

# Study applies neutrons to study hydrogen transfer in biological systems

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An innovative collaboration among scientists at Los Alamos National Laboratory, Fox Chase Cancer Center and the University of Tennessee has successfully applied neutron diffraction to create a three-dimensional map of the structure of the enzyme D-xylose isomerase. It is a model system for understanding other proteins involved in biological processes.

The first to locate the enzyme's active hydrogen atoms, the new research will be published on-line the week of May 15-19 in the early edition of *Proceedings of the National Academy of Sciences* as well as in the journal's June issue.

Hydrogen atoms are the workhorses of the enzyme, carrying out the chemical reactions it facilitates--such as the conversion of glucose to fructose to produce the high-fructose corn syrup widely used to sweeten sodas and other commercial foods.

Finding the hydrogen atoms reveals how water (H<sub>2</sub>O) molecules are bound in a protein. The way water interacts influences the protein's function.

Work in the Fox Chase laboratory of Jenny P. Glusker, D.Phil., first revealed the structure of D-xylose isomerase in 1984 using X-ray crystallography.

"However, this technique does a poor job of locating hydrogen atoms,

which make up about half of all atoms in a protein," explained Amy K. Katz, a Fox Chase visiting scientist from the University of Tennessee at Knoxville and a lead author of the new report along with Gerard J. Bunick, Ph.D., of the University of Tennessee.

"Now, using the world's only spallation neutron source equipped for protein diffraction studies, based at Los Alamos National Laboratory, it has been possible to locate the hydrogen atoms at active sites in crystals of D-xylose isomerase," Katz said. "This research demonstrates the potential for locating and understanding hydrogen-atom transfer processes in large biological systems, which could lead to improved and better-targeted medicines."

## **X-Rays Versus Neutrons**

The longest-used method of determining molecular structure, X-ray crystallography bombards crystallized molecules with X-rays, which scatter--diffract--to create patterns that are captured on film or electronically. The data and 3-D computer graphics allow researchers to study possible molecular models.

Neutrons--uncharged subatomic particles--are another tool for probing biological structures and complements X-ray diffraction and other microscopic studies. However, unlike X-rays, neutron scattering can detect heavy and light elements equally well and even sense vibrations of atoms as well as their positions.

An accelerator generates neutrons by driving an intense beam of particles, usually protons, into a target of heavy atoms. This knocks neutrons loose from the nuclei of the target, a process called spallation. The resulting neutron pulse can be directed into numerous experimental stations.

"The future of structural biology is in spallation sources," said study co-author Benno P. Schoenborn, Ph.D., of the Los Alamos, N.M., facility when it opened its protein crystallography station at the Los Alamos Neutron Science Center in 1997.

Source: Fox Chase Cancer Center

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