



## Press Release

August 15, 2002

### CCG Announces Winners of 5th CCG Excellence Award

BOSTON, October 20, 2002 - The American Chemical Society's (ACS) Division of Computers and Chemistry (COMP) and Chemical Computing Group (CCG), are pleased to announce the winners of the CCG Excellence Awards for the Fall ACS National Meeting, to be held in Boston, MA from August 19-21, 2002.

Chemical Computing Group ([www.chemcomp.com](http://www.chemcomp.com)) develops and markets MOE, the Molecular Operating Environment, a leading application for chemical researchers in the pharmaceutical and biotechnology fields. MOE's built-in applications cover the spectrum of drug discovery including: Protein/Homology modeling, High Throughput Screening Data Analysis, Combinatorial Library Design, Modeling/Simulations and Methods Development. MOE's unique architecture and platform independence allows it to be used enterprise-wide by a variety of researchers from methods developers, computational experts and medicinal chemists. CCG's customers include a worldwide roster of leading pharmaceutical and biotechnology companies.

The CCG Excellence Awards have been created to stimulate graduate student participation in COMP Division activities (symposia and poster sessions) at ACS National Meetings. Winners will receive a one-year software license of CCG's MOE (Molecular Operating Environment) for their academic research groups, in addition to travel costs associated with attending an ACS National Meeting to present their research.

In alphabetical order, the winners are:

- Srikanth Kidambi from the University of Michigan, for the paper entitled "Quantum chemical calculations of cadmium chemical shielding tensors in biologically relevant molecules"
- Qiong Luo from the Rensselaer Polytechnic Institute, for the paper entitled: "Prediction of Glass Transition Temperatures for Polymers Using TAE/RECON Method"
- Nathan R. McElroy from the Pennsylvania State University, for the paper entitled: "Classification of Cytogenetic Toxicity of Organic Compounds from Molecular Structure"
- Suhas J. Patankar from the Pennsylvania State University, for the paper entitled: "Classification of HIV Protease Inhibitors and Prediction of Their Antiviral Potency from Molecular Structure"
- Minghu Song from the Rensselaer Polytechnic Institute, for the paper entitled: "Prediction of Protein Retention Times in Anion-exchange System using Support Vector Machine Regression"

- Shixiang Yan from the New York University, for the paper entitled: "Molecular dynamics simulation and free energy analysis of polycyclic aromatic carcinogen-damaged DNA: accurate representation and new insights"

Awardees are chosen on the basis of the quality and significance of the research to be presented and the strength of the supporting materials. Please join us in congratulating the winners on Tuesday August 20, 2002, at the COMP General Poster Session held in Hall B at the Hines Convention Center between 7:00 p.m. and 10:00 p.m.

Applications for the next round of CCG Excellence Awards will be accepted shortly. Application for these awards is a two-step process. First, one must submit an abstract through the ACS OASYS system for online paper submissions. Secondly, an application for the Award must be submitted to the Treasurer of the COMP division for consideration.

Deadlines for these two steps are different to allow graduate students time to compile the additional paperwork needed to complete the application. Deadlines for the 2003 Spring National Meeting to be held in New Orleans, LA, will be announced shortly. The website for submissions will be [www.acs.org/meetings/neworleans2002](http://www.acs.org/meetings/neworleans2002). Supporting materials must include an extended 1-2 page abstract for your paper along with a letter of support from your research advisor, a two-page CV and a personal statement.

All graduate students are encouraged to submit applications for the Awards. Students from the same research group are encouraged to apply. Students from research groups that have won awards at previous ACS meetings are also encouraged to submit applications. Awards will be given only to those individuals making presentations, and not co-authors.