

Scripting & Programming: Cross Pharma Collaboration in High Performance Computing (Pharma HPCs): Zheng P Yang & Eugene Fluder

Scripting & Programming: HPC on the Cheap (GPU HPCs): Rajarshi Guha

Drug Discovery (Drug Disco): Y Jane Tseng & Scott Wildman

To reflect the interdisciplinary nature of computational chemistry, the **Molecular Mechanics** and **Quantum Chemistry** symposia have been unified into sessions that focus on: Proteins, Materials, Colloids, Waters, Membranes, Molecular Dynamics, Small Molecules, Data Analysis, Computational Experiments, Methodology, and Methodology Review.

Cosponsored symposia

Computer Modeling: The Wave of the Future and its Benefits for Small Business Owners (SCHB): Masha V Petrova

Data Intensive Drug Design (CINF): John Van Drie

Design, Discovery & Directed Evolution of Enzyme Activities (BIOL): Thomas Magliery

The Emerging Concepts of Activity Landscapes & Activity Cliffs and their Role in Drug Research (CINF): Jurgen Bajorath, Gerry Maggiora & Mic Lajiness

Semantic Web in Chemistry (CINF): Egon Willighagen & Martin Braendle

Simulation of Interfaces (PMSE): Hendrik Heinz

The COMP Division would like to recognize the following organizations that have provided financial support:

BioSolveIT

Cambridge Crystallographic Data Centre

ChemAxon

Chemical Computing Group

Dell

HP

Intel

Journal of Computer-Aided Molecular Design

The New Tripos

OpenEye

Pfizer

Pharsight

RCHSolutions

Schrödinger

Springer Publishing Company

Thomas-Reuters

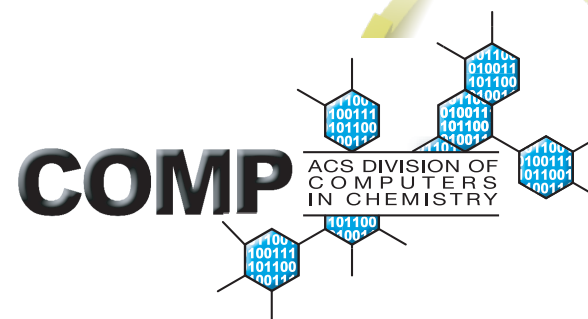
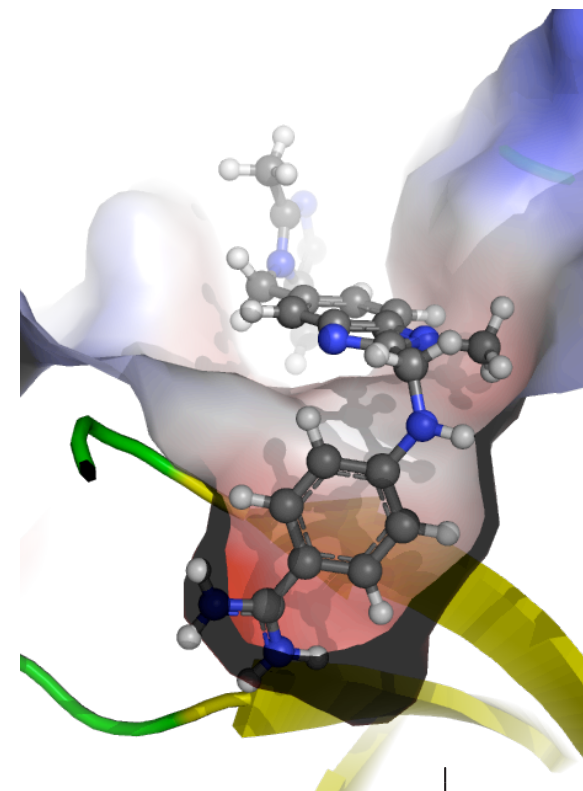


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Group Name: ACS Computers in Chemistry (ACS COMP)

All things COMP: www.acsCOMP.org



The Fall National Meeting
Boston, Massachusetts
August 22nd - 26th, 2010

Symposia

Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J Berne: Gregory Voth, Mark E Tuckerman & John Straub

An Emerging Challenge in Multiscale Modeling & Simulation: Mechanistic Understandings: Jih-Wei Chu & Hong Guo

The Journal of Chemical Information and Modeling's 50th Anniversary Symposium (JCIM's 50th): William Jorgensen. Corresponding AM session is in CINF.

The PDB & Chemistry (PDB): Terry Stouch

The Community Structure-Activity Resource Scoring Challenge (CSAR): Heather Carlson

Docking & Scoring: Neysa Nevins, Greg Warren & Georgia McGaughey

Success Stories in Computer-Guided Chemistry (Success stories): Abby Parrill

Using Waters Explicitly in Drug Discovery: Veerabahu Shanmugasundaram & Woody Sherman

Targeting Gram-Negative Pathogens (Pathogens): Veerabahu Shanmugasundaram & Jeremy Starr

Challenges in Industrial Computational Methods: Elizabeth Sourial & Anthony Nicholls

Emerging Technology: Curt Breneman

Tautomers in Biology: Yvonne Martin & Terry Stouch

COMP abstracts for the Spring 2011 National Meeting in Anaheim, California are due by October 30th, 2010!

AM	Sunday Aug 22 nd	Monday Aug 23 rd	Tuesday Aug 24 th	Wednesday Aug 25 th	Thursday Aug 26 th
156C	Tribute to Bruce J Berne				Materials
156B	Proteins	Emerging Challenge in Multiscale Modeling & Simulation			
157A	Colloids	Challenges in Industrial Comp Methods			Pathogens
157C	Tautomers in Biology			Success Stories	MD
157B	Comp Experiments	CSAR		Docking & Scoring	
154	Drug Discovery				
153C	Methodology	Waters	Small Molecules (Room 155)		

**Mentor Lunches! Tuesday, August 24th @ Noon!
Sign up at the COMP table outside of Room 154!**

PM	Sunday Aug 22 nd	Monday Aug 23 rd	Tuesday Aug 24 th	Wednesday Aug 25 th	Thursday Aug 26 th
156C	Tribute to Bruce J Berne				Materials
156B	Proteins	Emerging Challenge in Multiscale Modeling & Simulation			
157A	GPU HPCs	Challenges in Industrial Comp Methods			Pathogens
157C	PDB	JCIM's 50 th	Membranes	Pharma HPCs	Data Analysis
157B	Drug Disco	CSAR	Docking & Scoring		
154	Using Waters Explicitly in Drug Discovery			Emerg Tech	Drug Disco
153C	Methodology Rev				

SciMix :: Monday, August 23rd @ 8pm Hall C - BCEC

The COMP Poster Session with the CCG & HP Awards ::

Tuesday, August 24th @ 6pm Grand Ballroom Foyer (3rd Level BCEC)