchers employing high field strengths are unable to spin adequately, TOSS is sometimes used to remove the sidebands from the spectra. TOSS is clearly not a quantitative technique, and this further muddies any conclusions to be drawn from such work.

Several years ago we showed that CPMAS spectra with moderate levels of sideband interference could be corrected by using measured chemical shift anisotropy (csa) parameters from similar materials to predict the sideband intensities, and use those sideband intensities to correct the measured integral areas (3). To do this, we first performed the standard CPMAS experiment at a spinning rate such that the selected regions were separated by an integral number of spin rates. In what is shown here the regions were 15 ppm wide and covered the range 210-0 ppm, or 198–12 ppm (14 regions total numbered 0-13 with 0 being the most downfield). The sidebands were analyzed over these regions either by re-integrating the previously obtained sideband data (acquired using the method of Feaux deLacroix et al. (4) at a spinning rate of 3200 Hz), or re-measuring the sidebands for the sample of interest using the 5 pulse PASS method of Levitt et al. (5) at a slower spinning rate (2000 Hz). The analysis of the sideband intensities was accomplished using the very nice Mathematica notebook which is provided on the Levitt group website (http://www.fos.su.se/physical/mhl/science/research.html). These sideband intensities (up to third order) are then entered into the system of linear equations which describes how the centerbands and sidebands add to create the observed spectrum:

\[ A \cdot B_0 = B, \]

where \( A \) is a 14x14 matrix of normalized sideband intensities determined from the chemical shift parameters of each region and arranged with the rows indicating the sideband contribution to each region, and the columns containing the sideband intensities which originate in a particular region. The column vector \( B_0 \) contains the (unknown) centerband intensities, and \( B \) is a column vector of the observed uncorrected integral intensities of the standard CPMAS experiment. The matrix equation \( A \cdot B_0 = B \) does not give the corrected intensities directly. After \( B_0 \) is obtained, by numerical elimination, or a similar method, corrected integrals are generated by multiplying each element of \( B_0 \) by the sum of normalized sideband intensities for that region. For example, the corrected intensity of region (a) would be:

\[ (1 + a_{-3} + a_{-2} + a_{-1} + a_1 + a_2 + a_3) a_0, \]

where the subscripts indicate the sideband order. The question here is whether this procedure can be used for the larger sideband corrections which might be needed when operating at very high field.
As a test, CPMAS spectra were acquired at 3 spinning rates which were multiples of 15 ppm for $^{13}$C at 7.0 Tesla (2264, 3396, and 4528 Hz), and these were corrected as outlined above. We show below the resulting areas obtained from a series of standard 1 msec contact CPMAS spectra obtained at 3 different spinning rates on a fulvic acid from a shrub/sedge wetland in Western Washington. As can be seen, when the correction is applied using the csa parameters which were used in the previous study, there are wild deviations from reasonable integral area values in the corrected data for the slowest spinning rate. Since these csa parameters were obtained from ssb intensities at a spinning rate of 3200 Hz, it was thought that perhaps extrapolation of the values to obtain sideband intensities at much lower spinning rates was improper. To take care of this, we used the 5 pulse PASS method, and measured new sideband intensities at a much slower spinning rate of 2000 Hz. As you can also see below, these parameters (which are somewhat different from those previously obtained, but are not presented here due to space limitations) yield corrections that are still wildly outside of the range that most people would consider reasonable for the slowest spinning rate.

Perhaps it is not surprising that we cannot properly correct for sideband contributions in a series of spectra which have such similar integral areas across such a range of spinning rates. Because of the ill defined nature of these humic and fulvic acid spectra, it is possible that the method might work better on spectra that were more well defined; e.g. those of a polycrystalline sample. To test this we used anisic acid; which contains many of the same carbon types as humic and fulvic acids. Again, the 5 pulse PASS method was used to obtain the sideband
intensities and the Mathematica notebook (5) was used to fit the intensities to chemical shift parameters. In this case we also used published csa values for the aromatic carbons (6) to see if those yielded different results.

In this situation a reasonable correction is obtained at all spinning rates irrespective of which csa values we use, and the corrected data contain only positive intensities and only in those regions where intensity is expected (1,2,4,5 and 9).

There are potentially a couple of reasons for the poor performance of this method in the current application. First, the method may be unstable when applied to broad, poorly defined spectra such as those encountered in humic and fulvic acids, and this becomes particularly apparent when large corrections are applied. Second, the measured chemical shift parameters may be skewed toward carbon types which have a greater response in the experiment used (e.g. those with longer T2 s) and are thus not representative of the sample as a whole. Further investigation into these possibilities is underway.

References

Dr. Bernard L. Shapiro  
966 Elsinor Court  
Palo Alto, CA 94303  

September 1, Y2k-1  
(Received 9/4/Y1k+999)  

Liquid Nitrogen Level Indicator  

Dear Barry,  

A method of measuring the level of Liquid Nitrogen in a cryostat is sometimes done by immersing a wooden dowel rod in the Liquid Nitrogen, and then waving it in the air after removal from the cryostat. The level of LN2 is then indicated by moisture, in the form of frost, building up on the cold portion of the dowel rod. I, however, have not mastered this art.  

A much more precise and faster way to make this measurement is by using a non-magnetic metal tube (I use aluminum) which is terminated in a pneumatic switch*. (The switch has a specified sensitivity of 0.6 inches of water.) I used LED's (light emitting diodes) as visual indicators. Two LED’s are wired in series with the normally open contacts of the switch and a 1000 ohm resistor. A 9 volt battery is used to power the device. When the open end of the tube is immersed in the LN2, both LED’s will light. I placed one LED on the side of its box, and the other LED on the bottom. It has been my experience that the measurement precision of this technique is 4 mm.  

With best regards,  

Robert Dykstra  

- Micro Pneumatic Logic  
  Fort Lauderdale, FL 33309
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September 8, 1999

Bernard L. Shapiro, Ph.D.
Editor, The NMR Newsletter
966 Elsinore Court
Palo Alto, CA 94303

SMASH '99

Dear Barry,

As a follow-up to an announcement you published in The NMR Newsletter some months ago announcing the SMASH '99 Small Molecule NMR Meeting we thought it appropriate to share with the readership the outcome of the meeting.

Participation was significantly greater than the organizing committee had originally hoped. Final registration was a total of 174 scientists, with ~20% from outside of the US. The meeting was held from August 15-18 at the Argonne National Laboratory conference center outside of Chicago. Jim Shoolery, formerly of Varian NMR, gave the plenary introductory lecture Sunday night entitled “From Neat Liquids to Nanograms.” The Monday evening lecture, “A Tale of One Small Molecule,” was given by Ray Freeman, and Tom Farrar rounded out the after dinner program on Tuesday night with a lecture entitled “Antediluvian Anecdotes of Sensitivity Enhancement Advances in NMR Spectroscopy.” All three of the lectures from this well-known trio of NMR scientists were superb; the organizing committee would again like to thank Varian and ACD Laboratories for their sponsorship of the plenary lecturers.

The scientific program began Monday morning with sessions on Natural Products NMR followed by a session on Pulse Sequences. After an open session to allow attendees to interact or tour the Argonne National Laboratory’s Advanced Photo Source. There was a late afternoon session on New Probe and Magnet Developments followed by dinner and Ray Freeman’s plenary lecture. Tuesday’s scientific program began with a session devoted to Application of Flow NMR followed by a session on Metabolism. Tuesday afternoon provided a second open session for the exchange of techniques and ideas amongst participants and another opportunity for interested scientists to tour the Advanced Photo Source. The late afternoon session on Tuesday was Applications of NMR to High Throughput Screening and Combinatorial Chemistry. Tom Farrar gave the Tuesday after dinner lecture, which was humorously delayed for a few minutes by the need to “shim” the overhead projector – accomplished by vigorous application of the butt of a maintenance man’s hand to the projector! A Poster session followed on Tuesday night, with refreshments generously provided by Bruker Instruments. The final session of the meeting was held Wednesday morning and dealt with Post Acquisition Data Processing, Databasing, and Spectral Prediction.
During the meeting, the Organizing Committee discussed the prospects for SMASH 2000. Based on the very heavily positive feedback on the organization and content of this year’s meeting, it was decided to hold SMASH 2000 at the Argonne National Laboratory Conference Center again next year. Next year’s meeting will be held July 16-19, 2000. The organizing committee discussed session topics and potential session chairs for next year’s meeting. Details of the planned sessions and their respective chairs follow in this issue of The NMR Newsletter and will also be available in a few weeks on the web at www.smashnmr.org. From the perspective of the Organizing Committee, SMASH ’99 was a huge success! Attendance at this year’s meeting clearly underscored the need for a meeting and forum devoted to scientists working in the area of small molecule NMR.

On behalf of the attendees and the Organizing Committee, SMASH ’99, we would again like to thank the meeting’s sponsors whose backing and confidence in the goals of the SMASH meeting are greatly appreciated. Sponsors included the following: ACD (Advanced Chemistry Development, Inc.), Bruker Instruments, Cambridge Isotope Laboratories, Isotec, Nalorac Corporation, Schering-Plough, and Varian, Inc.

Sincerely,

Gary Martin for the SMASH ’99 Organizing Committee

Al Bach (bacha@war.wyeth.com)
Gwendolyn Chmumy (chmumy@ncifcrf.gov)
Robert Espina (j.robert.espina@dupontpharma.com)
Andy Evans (charlie.evans@spcorp.com)
Kevin Faccine (kf8589@glaxowellcome.com)
Krish Krishnamurthy (krish.krishnamurthy@varian.com)
Dave Lankin (david.c.lankin@monsanto.com)
Margaret Levenberg (mlevenberg@stepan.com), Secretary
Steven R. Maple (maple_steven_r@lilly.com)
Gary E. Martin (gary.e.martin@am.pnu.com)
Gene Mazzola (em105@umail.umd.edu)
Karen McCune (mccune_karen_a@lilly.com)
Greg Nemeth (gregory.a.nemeth@dupontpharma.com)
Alistair G. Swanson (alistair_swanson@sandwich.pfizer.com)
Michael Shapiro (michael.shapiro@pharma.novartis.com)
John Shockcor (john.p.shockcor@dupontpharma.com)
Tony Williams (tony@acdlabs.com)
Toby Zens (tzens@aol.com)
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- Ester bonded lipids for bicelle preparation
- Ether bonded lipids for bicelle preparation (pH stable)
- Anionic/Cationic lipids for bicelle preparation
- Lanthanide chelating lipid
- Pre-mixed lipids for bicelle preparation

References:

- Cavagnero S; Dyson HJ; Wright PE, (1999) Improved low pH bicelle system for orienting macromolecules over a wide temperature range., J Biomol NMR, 13:4, 187-91
- Struppe J; Komives EA; Taylor SS; Vold RR, (1998) 2H NMR studies of a myristoylated peptide in neutral and acidic phospholipid bicelles., Biochemistry, 37:44, 15523-7
- Prosser RS; Volkov VB; and Shiyamovskaya IV, (1998) Novel Chelate-Induced Magnetic Alignment of Biological Membranes. Biophys J. 75: 2163-2169

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# PRICE LIST

## Lipids for Bicelle Formation

<table>
<thead>
<tr>
<th>Product</th>
<th>M.W.</th>
<th>Quantity/Price</th>
<th>Catalog No.</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>25mg</td>
<td>200mg</td>
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<td>Acyl Zwitterionic Lipids</td>
<td></td>
<td></td>
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<tr>
<td>DHPC*</td>
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<tr>
<td>DMPC</td>
<td>677.94</td>
<td>$10</td>
<td>$20</td>
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<td>Acyl Anionic Lipids</td>
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<td>DMPC•Na</td>
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<tr>
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<td>$280</td>
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<td>12-0-PC</td>
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<td>DMPE-DTPA•(NH₄)₅</td>
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<td>$45</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>*DHPC is extremely hygroscopic; prepare solutions in dry box or dilute with buffer immediately after opening. Deuterated lipids are also available. Please inquire.</td>
<td></td>
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## Premixed Lipids for Bicelle Formation

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<tr>
<td>3.5</td>
<td>790575</td>
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</table>
As we all know, baseline correction can be a very essential step to obtain a high quality NMR spectra in some cases. Rolling baselines can make it difficult to identify peaks, as well as introduce a significant error into any quantitative measurements. The most convenient way of correcting baseline distortion is to construct a model of the baseline in the frequency domain and subtract it from the spectrum [1]. To this end, the majority of NMR desktop software allow the user to manually set the points belonging to the baseline and interpolate between them using analytical functions to model the baseline completely. While the results can often be good enough the method requires manual intervention and cannot be used for batch processing. On the other hand, the quality of automatic procedures is rarely sufficient when the baseline has severe distortions. The failures are generally due to both inadequate types of analytical functions used for modeling and the poor recognition of the baseline.

We have recently developed a new method for baseline correction which is governed by two easily adjustable parameters. The essence of the method is attributed to two parts: baseline modeling and baseline recognition.

It is a natural desire for visual inspection to have the baseline be a flat straight line with no constant offset. Our idea is to use the smoothed spectrum to model the baseline. We have used an averaging of neighboring data points of the spectrum, an operation equivalent to convolution with a rectangular function. The number N of points to average, or the width of the rectangle, is the first parameter of our procedure. It is evident that subtraction of the smoothed spectrum from the original one can give a relatively flat straight line, but it makes sense only for the area that does not contain peaks. As a result we have a fragmented model, which needs interpolation over the area where peaks are present. Interpolation can be as simple as connection by straight lines, or as complicated as we care to make it. The second important point is recognition of the baseline separately from the peaks.

Since the ultimate definition of “baseline” is “not containing peaks” it is natural to employ for its recognition the same tool that is used for peak identification. We have developed the following procedure. To decide whether the i-th point belongs to the baseline it is placed in the center of a rectangle with a width of N spectral points. Among these N points the minimal and maximal values are found. If their difference does not exceed the noise standard deviation multiplied by a definite factor (the second parameter of our technique) the i-th point is considered to belong to baseline. Finally the baseline model is then subtracted from the spectra.

Figures 1 and 2 below illustrate the results obtained with our approach. A characteristic rolling baseline can be observed in the spectrum in Figure 1 and can be accounted for by corruption of the first several points of FID. A well known algorithm was applied to this problem [2], and its performance is comparable with that of our method. However for the second case (Figure 2) our approach gives a far superior result. Due to adequate baseline modeling and recognition our technique has been shown to be superior and therefore of inherent value for desktop post-processing.
Figure 1. Original experimental (top) and baseline corrected (bottom) \(^1\)H NMR spectra of cyclopentanol in CDCl\(_3\). The rolling baseline is due to the first several points of the FID being corrupted.

Figure 2. Original (top) and baseline corrected (bottom) \(^1\)H NMR spectra of 6-bromo-1,5-dinitrobicyclo[3.3.1]non-6-ene-3-carboxylic acid in DMSO-D\(_6\). The hump in the original spectrum is due to non-optimal water suppression.

Yours sincerely,

Sergey Golotvin and Antony Williams,
Advanced Chemistry Development

P.S. Your readers may wish to take advantage of the FREE NMR viewer now posted at our website (www.acdlabs.com/download). This includes an integrated Structure Drawing Package, Chemsketch.

References:
**SMASH-2000**

"Small Molecules Are Still Hot"
Small Molecule NMR Conference
July 16-19, 2000
Argonne National Laboratory
Conference Center, Chicago, Illinois

**G.E. Martin – Program Chairman**

---

**Tentative Schedule**

**Sunday, July 16**

12:00-5:00 **Registration**

G. Nemeth, R. Espina, M. Levenberg, G. Chmurny

6:00-7:00 **Plenary Speaker**

TBA

7:00-10:00 **Dinner/Mixer**

**Monday, July 17**

7:00-8:15 **Breakfast**

8:25-8:30 **Opening Remarks**

8:30-10:30 **Natural Products**

P.J. Sidebottom

10:30-11:00 **Coffee Break**

11:00-12:30 **Pulse Sequences**

A.J. Shaka

12:30-2:00 **Lunch**

2:00-3:30 **Graduate Student/Post Doc Session**

R.T. Williamson

3:30-5:00 **Break/Advanced Photon Source Tours**

5:00-7:00 **Dinner**

7:00-? **Plenary Speaker**

TBA
Tuesday, July 18

7:00-8:15 Breakfast

8:30-10:30 Metabolism
   J.P. Shockcor

10:30-10:30 Coffee Break

11:00-12:30 Small Molecule
   Solid NMR
   A.G. Swanson

12:30-2:00 Lunch

2:00-5:00 Free Afternoon, Advanced Photon Source Tours
   or Workshop Attendance

Potential Workshops – individuals who have expressed
   interest in being involved
   Structure Elucidation – G. Chmurny, D.J. Russell
   LC/NMR – A. Swanson, S.R. Maple
   Metabolism NMR – J.P. Shockcor
   CombiChem/HTS – M. Shapiro, G. Nemeth
   FDM – A.J. Shaka

6:00-11:00 Poster Session/Buffet Dinner in Poster Area
   D. Lankin,
   Poster Session Co-ordinator

Wednesday, July 19

7:00-8:15 Breakfast

8:30-10:30 Tips & Techniques
   D. Lankin
   (8x15 min presentations)

10:30-11:00 Coffee Break

11:00-12:30 Forensic NMR
   J. Myers & P. Hays
   Co-chairs

12:30-12:45 Closing Remarks

12:45 Box lunch & departure
Position Available

An immediate one-year post-doctoral position is open in our lab for the following MRI investigations:

- mixing flows of highly concentrated (model) suspensions in relation to the preparation of cement and concrete;
- flow of water through either model porous materials (bead packing) or concrete during infusion and drying processes.

The research will be carried out using our unique MRI set-up (a 0.5 T vertical magnet with a 40 cm bore) which is devoted to the study of civil engineering materials. The work will be done in close collaboration with two researchers in our lab who are involved in the rheology of granular pastes and water transfer in concrete. The experimental set-up for the first part of the work is now ready.

The successful candidate should have a Ph.D. in physics or a related field and a wide experience in NMR (and possibly MRI) of highly heterogeneous porous materials.

Applications should be sent to:
Ph. Coussot, LMSGC, 2 Allée Kepler, 77420 Champs-sur-Marne, France.
Tel.: 01 40 43 65 41 email: philippe.coussot@lcpc.fr

Field of Dreams

By Kip Shaffer

SHIMMING FOR INSOMNIACS

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NMR TECHNOLOGIES: Development and Applications for Drug Discovery

November 4-5, 1999 • Sheraton Inner Harbor Hotel • Baltimore, Maryland

Major advances in NMR technologies continue to enable dynamic, molecular structure (SAR) studies leading to a greater understanding of some of the mechanisms of various diseases as well as targeted therapeutic drug design and discovery programs. New biomedical and materials sciences are fueling the development of high-field NMR spectroscopy as a more accessible tool for researchers. Researchers are continuing to develop new ways to share their NMR resources more efficiently and creatively, primarily over the Internet. Driving the interest in faster access to SAR analyses is genome research. Major emphasis will be placed on the application of NMR to drug discovery processes this year, including case studies and other examples from large pharmaceutical and biotech organizations.

SESSION TOPICS INCLUDE:
ADVANCES IN NMR TECHNOLOGIES AND METHODOLOGIES
Flow NMR Spectroscopy
Cryoprobe for NMR
Capillary-Based Microliter-Volume NMR
Solid-State NMR Approaches to the Study of Biomolecular Self-Assemblies
Autoscreen: Automated Processing and Analysis of Receptor/Ligand Binding NMR Data
Automated Analysis of Protein NMR Spectra
ASTER: Fast and Accurate NMR Structure Determination
High-Efficiency NOE Assignments and Structure Calculations

NMR FOR DRUG DISCOVERY
NMR Pattern Recognition of Biofluids
Structure-Based Drug Design
Structures, Interactions, and Dynamics of Protein-Ligand Complexes of Therapeutic Interest
PFG-NMR Detection of Anticancer Drugs Bound to Okazaki Fragments
Interaction of Cyclic Peptides with HIV-1 TAR RNA
SAR by NMR
Novel Applications of NMR SHAPES Screening in Drug Discovery
Application of NMR in High-Throughput Pharmaceutical Research and Development
Development of Affinity NMR
Alignment of Small Molecule Fragments That Interact with Protein Targets

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□ Molecular Diversity (MLD)
□ Phage Display (PGD)
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• Request a refund minus the cost ($195) of ordering a copy of the document binder

NOTE: Cancellations will only be accepted up to one week prior to the conference.

Program and speakers are subject to change.
The NMR Newsletter (formerly the TAMU NMR Newsletter, the IIT NMR Newsletter, and originally, the Mellon Institute NMR Newsletter), now in its forty-second year of consecutive monthly publication, continues under the same general policies as in the past.

1. Policy:

The NMR Newsletter is a means for the rapid exchange of information among active workers in the field of NMR spectroscopy, as defined broadly, including imaging. As such, the Newsletter serves its purpose best if the participants impart whatever they feel will interest their colleagues, and inquire about whatever matters concern them. Technical contributions should always contain a significant amount of information that has not already been published or that will appear in the formal literature within a few weeks of the appearance in the Newsletter.

Since the subscriber/participant clearly is the best judge of what he or she considers interesting, our first statement of policy is "We print anything." (This is followed by the reservation, "that won't land us in jail or bankruptcy court.") Virtually no editorial functions are performed, although on rare occasions there is the need to classify a contribution as 'not for credit'. The Newsletter is not, and will not become, a journal. We merely reproduce and disseminate exactly what is submitted.

2. Public Quotation and Referencing:

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

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

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

Frequent contributions are encouraged, but no advance credit can be obtained for them. In cases of joint authorship, only one contributor may be credited. Meeting announcements, as well as "Position Available," "Equipment Wanted" (or "For Sale"), etc., notices are very welcome, but only on a not-for-credit basis, i.e., such items do not substitute for a bona fide technical contribution.

4. Finances: The Newsletter is wholly self-supporting, and its funding depends on Advertising, Sponsorships, and individual Subscriptions. The Subscription fee for the October 1999 - September 2000 year is US$190, with a 50% academic or personal subscription discount. Subscriptions are available for a minimum of the twelve monthly issues which end with a September issue. However, a subscription can be initiated at any time, with the price for more than twelve issues being prorated.

continued
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5. Practical Considerations:

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

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

c) Contributions should be on 8.5 x 11" (21 x 27.5 cm) pages, printed on one side only. Contributions should be submitted in camera-ready condition. Contributions may not exceed three pages without prior approval. Each page must have margins of at least 0.5" (1.3 cm) on all four edges. Black ink for typing, drawings, etc., is essential. All drawings, figures, etc., should be mounted in place on the 8.5 x 11" pages. We are not equipped to handle pieces of paper larger than 8.5 x 11" (21 x 27.5 cm).

d) Please include your e-mail address on your contribution.

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

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

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i) Try using a smaller type font: The body of this page is printed in 10 point type, which I believe is adequate for most purposes. Even 11 or 12 point type is acceptable if the particular font is not too large. Type smaller than 8 point should not be used.

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

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

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

iv) AVOID DOUBLE SPACING LIKE THE BLACK PLAGUE !!! This is extremely wasteful of space.

6. Suggestions: They are always welcome.

October 1999

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