Proudly sponsored by

WHITING-TURNER

EMJAY ENGINEERING AND CONSTRUCTION CO., INC.

RMF Engineering
Reliability. Efficiency. Integrity.

UNIVERSITY of MARYLAND
THE FOUNDING CAMPUS

PRODUCED BY THE OFFICE OF COMMUNICATIONS AND PUBLIC AFFAIRS, 2012

UNIVERSITY OF MARYLAND

Founders Week 2012

Researcher of the Year

ALEXANDER MACKERELL JR., PHD

"From Balls on Springs to Drugs and Things"

WEDNESDAY, OCTOBER 24, 2012
4 P.M.

PHARMACY HALL | 20 N. PINE STREET
N103 LECTURE HALL

Alexander MacKerell Jr., PhD

"From Balls on Springs to Drugs and Things"

The Faculty Research Lecture for Founders Week 2012 highlights Alexander MacKerell Jr.'s 25-year quest to improve the mathematical models used to simulate biological and pharmaceutical molecules using computers and apply them toward drug design. The lecture will introduce molecular models and how they can be improved to better understand chemical and biological systems. The application of such models in computer-aided drug design will be presented in the context of a collaborative study to develop chemicals that can inhibit the protein BCL6, with the goal of developing drugs for the treatment of diffuse large B-cell lymphoma (DLBCL).

If imitation is the sincerest form of flattery, Alexander MacKerell Jr., Grollman-Glick Professor of Pharmaceutical Sciences at the University of Maryland School of Pharmacy, should feel flattered indeed.

At last count, his work has been cited 13,000 times by fellow researchers, with his 1998 paper "All-Atom Empirical Potential for Molecular Modeling and Dynamics Studies of Protein" being cited more than 4,500 times alone.

At the School of Pharmacy's Computer-Aided Drug Design (CADD) Center, which he directs, MacKerell has used his improved computational models of chemicals to facilitate the identification of novel compounds for development into therapeutic agents for the treatment of pain, cancer, and bacterial infections.

"The field of research I'm in allows me to understand the molecular details that control a range of biological functions," says MacKerell. "Obtaining such an understanding requires a variety of tools that allow us to 'see' the molecular phenomena. One of these tools is computational chemistry, a field to which we have made a nice contribution."

"Nice" is an understatement. "It is no overestimation to state that Dr. MacKerell is a world leader in the area of computational chemistry," says Andrew Coop, PhD, chair of the School's Department of Pharmaceutical Sciences.

MacKerell's global impact is borne out by his nomination letters from scientists in places like Sweden and Switzerland. His research has attracted substantial funding (more than $9 million from the National Institutes of Health alone) and numerous patents and patent applications. He is committed to the training of postdoctoral fellows and graduate students and is a willing interdisciplinary research partner even before funding has been secured.

"The CADD Center has been involved in a wide range of collaborations that have allowed a number of biologists at the University of Maryland as well as at other institutions to extend their research programs into the area of drug design and discovery," says MacKerell. "Importantly, these collaborative efforts have led to grant funding, which is good for the institution as a whole as well as for the individual scientists."