



**Trip Report:
Northeast Users Meeting
Bruker BioSpin, Inc.
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***Abstract:** Bruker BioSpin, Inc. hosts regional users' group meetings annually. The NE Users Meeting was held on November 3-4, 2005 in Cambridge, MA. The users meetings are a forum where application engineers and customers have the opportunity to report on specific areas of interest or problems that they were able to correct. There were approximately 60 attendees present from both industry and academia. This report provides a brief summary of the presentations given*

The first presentation was an introduction by Paul Cope, our Sales Representative. He discussed all the new products Bruker introduced this year. He spoke on the AVANCE II Spectrometers, which are 2nd generation digital receivers. The new receivers give improved S/N, flatter baselines

and larger band widths with digital quadrature detection (DQD). He then mentioned Bruker released version 1.3 of the new NMR software, TopSpin. The software operates all AVANCE style spectrometers. Bruker also introduced a new samplechanger for both 5 mm and 1 mm sample tubes. The changer can draw sample right from a 96 well plate when equipped with the 1 mm accessory. Bruker introduced several new probes for solution analysis. They were a 400 MHz BBOF, which is a broad band probe with can observe ^{19}F ; a 400 MHz Cyro-probe; a 1 mm Z-Grad using a sample funnel and a Gilson LC autosampler; and 10 mm cyro probe with Z-gradients, used mostly for polymers.

The next presentation was the second in a series on pulse programming. The nomenclature for pulses and power levels was discussed. Fortunately, the nomenclature has not changed for new NMR operating software, called "TopSpin," so the commands from the present software, XWIN-NMR, will still function correctly. The presenter discussed high power pulses, on both channels; shaped pulses, gradient pulses, pulse trains as in MELV-17 in variable pulse (vp) lists; and power levels for shaped pulses.

The next presentation was on ^{19}F Data acquisitions. The presenter discussed the different field strength consoles require different amplifiers and he also mentioned the special pulse programs written for ^{19}F analysis for a quad-nuclear (QNP) probe. Two ^{19}F heteronuclear 2D experiments (HOESY and HSQC) were discussed and examples of how they are used in structural elucidation. Procedures on how to correct poor baselines in ^{19}F spectra were described. The presenter also described how to perform ^{13}C experiments with ^{19}F decoupling.

The next presentation was on solvent suppression. Several pulse programs for solution NMR and best application of each one were discussed. The pulse program, wet, is most commonly used in LC/NMR. This experiment achieves solvent suppression of multiple resonances and can be setup in automation. The presenter also described a new pulse program called **Purge**, which stands for **P**restaturation using **R**elaxation **G**radients and **E**choes, and was detailed in *J. Magnetic Resonance*, **175** (2005) 340-346. The advantages over the other techniques are the resonances close to the water resonance are not lost because of a stable narrow null on the water resonance; and the experiment produces a flat baseline over the entire spectral width.

The next presentation was the advantages of new version of the NMR acquisition and processing software, "TopSpin." TopSpin includes a new version of the automated acquisition software called ICON-NMR. Remote operation of TopSpin and ICON-NMR are now available through the TopSpin software. The web browser employed uses Corba Technology, which is state of the art in high security remote access. The NMR software administrator sets up user access, continuing to preserve security through out the operation. There are no slow refresh rate issues as with third party software packages (VNC), and the accessed computer is not locked by the remote computer as is with the computer's operating software remote feature (Windows™ Remote Desktop). Another time saving advantage of TopSpin is that the software allows for user created function buttons in the tool bar. A button can be created that performs several processes at once, i.e., exponential multiplication, Fourier transform and phasing are performed with the press of one button. The cost of TopSpin is \$1,500.00 for each license upgrade from XWIN-NMR. A new acquisition computer can be purchased from Bruker that is already configured to operate TopSpin properly for \$4,500.00, plus the cost of the new license. The presentation of TopSpin was so interesting; a copy of the software was obtained for a 3 month demonstration.

The last presentation was on identifying the causes of 2D NMR artifacts. There are environmental and hardware factors such as temperature, vibrations, DC offset, quad image, and poor amplifier/gradient performance which produce the artifacts. There are also programming errors that can cause poor quality spectra. Incorrectly set ninety degree pulses and cause T1 noise and poor sensitivity. An incorrectly set receiver gain can cause diamond pattern in DFQ-COSY spectra. The presenter discussed ways to correct all of these artifacts.

In conclusion, this user meeting was most informative and quite useful to the everyday user of Bruker NMR instruments and software. I highly recommend we attend every year.