Center For Computational And Structural Biology

Campus-wide effort focuses on structure of living systems

With expertise from scientists in diverse disciplines, including medicine, microbiology, mathematics, physics, engineering, and chemistry, UAB’s Center for Computational and Structural Biology (CCSB) brings together computer-intensive, structure-based approaches aimed at uncovering functional and interactive mechanisms of complex living systems, Professor of Medicine and CCSB Director Jere Segrest, MD, PhD, says.

“The center is combining powerful tools — X-ray crystallography, nuclear magnetic resonance spectroscopy, ... continued on page 2

DISCHARGE GROWTH PROJECTIONS AND UAB MARKET SHARE — BIRMINGHAM MSA*

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<th>County</th>
<th>2004 Discharge Estimates</th>
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<th>% Growth 2004-2009</th>
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*Though not included in the Census Bureau definition, Walker is a county from which UAB receives substantial admissions.

Source: Solucient Growth Estimates and UAB Discharge data
Prepared by: UABHS Dept of Strategic Planning
cryo-electron microscopy, and computational biology — to develop detailed molecular models of a gene’s protein products. Structural images can tell us how proteins function and interact in health and disease and will foster rational drug design,” he says.

Dr. Segrest and Director of UAB’s Center for Biophysical Sciences and Engineering Larry DeLucas, OD, PhD, who is contributing X-ray crystallography expertise to CCSB, share an interest in determining membrane protein structures.

“Half of all therapeutic drugs target membrane proteins, but only about 20 of 300,000 have been crystallized, so we know very little about their structure,” Dr. Segrest says. “Computational biology, which uses the linked power of high-performance computers to mimic movements of individual molecules, is poised to give us meaningful information about membrane proteins, predicting their structure and telling us how they interact with each other.”

Dr. Segrest cites cystic fibrosis transmembrane regulator (CFTR), the protein defective in cystic fibrosis, as an example of a membrane protein of interest at UAB whose structure could be predicted by computational biology. “The crystallography group has been working to crystallize CFTR but has not yet determined its structure. Creating predictive computer models of CFTR could provide clues that ultimately lead to its crystallization.”

UAB’s Enabling Technology Laboratory (ETL) in the Department of Mechanical Engineering provides the massive computing power required by such modeling. ETL’s cluster of 124 high-performance computers will increase to 512 in the next few months, Dr. Segrest says.

TRANS-CAMPUS EFFORT

Professor of Microbiology Peter Prevelige, PhD, is CCSB associate director. His work focuses on hydrogen deuterium exchange, which can help quantify protein structure changes and is part of the center’s efforts to develop methods of mapping protein-lipid interactions, Dr. Segrest says.

“The center coordinates UAB’s efforts in structural biology, bringing together scientists from the medical and academic sides of the campus,” says Dr. Segrest, who gives credit to the CCSB’s influential “trans-institutional” advisory committee for helping make the center possible.

Committee members include Drs. DeLucas and Prevelige, Vice President for Research Richard Marchase, PhD; Dean of the School of Engineering Linda Lucas, PhD; Dean of the School of Natural Sciences and Mathematics Lowell Wenger, PhD; Associate Dean of Medicine Samuel Brown, EdD; Department Chairs David David, MD, PhD, microbiology; David Graves, PhD, chemistry; William Koopman, MD, medicine; Jay M. McDonald, MD, pathology; David Shealy, PhD, physics; Anthony Skjellum, PhD, computer and information sciences, Bharat Soni, PhD, mechanical engineering; and Tim M. Townes, PhD, biochemistry and molecular genetics.

“Combining different approaches to solve the extremely complex problems of structural biology can lead to extraordinary new drugs and procedures targeting humans’ most persistent and difficult medical problems,” Dr. Segrest says.

“Ultimately, the answers to the questions we ask could tell us everything we want to know about living organisms, wellness, treatment of disease, and aging.”

Riley Joins Neurosurgery

UAB Professor and Director of the Division of Neurosurgery Richard B. Morawetz, MD, announces the appointment of Kristen Riley, MD, as assistant professor.

A Phi Beta Kappa graduate of the University of North Carolina at Chapel Hill, Dr. Riley completed her MD degree at the School of Medicine at UAB, where she was inducted into Alpha Omega Alpha. She completed a neurosurgery residency at UAB and a 6-month fellowship in epilepsy at The Great Ormond Street Hospital for Children in London, England.

Dr. Riley’s clinical interests center on surgery for epilepsy, as well as surgery for pituitary tumors. She is accepting patients at The Kirklin Clinic®. For patient appointments, call 996-2461; e-mail kroriley@uabmc.edu.

Appointments

ALLIED HEALTH PROFESSIONAL
Paul D. Blanton, PhD, 934-3537, RWUH M001, Neuropsychology, Effective March
University Hospital’s Pediatric Unit

A SAFE HAVEN

A bright, cheerful pediatric unit, structured to meet the special needs of children and adolescents, awaits University Hospital’s pediatric patients. Located on the 5th floor of Spain Wallace, the unit cares for children undergoing transplantation, those with heart disease requiring catheterization or surgery, and those with complex dental problems requiring surgery, among others, according to Child Life Coordinator Jane Love.

“When possible, we visit other hospital units to see pediatric patients, as well,” she says.

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All medical equipment, including that used for resuscitation, is age-specific. The 17-bed unit features private rooms with televisions, video machines, guest sleeping accommodations, pediatric chairs, and a kitchen, as well as a laundry area, activity and play room, and family room.

Child life specialists on the unit demystify procedures and help patients psychologically prepare for tests and treatments. “We see patients and families often during hospitalization to monitor reactions to medical activities, provide information, help families understand children’s response to treatment, and arrange for appropriate play activities,” Love says.

The American Academy of Pediatrics (AAP) policy on Child Life Services (Pediatrics. 2000;106:1156-1159), says “play is the primary modality of a child life program, which makes pediatric patients’ hospital stays more comfortable and less intimidating. “We use medical play, games, or puzzles to explore intimidating medical equipment and address specifics of procedures or therapy to ease anxiety and give children some sense of control over these encounters,” Love says.

AAP policy defines children as individuals aged 18 years or younger and specifies that they would benefit from a child life program that addresses the psychosocial concerns that accompany hospitalization of children and adolescents. The policy also states that a child-life program can help organizations meet Joint Commission on Accreditation of Healthcare Organization standards to provide developmentally appropriate care, patient education, and patient assessments.

“It is important that hospitalized children have somewhere to go outside their hospital rooms to relax and spend time with other children. Since they cannot play outside, activity and play rooms meet that need,” Love says. Patients can paint, draw, play with toys and games, participate in music therapy, or use the activity room computer. Research confirms that play helps children to work through the stresses of hospitalization.

“We work closely with nurses when preparing patients for invasive procedures or painful treatments by telling them what to expect in an age-appropriate manner. For instance, before starting an IV, we go through the entire procedure using a teddy bear or doll to ease their fears. While the procedure is under way, we stay in the room and distract the patient,” Love says. “Instead of holding a child down for a venipuncture, for example, we encourage parents to use a comforting position, such as a hug—which is far less traumatic.”

For information about admitting policies for the unit, call Nurse Manager Candace Smiley at 934-4267.