



Press Release

November 11, 2003

CCG Honors Excellence Award Winners at the Spring ACS in Anaheim, CA

MONTREAL, November 11, 2003 - Chemical Computing Group (CCG) and the American Chemical Society's (ACS) Division of Computers in Chemistry (COMP) are proud to announce the latest winners of the CCG Excellence Awards for the 227th ACS National Meeting in Anaheim, California.

The CCG Excellence Awards are intended to encourage graduate student participation and interaction among computational chemists in the COMP Division activities at ACS National Meetings. Winners are selected according to the high quality and relevance of their research, as well as the caliber of supporting materials. The winners will receive a one-year software license for the most recent version of MOE, the Molecular Operating Environment, in addition to reimbursement for travel expenses to Anaheim, California for the ACS National Meeting.

Congratulations to the following winners!

Cheng, Xiaolin - "*Molecular Dynamics Simulations of 8-oxoguanine: A mismatch DNA*". Department of Chemistry and Center for Structural Biology, Stony Brook University.

Perryman, Alexander - "*HIV-1 Protease Molecular Dynamics of a Wild-Type and of the V82F/I84V Mutant: Possible Contributions to Drug Resistance and a Potential New Target Site for Drugs*". Howard Hughes Medical Institute, Department of Pharmacology, & Dept. of Chemistry and Biochemistry, University of California at San Diego.

Ladiwala, Asif - "*Prediction of Protein Affinity in Hydrophobic Interaction Chromatography using Quantitative Structure-Retention Relationship (QSRR) Models*". Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute.

Okur, Asim - "*Multiple pathways in beta-hairpin folding and unfolding simulations*". Department of Chemistry, Stony Brook University.

Swanson, Jessica - "*Revisiting Free Energy Calculations: One Step Closer to Rigorous Scoring Functions and One Step beyond MM/PBSA*". Department of Chemistry & Biochemistry, University of California.

Tubert-Brohman, Ivan - "*Improved Semiempirical Methods: Parameterization of PDDG/PM3 for Sulfur*". Department of Chemistry, Yale

University.

Mueller Stein, Sarah A. - "*The Influence of Steric Congestion on the Dynamics and Geometry of DNA*". Duquesne University.

Deng, Wei (David) - "*Predicting Protein-Ligand Binding Affinities using Transferable Atom Equivalent (TAE) Techniques And Machine-Learning Methods*". Department of Chemistry, Rensselaer Polytechnic Institute.

Bender, Andreas - "*Similarity Searching using Atom Environments, Information Gain based Feature Selection and the Naive Bayesian Classifier*". Unilever Centre for Molecular Informatics, Department of Chemistry, University of Cambridge.

Loccisano, Anne E. - "*Development of New CHARMM Force Field Parameters for Novel DNA Bending Agents*". Duquesne University.

CCG acknowledges all of the applications submitted, and continues to promote graduate students working in the field of Computational Chemistry.

For more information, please contact:

