

A CASE STUDY

## University of Houston NMR facility manager discusses the merits of JEOL's NMR platform, technology and software

From undergraduate teaching to research into the structure and dynamics of complex systems in chemistry, material science, and medicine – a look at NMR spectrometry at University of Houston.



Flexible, robust and easy-to-use – all words that describe important properties of a Nuclear Magnetic Resonance (NMR) spectrometer that is used for teaching in a large university.

But, in addition, the research interests of post-grads and faculty members demand higher specification, and the ability to perform across a broad range of applications. Here, Scott K. Smith Ph.D., NMR Lab Manager, Dept of Chemistry, University of Houston, explains how his JEOL NMR systems meet the diverse needs of an active academic community.

The University of Houston's chemistry department has four NMR systems and the pharmacy department has one – all from JEOL Inc. Our users come from a range of disciplines, with biology, physics, and engineering groups making up a total user group of over 100 students and 30 faculty staff at any given time.

I am responsible for the stewardship of all aspects of the NMR facility, including but not limited to: maintenance, calibration, training, software customization, new method development, and testing.

Having started in NMR back in the late 80s, I worked in a series of academic labs, before making a move into pharma, where I stayed for 13 years, specializing in structural elucidation of natural products. Having gained subsequent experience with an NMR manufacturer, I moved back to academia to take up this role in Houston around two years ago.

Being back in a university environment is great. I'm enjoying all the benefits of the last 30 years of instrument development in NMR; advances that have improved all aspects of system hardware, software, and applications capability.

Of course, routine 1D and 2D NMR are as they were – but simpler to do on the new spectrometers – and now it's quite straightforward to acquire diffusion, protein solid state, and quantitative NMR data. In my opinion, this university has a state-of-the-art instrumentation lab and the students are the real beneficiaries of that.

## A core role for NMR in a growing facility

In the last year, we have added two new NMR systems. Of course, we are bound by University funding rules and their process and procedures when we look to make such a significant capital purchase. In this case, we reviewed the market and had offers from all relevant vendors. We also considered benchtop instruments for the undergrad labs but, in my view, the best route was for us to go for a dual purpose set up that would handle both research and undergraduate work. We felt that JEOL offered us the best solution, as well as a favourable price compared to the competition. We chose to add an ECZ400L/S1 for undergraduate teaching and university research and the pharmacy department acquired its own ECZ600R/S1 for research.



Right out of the box, the system and user interface were easy to learn and use, and have been especially easy with respect to new user training. Simple and robust automation along with the flexible user interface allowed for focused customization for several different undergraduate classes, from first year organic to upper level PChem lab experiments.

## In daily use

As one would expect, the majority of NMR work here is routine 1D proton and carbon, which aid studies of natural or medicinal chemistry, super-molecular complex formation, in-solution catalysts for improved industrial processes, and polymer formation, for example.

I am pleased that the requirement for six weeks' NMR training when I was in graduate school is no longer needed. Because of the robust and reproducible pulse sequences, automated shimming, automated probe tuning and the customizable user interface that we have, I can give a basic training and documentation that guides a student through their experiments and process data without the depth of NMR knowledge formerly needed. For me, these are all tangible benefits of the current JEOL platform.

Installation, set-up and maintenance of the new spectrometers has been straightforward, and I believe that is largely due to the calibre of engineers and support staff JEOL makes available.

In particular, I have found the applications scientists to be extremely helpful and generous when I have needed support with troubleshooting or hardware specifics or application direction. I have also had the chance to speak to lead JEOL software developers, which was extremely useful. I have learned more in the last two years than probably the last ten before that. It's quite phenomenal the amount of support I have had from JEOL!

When doing new experiments, I have found them reasonably easy to implement and have obtained useful results quickly. I'd not previously done protein / diffusion work before and when I tested the system for these requirements, it just worked. I was impressed.

## In conclusion

For me, it's exciting to be helping the current generation of graduates and undergraduates at the University of Houston to discover the advantages of NMR for non-destructive structural elucidation, direct quantitative analysis, physical property measurements, and straightforward method development. In my experience, the JEOL systems provide a cost-effective, solid platform for a range of research activities across chemistry, polymer science, and engineering/material sciences.

