

# Science goes through the roof

## Specialized NMR equipment delivered

COLLEGE STATION – Top-notch molecular research swung into gear at Texas A&M University this week – literally.

A crane lowered a high-field 800 megahertz Nuclear Magnetic Resonance spectrometer through an opening in the roof of a biochemistry and biophysics building Wednesday, putting the university on par with leading U.S. research institutions, according to Dr. Gregory Reinhart, department head.

The German-made instrument, which was flown on a cargo plane accompanied by an engineer and transported to the Texas A&M campus on a special truck, is expected to be fully operational by the first of September.

The Nuclear Magnetic Resonance technique, commonly called NMR, is the forerunner of the more widely known MRI. Reinhart explained that an MRI makes images of human tissue for medical diagnostics, but NMR makes images at the molecular level for scientific exploration.

"This is a major step forward in the capability of the university in the general area of structural biology," said Reinhart, whose department collaborated with Texas AgriLife Research, a part of the Texas A&M System, to obtain the equipment.

The equipment will benefit researchers from across Texas A&M, officials noted.

"We are excited to partner with Texas A&M University to bring this powerful instrument to campus," said Dr. Craig Nessler, AgriLife Research director. "It is critical that we find ways to collaboratively provide such state of the art equipment to our scientists to maintain our research competitiveness."

Structural biology means looking at macromolecules which consist of hundreds or thousands of atoms and then deducing the way these are built and how they move, Reinhart said. Knowing how the molecules work helps scientists create solutions for a variety of needs.

"Macromolecules are important in disease research as well as for studying all biological problems, from plant growth control to waste management in feedlots," Reinhart said.

Prior to obtaining the \$2.7 million NMR, Texas A&M researchers had access to two 600 megahertz and one 500 megahertz NMRs, he noted. Those will remain operable in the biochemistry department's new NMR wing, but the new larger magnet will provide faster, more detailed results.

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"The business component of an NMR spectrometer is a very large, super-conducting magnet the strength of which is measured by the frequency of protons that resonate in it," said Dr. Tatyana Igumenova, a biochemist and director of the Biomolecular NMR facility. "By today's standards this is considered to be a very high-field instrument."

One common application of the high-field NMR, she said, is in drug design.

"NMR offers a very quick and easy way to test if a drug candidate binds to a particular protein or enzyme, for example," she said. "If you can map the binding site and understand what a particular drug candidate is doing to the protein structure and dynamics, this in turn would enable you to design even better therapeutic agents."

Because the new equipment also has a CryoProbe, or cold probe that keeps the electronics responsible for signal detection at the temperature of helium gas, less noise is generated and that leads to improved signals, Igumenova said. In essence, what would have been a two-day experiment on the existing equipment could now be done in half a day.

Reinhart said Texas A&M researchers will now have better access to three complementary methods in structural biology research: x-ray crystallography, electron microscopy, and NMR spectroscopy.

"These methods serve different purposes," he said. "With x-ray crystallography, the sample is immobile because it has been crystallized so that limits what can be studied about function but the structural information is very precise. Electron microscopy doesn't afford the atomic resolution but it images anything so one doesn't have to have pure samples.

"The NMR does not quite have the precision of X-ray but it comes close, and one can observe the molecule in solution which is more like its native environment and with motion which is important to understanding function."

Igumenova said graduate and undergraduate students will be trained to use the equipment as well as to process and interpret the data. She also plans to use a portion of her National Science Foundation Faculty Early Career Development Grant to provide opportunities for underrepresented students to use the equipment in studies.

"It's a stepping stone into even greater research opportunities in the future," Reinhart said.

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