To: All Facility Users

From: John Harwood (jharwood@purdue.edu)

Date: July 11, 2006

Subject: 1) Bruker ARX-400 (369 WTHR) Open For Use

2) Revisions to Bruker Training Procedures

1) I am very pleased to announce that our most recently acquired NMR spectrometer is now available for general usage. The installation of the Bruker ARX-400 spectrometer in 369 WTHR is finally completed, after being beset by many problems. This spectrometer is equipped with a 4-nucleus (“QNP”) probe and is capable of observing $^1$H, $^{19}$F, $^{31}$P and $^{13}$C nuclei. I am happy to report that this spectrometer is now returning very good figures for $^1$H and $^{13}$C sensitivity, and I am confident that it will prove to be a useful addition to our Facility, particularly for $^{13}$C acquisitions. Indeed, the $^{13}$C sensitivity is about twice that of the Facility’s 300-MHz Varian systems located in BRWN/WTHR. In addition, the ARX-400 will provide better $^{13}$C spectra overall than does the DRX-500-1, at a lower cost-per-hour.

For those of you who might be interested, here is a comparison of $^1$H and $^{13}$C sensitivity for our Facility’s routine-use spectrometers.

<table>
<thead>
<tr>
<th>Console/Probe</th>
<th>$^1$H sensitivity</th>
<th>$^{13}$C sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Varian 300’s, 4-nucleus probes</td>
<td>100:1</td>
<td>90:1</td>
</tr>
<tr>
<td>ARX/DPX-300’s, QNP probe</td>
<td>130:1</td>
<td>120:1</td>
</tr>
<tr>
<td><strong>ARX-400, QNP probe</strong></td>
<td><strong>230:1</strong></td>
<td><strong>190:1</strong></td>
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<tr>
<td>DRX-500-1, Cryoprobe</td>
<td>3800:1</td>
<td>200:1*</td>
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<tr>
<td>DRX-500-2, TXI probe</td>
<td>800:1</td>
<td>90:1*</td>
</tr>
<tr>
<td>DRX500-2, BBO probe</td>
<td>350:1</td>
<td>300:1</td>
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</tbody>
</table>

*These probes will show a background signal or rolling baseline when used for $^{13}$C acquisition.

All current Bruker users will have access to this spectrometer without further training. However, because of the differences in operation between this spectrometer and our Bruker Avance spectrometers, each current user must attend a 30-45 minute overview session prior to being allowed to use the ARX-400. I would like to schedule these overview sessions in a group-wise fashion. Please contact Donna Bertram (dbertram@purdue.edu, 4-7850) regarding the scheduling of these overview sessions.
2) Along with the ARX-400 becoming available, we are taking this opportunity to introduce new operating and training procedures for the Facility’s Bruker NMR spectrometers. From now on, a single training procedure will be followed to train users on any PINMRF Bruker spectrometer. Once the user is checked out on one PINMRF Bruker spectrometer, that user will have access to all the Facility’s Bruker spectrometers. The only other condition extant is that the user must attend a 30-minute cryoprobe overview session prior to getting their account opened on the DRX-500-1.

There are three other items of note that are related to this new training procedure. First, it is not required that a user be checked out on the Varian Mercury-200 prior to obtaining Bruker training. Second, we will no longer train new users in the use of IconNMR. Current users who use IconNMR may still use this automated system to obtain spectra, however, all new users will be trained using XWinNMR. This change is critical to the overall efficiency of the new training plan. Third, we will now allow new Bruker users to be trained by their fellow group members, provided that two conditions are met:

a) the trainer is a checked-out user with a reasonable amount of experience, and

b) the training follows the currently published PINMRF training methods.

This change will eliminate the need for new Bruker users to have to schedule training meetings with PINMRF staff, however, PINMRF staff will gladly provide new-user training if desired. All new Bruker users, whether trained by PINMRF staff or by their fellow group members, must complete a safety briefing and pass both a written and a practical exam in order to get checked out for spectrometer operation.

The new training materials will be printed and placed in a binder adjacent to each Bruker spectrometer. These materials also will be available for download from the PINMRF website, and can be obtained from Donna Bertram (dbertram@purdue.edu, 4-7850).

We are currently working on rationalizing our Varian 200/300 training procedures in a similar fashion. I will send out another memo when this is completed.

In closing, I would like to thank Eli Lilly and Company for the donation of the Bruker ARX-400 spectrometer and Jerry Hirschinger for all of his work on the renovation of 369 WTHR and the spectrometer installation.

If you have any questions or concerns that I may be able to address, please feel free to contact me.

cc:  Department Heads
     F. Lytle
     D. Raftery
     NMR Support Staff