



## Press Release

August 28, 2001

### **CCG Excellence Award Winners Announced at the Fall 2001 National ACS Meeting in Chicago**

MONTREAL and CHICAGO, August 28, 2001 -- The American Chemical Society (ACS) Division of Computers in Chemistry (COMP) and Chemical Computing Group (CCG), announced the winners of the CCG Excellence Awards for the Fall ACS National Meeting, held in Chicago, IL from August 26-30, 2001. The awards were created by CCG in conjunction with the COMP division. They were created to stimulate graduate student participation in COMP division activities (symposia & poster sessions) at ACS National Meetings. Winners receive a one-year software license for CCG's MOE (Molecular Operating Environment) for their academic research groups, in addition to reimbursement for travel costs associated with attending an ACS National Meeting to present their research.

We are very happy to once again have the opportunity to work with COMP to reward deserving students for their exceptional scientific work and encourage everyone to participate in ACS functions such as the National Meetings," said Bill Hayden, Vice President of CCG.

In alphabetical order, this sessions winners are:

- Caterina Bissantz, Dept. of Applied Bioscience, Swiss Federal Institute of Technology, Zurich, for her poster: *Virtual Screening of Chemical Databases: Application of G-protein Coupled Receptors*. Advisor: Gerd Folkers.
- Catherine Check, Dept. of Chemistry, Northern Illinois University, for her poster: *Augmentation of the LANL2DZ Basis Set Under B3LYP and MP2 Models to Improve Calculated Results for p Block Elements*. Advisors: Thomas M. Gilbert and Lee S. Sunderlin.
- Norge Cruz Hernandez, Dept. of Physical Chemistry, University of Seville, Spain, for his poster: *DFGT and Molecular Dynamic Study of ScN, TiN, and VN Materials*. Advisor: Javier Fernandez Sanz.
- Ohyun Kwon, Dept. of Chemistry, Auburn University, for his poster: *Theoretical Studies of Main-Group Metallocenes*. Advisor: Michael L. McKee.
- Nelaine Mora-Diez, Dept. of Chemistry, Dalhousie University, Halifax, Nova Scotia for her poster: *Theoretical Calculations in Atmospheric Chemistry: OH and NO Hydrogen-Abstraction Reactions from Aldehydes*. Advisor: Russell J. Boyd.

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 28, 2001 at the COMP General Poster Session between 7:00 p.m. and 10:00 p.m.

Applications for the next round of CCG Excellence Awards (Orlando - April 2002) are currently being accepted. 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.

**ABOUT CCG:**

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