

2006 Press Release

Chemical Computing Group Announces Excellence Award Winners at the 2006 ACS in San Francisco, CA.

MONTREAL, May 30, 2006 - Chemical Computing Group (CCG) and the American Chemical Society's (ACS) Division of Computers in Chemistry (COMP) congratulate the winners of the CCG Excellence Awards at the 232nd ACS National Meeting in San Francisco, California.

The well-regarded CCG Excellence Award honors graduate students who have excelled in the field of computational chemistry. Winners are selected according to the distinction and relevance of their research, as well as the quality of supporting materials. CCG will finance each awardee for travel costs to San Francisco for the Fall 2006 ACS; will recognize their research at the Awards Presentation during the COMP Division Poster Session on Tuesday September 12, 2006; and will give a one-year license for their software, the Molecular Operating Environment. For more information on how to submit for the 2007 ACS Award in Chicago, please contact Andrew Good at: Andrew.Good@bms.com

Fall 2006 ACS San Francisco, CA Winners:

Ying Wei, Northeastern University

High-recall, high-precision prediction of protein binding sites from 3D structure

Sara E. Nichols, Yale University

Shrinking residues for enhanced Monte Carlo sampling for proteins

Timothy H. Click, University of Oklahoma

Locating alpha-helices and beta-strands using recently-developed protocols

Johannes Hachmann, Cornell University

Quadratic Scaling Multireference Correlation in Polyenes and Long Molecules with the Local Density Matrix Renormalization Group

Zhi Wang, Emory University

Quantum Chemical Molecular Dynamics Study of Catalyst-Free SWNT Growth from SiC-derived Carbon