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DEVELOPERS



Monday,
January 13, 2003

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Blowing
Snow
28°F / -2°C
Wind Chill
13°F /
-11°C



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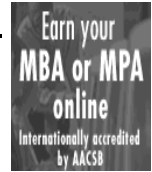
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HIGH TECHNOLOGY
Breakthrough at UB



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New techniques determine the structure of a protein molecule 250 times faster than conventional nuclear magnetic resonance methods

By FRED O. WILLIAMS
News Business Reporter
1/13/2003

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BILL WIPPERT/Buffalo News
Dr. Thomas Szyperski works with Nuclear Magnetic Resonance Spectrometers, which determine protein structures.

Society describing a breakthrough in NMR technology. He and another scientist developed computational techniques that determined the structure of a protein molecule 250 times faster than conventional NMR methods, according to UB.

"I think the main story is, it makes optimal use of the NMR," Szyperski said.

The drawback for conventional NMR research has been its slow pace, taking days or even months to produce a molecular picture, he said.

Doctors use nuclear magnetic resonance - NMR machines - to peer into patients, looking for problems.

Now a development at the University at Buffalo makes NMR technology better at seeing the structure of molecules - a key step toward finding disease-fighting drugs.

UB chemist Thomas Szyperski published a paper Friday in the Journal of the American Chemical



taking days or even months to produce a molecular picture, he said.

UB has filed a patent application on the computational technique, called G-matrix Fourier Transformation, that Szyperski developed with Seho Kim, formerly a postdoctorate fellow at UB.

With a Rutgers University scientist, Szyperski plans to develop a software package that incorporates the technique, for use by researchers and pharmaceutical companies.

The work extends Buffalo's presence in molecular structure research. X-ray crystallography, also used for structural research, was pioneered by Nobel laureate Herbert Hauptman, founder of the Hauptman-Woodward Research Institute.

Scientists familiar with the development at UB said it will boost NMR imaging's role in mapping protein molecules, a task seen as the follow-up to sequencing the human genome.

NMR provides "a different way of modeling the shape of a protein," said Cheryl Arrowsmith, senior scientist at Ontario Cancer Institute in Toronto.

She has used NMR imaging to study the shape of protein p53, which figures highly in cancer research because of its role in regulating cell growth.

Stronger NMR techniques developed at UB should complement work by researchers using other methods, she said. For example, X-ray crystallography was unable to image the entire p53 molecule, leaving some of its active sites undetermined.

Szyperski's lab is a member of the Northeast Structural Genomics Consortium, nine research groups working to capitalize on the results of the human genome project.

NMR imaging works on molecules in solution - the way they are found in the body - while X-ray techniques require painstaking preparation of a crystal containing the molecule.

To image molecular structures, NMR measures resonance frequencies of atomic nuclei within a magnetic field. Using computational methods and spectrum analysis, the Szyperski group's G-matrix method arrives at resonance frequencies faster than determining them through lengthy sampling, according to the research paper.

NMR has been used for protein imaging since the mid-1980s, according to UB. In that time it has determined about 20 percent of the

structures in the global scientific protein databank.

The UB technique should leverage the research ability of new, more powerful magnets coming into research use. UB researchers will have access to a \$5 million NMR machine at the New York Structural Biology Center in New York City, said Szyperski, an associate professor of chemistry and biochemistry.

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