

## Highest prize in scientific computing goes to chemists from UCSD and SDSC

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### HIGHEST PRIZE IN SCIENTIFIC COMPUTING GOES TO CHEMISTS FROM UCSD AND SDSC

A team of chemists from the University of California, San Diego and the San Diego Supercomputer Center has been awarded the Fifth Annual Forefronts of Large-scale Computation Award, the nation's highest prize in scientific computing.

Recipients of the award include UCSD chemists Susan Taylor, Daniel Knighton, Janusz Sowadski and Lynn Ten Eyck, who holds a joint appointment with UCSD and the San Diego Supercomputer Center.

The group was awarded for its studies of protein kinases, essential proteins that play important roles in regulating cell growth and behavior.

"This work represents an outstanding example of the interdisciplinary approach to the use of large-scale computation in the solution of important problems in science and engineering," said David S. Wehrly, chairman of the Forefronts board.

With the help of the center's supercomputers and graphics workstations, in 1991 the team solved and published the three-dimensional structure of a member of the kinase family, a large group of proteins. Since then, the structure has been used as a template to solve and model the structures of other kinase molecules.

"Since some kinases are known to play a role in disease processes, including immunodeficiency diseases, diabetes, cancers, Alzheimer's disease, Lou Gehrig's disease, and myotonic dystrophy, knowledge of their structures will help scientists find ways to deal with these diseases," said Taylor.

"Most of the kinase-related diseases seem to be due to loss of control over the action of the kinase," she added. "The result can be too much activity, too little activity, or activity at the wrong time.

"One way to deal with these situations is to find or construct other molecules that will bind with the uncontrolled kinases and interfere with or stop their activities."

To help accomplish that goal, Taylor's research group has turned to the SDSC's new CRAY C-90, which has roughly twice the speed and twice the memory of the center's previous system.

Taylor was elected a Fellow of the American Academy of Arts and Sciences in 1992 in recognition of her work. The work also constituted Knighton's doctoral dissertation and, in 1991, won the UCSD Martin Kamen Prize for the best dissertation in the areas of biology and chemistry. Knighton is now a postdoctoral fellow at Agouron Institute in La Jolla.

Ten Eyck is co-director with Taylor and John Tainer, of The Scripps Research Foundation, of the Computational Center for Macromolecular Structure--a joint project between UCSD, SDSC, and Scripps for the development and distribution of software for the study of biological macromolecules. Ten Eyck, a senior staff scientist with SDSC who has a joint appointment in the chemistry department at UCSD, was one of the early developers of software for the determination of accurate three-dimensional structures of proteins.

Administered by General Atomics, the SDSC is one of four National Science Foundation centers. With a staff of more than 100 scientists and researchers, the center serves 3,000 researchers from 355 academic and research institutions and more than 50 industrial partners.

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