CHEMICAL COMPUTING GROUP
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Press Release

July 22, 2003

CCG Honors Excellence Award Winners at the Fall ACS in New York

MONTREAL, July 30, 2003 - Chemical Computing Group (CCG) and the American Chemical Society's (ACS) Division of Computers in Chemistry (COMP) congratulate the latest winners of the CCG Excellence Awards for graduate student research. A presentation of the awards will take place during the COMP division poster session on Tuesday, September 9th in New York.

"We at CCG have enjoyed watching this award develop over the past few years. Helping to nurture the relationship between academia and industry will continue to be a priority for us", says Pamela Newton, Director of Sales and Marketing at CCG. "We are especially pleased with the response and high quality of the applicants the competition has received." The award was initially developed to promote interaction between graduate students and computational chemists. This has been successful through encouraging student participation in the COMP Division activities at ACS National Meetings.

The winners were selected based upon the high quality and significance of the research they will be presenting in New York, as well as the strength of supporting letter and other materials submitted. Each winner will receive reimbursement for travel expenses to the ACS and a license for MOE, the Molecular Operating Environment.

GHOSH, Tuhin
Department of Chemical Engineering, Rensselaer Polytechnic Institute
Proteins Under Stress: Molecular Studies of Pressure Effects on Proteins
Sekhar Garde

THOMPSON, Jason
Department of Chemistry and Supercomputer Center, University of Minnesota
Predicting Aqueous Solubility: A Fundamental Approach
Christopher J Cramer

UDIER-BLAGOVIC, Marina
Department of Chemistry, Yale University
Validation of A Model for the Complex of HIV-1 Reverse Transcriptase with Non-Nucleoside Inhibitor TMC125
William L. Jorgensen

MATTIONI, BRIAN
Department of Chemistry, Pennsylvania State University
Classifying the Mutagenicity of Two Diverse Sets of Organic Compounds Using Ames Test Data for Salmonella Typhimurium TA100 and TA98

Peter C. Jurs

RATHORE, Nitin
Department of Chemical Engineering, University of Wisconsin
Density of States Simulations of Proteins in a Continuum
Juan J. de Pablo

SHEN, Min
Division of Medicinal Chemistry and Natural Products School of Pharmacy, University of North Carolina, Chapel Hill
Discovery and Experimental Validation of Novel Functionalized Amino Acid Anticonvulsant Compounds: A Success Story of QSAR-Based Database Mining
Alex Tropsha

WANG, DONG-QI
Department of Chemistry, University of Hong Kong
A DFT Investigation of the Remarkable Reactivity of the Gem-Dizinc Carbenoid (IZn) 2CHI as a Cyclopropanation Reagent with Ethylene Compared to its Mono Zinc Carbenoid IZnCHI2
David Lee Phillips

WU, YUDONG
Department of Chemistry, Princeton University
Application of a Coarse-Grained Dynamical Method to Explore the Conformational Space of Small Molecules
Roberto Car

SHEN, LING-LING
Department of Chemistry, Rensselaer Polytechnic Institute
Modeling the mu-opiod receptor affinity of synthetic 8-aminocyclazocine analogues using TAE, PEST and PAD descriptors and machine-learning methods
Curt M. Breneman.

TSCHAMPEL, SARAH
Department of Chemistry, University of Georgia
Rational Development of a Lone Pair Inclusive Force Field
Robert J. Woods

Applicants first submit an application to the Treasurer of the COMP division for consideration. This includes an abstract of the poster or presentation along with a letter of support from the research advisor, a CV and a personal statement. An abstract must also be submitted through the ACS OASYS system for online submissions prior to the deadline for the meeting.

All graduate students are encouraged to submit applications for the awards. Students from the same research groups, or who have won in the past are also encouraged to apply. Awards will be given only to those individuals making the presentations and not co-authors.

Chemical Computing Group Inc. is a leading provider of computational applications for the Life Sciences. CCG's develops and markets MOE - Molecular Operating Environment, which offers visualization, simulation, and methodology development in one package. MOE provides an integrated suite of powerful, yet intuitive chemistry software tools for HTS, Structure Based

Design, Molecular modeling and Protein and Homology modeling as well as an embedded programming language for the rapid prototyping of scientific methods. Computational chemists, medicinal chemists and biologists use MOE in pharmaceutical companies, biotechnology companies, and universities worldwide.

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