# COMP

# DIVISION OF COMPUTERS IN CHEMISTRY

## Final Program, 238th ACS National Meeting, Washington, DC, August 16-20, 2009

J. D. Madura, E. X. Esposito, and A. E. Roitberg, *Program Chairs*

**SOCIAL EVENT:**
**Academia & Industrial Mentor Lunches. Please meet outside Room A:** Tue

## SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Binding and Recognition**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**8:15 —** Introductory Remarks.

**8:20 —1.** The effects of active site solvation and protein conformational flexibility on protein-ligand binding. **R. A. Friesner**

**9:00 —2.** Gated binding of ligands to proteins. **J. A. McCammon**

**9:40 —3.** Following biomolecular recognition and association at the microsecond/atomic scale. **R. Baron**, C. A. F. de Oliveira, J. A. McCammon

**10:00 —** Intermission.

**10:20 —4.** Dynamics and conformational changes in DNA-binding proteins. **M. Ikeguchi**

**11:00 —5.** Functionally important conformations of enzymes are populated by rapid thermal fluctuations. **K. Arora**, C. L. Brooks III

**11:20 —6.** Modeling of synergistic regulation and ligand-induced conformational changes of

tryptophan synthase. **C -E. A. Chang**, M. Q. Fatmi, R. Ai

**11:40 —7.** Human Glutathione Synthetase (hGS) and its mechanism of negative cooperativity. **B. Wilson**, M. E. Anderson, T. Brown, S. Hernandez, A. K. Wilson, T. R. Cundari

Section B

Unknown Site -- Unknown Room

**Structure Activity Relationship Knowledgebases**

*Cosponsored by CINF*
E. Bolton and S. Senger, *Organizers, Presiding*

**9:00 —** Introductory Remarks.

**9:05 —8.** Detection, assignment and analysis of multiple scaffolds for medicinal chemistry project databases. **A. M. Clark**

**9:35 —9.** Online chemical modeling environment: models. **I. Sushko**, S. Novotarskyi, A. K. Pandey, R. Körner, **I. V. Tetko**

**10:05 —10.** In silico profiling based on Aureus Global Pharmacology Space Knowledgebase. **F. Petitet**

**10:35 —** Intermission.

**10:50 —11.** BIDATA: An SAR Knowledgebase for data retrieval and new compound suggestions. **S. Oloff**

**11:20 —12.** Using knowledgebases of structure-activity-data, receptor-site and protein structural similarity to generate new matter ideas. **S. M. Muskal**

Section C

Unknown Site -- Unknown Room

**Quantum Chemistry**

**Pushing the Envelope... and Electrons**

A. E. Roitberg, *Organizer*
J. R. Hammond, *Presiding*

**8:30 —13.** Density Matrix Renormalization Group Self Consistent Field - Canonical Transformation calculation on conjugated polyenes. **D. Ghosh**, E. Neuscamman, T. Yanai, G. K. Chan

**9:00 —14.** Continuous and smooth potential energy surface for conductor-like screening solvation model using fixed points with variable areas. **P. Su**, H. Li

**9:30 —15.** Energy decomposition analysis of bonding and nonbonding interactions. **H. Li**, P. Su

**10:00 —** Intermission.

**10:10 —16.** Heterogeneous conductor-like screening solvation model for quantum chemical calculation: Implementation and application. **H. Li**, D. Si

**10:40 —17.** Excitation energy in solution at EOM-CCSD level, a state specific approach within the polarizable continuum model. **M. Caricato**, B. Mennucci, G. Scalmani, G. Trucks, M. Frisch

**11:10 —18.** O+ethylene potential energy surface: Theoretical study at the MCSCF and MRMP2 levels. **A. C. West**, J. S. Kretchmer, K. Park, H. Lischka, W. L. Hase, T. L. Windus

**11:40 —19.** Orbital ordering in Density Matrix Renormalization Group methods. **C. C. Ralph**, D. Zgid, G. K. Chan

Section D

Unknown Site -- Unknown Room

**The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry**

**Reaction Mechanisms in Biological Systems**

*Cosponsored by St. Jude Children's Research Hospital*
A. M. Ferreira, *Organizer, Presiding*

**8:30 —** Introductory Remarks.

**8:50 —20.** DFT and ONIOM(DFT:MM) computational studies of *myo*-inositol oxygenase: Insights into the (superoxo)diiron(III/III) intermediate and reaction mechanism. **H. Hirao**, K. Morokuma

**9:40 —** Intermission.

**10:30 —21.** Quantum mechanics-coupled AMBER ff99 compatible heme parameters for the P450 catalytic cycle. **K. Shahrokh**, G. S. Yost, T. E. Cheatham III

**11:20 —22.** Substrate hydroxylation by the P450s: Is there any consensus mechanism? **N. R. Jena**

Section E

Unknown Site -- Unknown Room

**Computational Chemistry in the Discovery & Development of Novel Anti-Infective Agents**

*Cosponsored by CINF*
G. S. Weston, R. J. Czerminski, and J. I. Manchester, *Organizers, Presiding*

**8:20 —** Introductory Remarks.

**8:30 —23.** 2'-F-2'-C-Methyl nucleosides for the treatment of HCV: From discovery to the clinic. **M. J. Sofia**

**9:00 —24.** Modeling binding modes of HIV integrase inhibitors. **X. Chen**, S. Swaminathan, J. M. Chen

**9:30 —25.** Identifying novel anthrax toxin lethal factor inhibitors via topomeric searching and docking/scoring. **E. A. Amin**, T -L. Chiu, D. Hook, M. A. Walters, S. Patil

**10:00 —** Intermission.

**10:15 —26.** Fragment-based molecular docking in inhibitor discovery against CTX-M class A β-lactamase. **Y. Chen**, B. Shoichet

**10:45 —27.** Design and optimization of novel peptide deformylase inhibitors as new antibacterial agents . **K. M. Aubart**, D. Qin, A. B. Benowitz, X. Liao, J. M. Karpinski, J. Lee, J. Dreabit, Y. Fang, A. Knox, S. Kelly, N. Campobasso, C. Duraiswami, K. J. Smith, M. Cummings, J. Briand, S. Kulkarni, T. F. Lewandowski, P. DeMarsh, R. Zonis, L. McCloskey, S. Rittenhouse, S. B. Christensen, M. Zalacain

**11:15 —28.** De novo design of novel Polypeptide Deformylase (PDF) inhibitor templates with broad spectrum antibacterial activity. **C. Duraiswami**, R. A. Daines, N. Campobasso, M. Vimal, I. Pendrak, M. Zalacain, K. M. Aubart

**11:45 —29.** Discovery of Novel Small-Molecule Inhibitors of P. falciparum using the Hybrid Structure Based Method. **S. Kortagere**, J. Morrisey, J. Bosch, K. Laroiya, T. Daly, W. Welsh, E. Fan, W. Hol, P. Sinnis, I. Ejigiri, L. Bergman, A. Vaidya

**Chemical Text Mining and Public Molecular Databases**

*Sponsored by CINF, Cosponsored by COMP*

# SUNDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Binding and Recognition**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**1:20 —30.** Visualizing lowly-populated regions of the free energy landscape of macromolecular complexes by paramagnetic relaxation enhancement . **G. M. Clore**

**2:00 —31.** All-atom simulations of coupled folding-binding of unstructured proteins. **R. B. Best**

**2:40 —32.** Assembly/Disassembly Mechanisms of Multidomain Src Kinase Revealed by X-ray Solution Scattering and LRET. **S. Yang**, L. Blachowicz, W. Sandter, F. Bezanilla, L. Makowski, B. Roux

**3:00 —** Intermission.

**3:20 —33.** Flexible Biomolecular Recognition and Conformational Changes. **J. Wang**, Q. Lu

**4:00 —34.** Binding cooperativity in R67DHFR. **J. L. Poutsma**

**4:20 —35.** Conformational Coupling in an Effector-GTPase Interaction: Differences in the Complex Formation of the Plexin GTPase Binding Domain with Rac1 and Rnd1. **M. Buck**

**4:40 —36.** Deciphering the post-replication DNA-mismatch recognition cycle in prokaryotic MutS and eukaryotic MSH2-MSH6. **S. Mukherjee**, S. M. Law, M. Feig

Section B

Unknown Site -- Unknown Room

**Structure Activity Relationship Knowledgebases**

*Cosponsored by CINF*
E. Bolton and S. Senger, *Organizers, Presiding*

**1:30 —37.** Structure activity relationship analysis using PubChem. **E. Bolton**

**2:00 —38.** GOSTAR: GVKBIO Online Structure Activity Relationship Database – Data and its Utility. **J. Sarma**

**2:30 —** Intermission.

**2:45 —39.** ChEMBL: Large-scale Mapping of Medicinal Chemistry and Pharmacology Data to Genomes. **J. P. Overington**

**3:15 —40.** Pharmacoinformatics on very large annotated ligand databases. **R. Jain**, A. Ausekar

Section C

Unknown Site -- Unknown Room

**Molecular Mechanics**

**Our Blood, Sweat, and Tears**

E. X. Esposito, *Organizer*
S. E. Nichols, *Presiding*

**1:30 —41.** An image-based reaction field method for electrostatic interactions in molecular dynamics simulations of aqueous solutions. **Y. Lin**, A. Baumketner, S. Deng, Z. Xu, D. Jacobs, W. Cai

**2:00 —42.** Aromatic oligoamide foldamers: Conformational insights from molecular dynamics simulation using reparameterized molecular mechanics force fields regarding aromatic-amide torsions. **Z. Liu**, J. Galan, V. Pophristic

**2:30 —43.** Fully-flexible polarizable water model for classical and multiscale Molecular Dynamics simulations. **P. K. Biswas**

**3:00 —** Intermission.

**3:10 —44.** POLARIS: software and alanine parameters for fast polarizable calculations. **G. A. Kaminski**

**3:40 —45.** PRIMO: A transferable physics-based coarse-grained model for peptides and proteins. **M. Feig**, S. M. Gopal

**4:10 —46.** Statistically optimal multidimensional potentials of mean force with large data sets. **M. Shirts**, J. D. Chodera, Z. Tan

Section D

Unknown Site -- Unknown Room

**Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches**

**Nanoscale Interfaces and Energy Transport**

*Cosponsored by PMSE*
H. Heinz, *Organizer, Presiding*

**1:00 —** Introductory Remarks.

**1:05 —47.** Simulations of interfaces and nanostructures using first principles based methods. **W. A. Goddard III**

**1:40 —48.** Simulation of organic-inorganic interfaces: The case of self-assembled monolayers on metal oxides in organic opto-electronic devices. **J -L. Brédas**

**2:15 —49.** The workings of nitrogenase and new developments of the projector augmented wave method . **P. E. Bloechl**, J. Kaestner, S. Hemmen

**2:50 —** Intermission.

**3:05 —50.** Molecular Dynamics study of the effect of inorganic ions on the aggregation of carbocyanine dyes in aqueous solution. **A. E. Masunov**

**3:40 —51.** Conservative algorithm for an adaptive change of resolution in mixed atomistic / coarse-grained multiscale simulations. **A. Heyden**

**4:00 —52.** Density dependence of azobenzene switching on gold: A mean field/quantum chemistry study . C. Chapman, **I. Paci**

Section E

Unknown Site -- Unknown Room

**Computational Chemistry in the Discovery & Development of Novel Anti-Infective Agents**

**Part II**

*Cosponsored by CINF*
G. S. Weston, R. J. Czerminski, and J. I. Manchester, *Organizers, Presiding*

**1:30 —** Introductory Remarks.

**1:40 —53.** Some observations on the quality of 3D QSAR data sets. **R. J. Czerminski**, C. Eyermann, J. I. Manchester

**2:10 —54.** AutoGrow: A novel algorithm for protein inhibitor design. **J. D. Durrant**, R. E. Amaro, J. A. McCammon

**2:40 —55.** Computational Models of the Action of Protegrin Antimicrobial Peptides: Transient Ion Diffusion and Osmotic Swelling . **D. Bolintineanu**, E. Hazrati, A. A. Langham, R. I. Lehrer, H. T. Davis, Y. N. Kaznessis

**3:10 —** Intermission.

**3:25 —56.** Design of new antibacterial drugs: Computational approaches that take advantage of the rapid generation of multiple co-crystal structures. **J. Finn**

**3:55 —57.** Heme oxygenase as antimicrobial target: Results from computer-aided drug design and experiment. **P. E. M. Lopes**, A. Wilks, A. D. MacKerell Jr.

**4:25 —58.** Methodologies for efficient knowledge-based antibody homology modeling. **J. Maier**

**4:55 —59.** Prediction of drug resistance using all-atom molecular simulations. **R. C. Rizzo**

**Chemical Text Mining and Public Molecular Databases**

*Sponsored by CINF, Cosponsored by COMP*

## MONDAY MORNING

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Coarse Graining and Multiscale Methods**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**8:20 —60.** Unveiling conformational changes of biological molecules using multiscale modeling and multiresolution experiments. **F. Tama**

**9:00 —61.** Examining protein dynamics and function using multiscale methods. **B. R. Brooks**

**9:40 —62.** Extracting multiscale information from time series characterizing proteins under the influence of time dependent external forces. **C. P. Calderon**

**10:00 —** Intermission.

**10:20 —63.** Mixing Structure-Based and Physics-Based Coarse-Grained Models: Application to Membrane Proteins. **X. Periole**, S. J. Marrink

**11:00 —64.** Modeling of transmembrane proteins and peptides: All-atom and coarse grain molecular dynamics simulations of helical bundles in palmitoyloleoylphosphatidylcholine (POPC) lipid bilayer. **Z. Liu**, T. H. Nguyen, J. Galan, R. DeVane, P. B. Moore

**11:20 —65.** Systematic coarse-craining of biomolecules. **L. Larini**, G. A. Voth

**11:40 —66.** Conserved networks underlying protein structure, folding and dynamics. **L. H. Greene**, J. Pothen, J. A. Tibbitt, H. Li

Section B

Unknown Site -- Unknown Room

**Structure Activity Relationship Knowledgebases**

*Cosponsored by CINF*
E. Bolton and S. Senger, *Organizers, Presiding*

**9:00 —67.** Linking genomic knowledge to natural products and drugs. **M. Kanehisa**

**9:30 —68.** Metabolic Liability and SAR Analyses Derived from Bioactivity Databases. **R. Hillard**

**10:00 —** Intermission.

**10:15 —69.** Discovery and data mining using the NCBI BioSystems database, a centralized repository linking small molecules to their biological function. **L. Geer**

**10:45 —70.** SAR studies using ‘ChemBioBase', a knowledge base on Target centric small molecules. **S. Kumar**

**11:15 —** Panel Discussion.

Section C

Unknown Site -- Unknown Room

**Quantum Chemistry**

**Quantum Chemistry & Proteins. That's Like Congress & The Senate Getting Along**

A. E. Roitberg, *Organizer*
F. Ding, *Presiding*

**8:30 —71.** Ab initio transition state optimizations of the peptidyl transfer reaction in the ribosome. **G. Wallin**, S. Trobro, J. Åqvist

**9:00 —72.** Artificial reaction coordinate “tunneling” in free energy calculations: the catalytic reaction of RNase H. **E. Rosta**, H. L. Woodcock III, B. R. Brooks, G. Hummer

**9:30 —73.** Improvements of a fragment-based quantum chemical approach: The border region problem. **T. E. Exner**, S. Eckard, A. Frank

**10:00 —** Intermission.

**10:10 —74.** QM/MM Studies of Interaction Mode of B12-Independent Dehydratase with Glycerol. **Y. Liu**, A. A. Gallo, W. xu

**10:40 —75.** Using semiempirical methods to predict Young's moduli of elastomeric proteins. **J. J. P. Stewart**

**11:10 —76.** What happens to amino acids' hydrogen bonding in variable pH? **M. D. Bojin**

Section D

Unknown Site -- Unknown Room

**The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry**

**Methods Development**

*Cosponsored by St. Jude Children’s Research Hospital*
A. M. Ferreira, *Organizer, Presiding*

**8:30 —77.** Dynamic Contributions to Enzyme Catalysis as Illustrated by Orotidine Monophosphate Decarboxylase. **J. Gao**, A. Cenbran

**9:15 —78.** Integrating Electronic-Embedding QM/MM approaches with a conductor-like screening

model . **J. A. Gascon**

**10:00 —79.** Intramolecular hydrogen bonding of ortho-substituted arylamide oligomers: Model compound study. **J. Galan**, J. Brown, Z. Liu, J. L. Wildin, C. N. Tang, V. Pophristic

**10:45 —** Intermission.

**11:00 —80.** Quantum Chemistry for Protein Structure and Dynamics. **J. Z. Zhang**

**11:45 —81.** Post density functional theory approaches for elucidating metalloenzyme function and reactivity. **J. H. Rodriguez**

Section E

Unknown Site -- Unknown Room

**Scripting & Programming**

**Tools of the Trade**

J. M. Leonard, J. R. Hammond, C. Harwell, R. E. Amaro, and R. Guha, *Organizers*
E. X. Esposito, *Organizer, Presiding*

**8:30 —** Introductory Remarks.

**8:35 —82.** The snake that fits your brain: Python for computational chemists. **G. A. Landrum**

**9:10 —83.** The Cactvs Chemoinformatics Toolkit – Universal chemical information processing with Tcl scripts. **W -D. Ihlenfeldt**

**9:45 —84.** Vision: A software tool for visual programming and scientific workflows. **M. F. Sanner**

**10:20 —** Intermission.

**10:30 —** place holder for talk.

**11:05 —85.** Crunching molecules and numbers in R. **R. Guha**

**11:40 —86.** Optical Structure Recognition Application. **I. V. Filippov**, M. C. Nicklaus

**12:15 —** Concluding Remarks.

**Federated Search**

**Beyond Traditional A&I Services**

*Sponsored by CINF, Cosponsored by COMP*

## MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Enzyme Catalysis**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**1:20 —87.** Free energies and mechanisms of chemical reactions in enzymes and in solution with QMMM minimum free energy path. **W. Yang**

**2:00 —88.** Dynamical effects are important in ultrafast reactions but not in enzyme catalysis; advances in modeling long time enzyme dynamics . **A. Warshel**

**2:40 —89.** Computational delineation of the influence of slow modes on the catalytic step in DNA replication in a high fidelity polymerase . **R. Venkatramani**, R. Radhakrishnan

**3:00 —** Intermission.

**3:20 —90.** Engineering enzyme:substrate specificity: From free energy simulations to computational protein design. **T. Simonson**, D. Thompson, A. Lopes

**4:00 —91.** Proton transfer reactions in ketosteroid isomerase. **D. K. Chakravorty**, A. V. Soudackov, S. Hammes-Schiffer

**4:20 —92.** Linking enzyme structure, dynamics and catalysis. **P. K. Agarwal**

**4:40 —93.** Protein flexibility and energy flow during enzyme catalysis. **A. Ramanathan**, J. M. Borroguero, C. J. Langmead, P. K. Agarwal

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Drug Discovery I**

I. Visiers, *Organizer, Presiding*

**1:30 —94.** Binding free energy prediction by molecular dynamics based docking and volunteer computing. **O. Rahaman**, R. S. Armen, T. Estrada, D. J. Doren, M. taufer, C. L. Brooks III

**2:00 —95.** A Fresh Look on 3D Database Searching: Towards a Unified Description of Pharmacophoric Features and Shape. **M. Rarey**, J. Schlosser, C. Schärfer

**2:30 —96.** A gradient-directed Monte Carlo approach to molecular design. **X. Hu**, D. N. Beratan, W. Yang

**3:00 —** Intermission.

**3:10 —97.** Validating conformer generators using experimental structures: Promise and Problems. **P. Hawkins**

**3:40 —98.** Binding of ruthenium-based organometalic protein kinase inhibitors to PIM1, GSK-3, and CDK2 protein kinases evaluated through ensemble molecular docking simulations. Y. Liu, N. Agrawal, **R. Radhakrishnan**

**4:10 —99.** CNS library design using multiple parameter optimization. **S. Mente**, H. Berke, T. T. Wager

**4:40 —100.** Lead optimization of progesterone receptor partial-agonists by structure-based design and QSAR approaches in tandem . **C. Duraiswami**, D. Washburn, K. Madauss, M. Hammond, J. Frazee, T. H. Hoang, L. C. Johnson, S. Manns, J. R. Patterson, P. Stoy, J. D. Bray, N. J. Laping, E. T. Grygielko, L. Glace, W. Trizna, S -J. Deng, L. M. Azzarano, L. J. Jolivette, R. Nagilla, L. Barton, L. Kallander, Q. Lu, S. K. Thompson

Section C

Unknown Site -- Unknown Room

**Molecular Mechanics**

**BIG CALCULATIONS for small molecules**

E. X. Esposito, *Organizer*

X. Cang, *Presiding*

**1:30 —101.** Prediction of environmental impact of energetic materials with atomistic computer simulation. **N. Sokkalingam**, J. J. Potoff

**2:00 —102.** Investigating intramolecular hydrogen bonding in aromatic oligoamide foldamers . **J. A. Geer**, J. L. Wildin, G. Moyna, J. Galan, Z. Liu, V. Pophristic

**2:30 —103.** Modeling the reactivity of acid amplifiers. **R. L. Brainard**, S. A. Kruger, C. Higgins, S. Revuru, S. Gibbons, D. A. Freedman, W. Yueh, T. R. Younkin

**3:00 —** Intermission.

**3:10 —104.** Thermodynamically dominant hydration structures of aqueous ions. **S. Merchant**, D. Asthagiri

**3:40 —105.** Solvent-dependent mechanisms for triazolinedione and singlet oxygen ene reactions from QM/MM simulations. **O. Acevedo**

**4:10 —106.** Reactive force field modeling of Cu2+ and CuCl+ in aqueous solutions. **O. Rahaman**, A. C. van Duin, D. J. Doren

Section D

Unknown Site -- Unknown Room

**Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches**

**Polymers and Polymer Interfaces**

*Cosponsored by PMSE*
H. Heinz, *Organizer, Presiding*

**1:00 —107.** Simulating macromolecules by structure based coarse graining and adaptive resolution methods. **K. Kremer**, C. Peter, N. van der Vegt, L. Delle Site, M. Praprotnik

**1:35 —108.** Designing self-propelled trains of microcapsules. **A. C. Balazs**, O. B. Usta, A. Bhattacharya

**2:10 —109.** Single-chain dynamics in a homogeneous melt and a lamellar microphase: a comparison between Smart-Monte-Carlo dynamics, slithering-snake dynamics, and slip-link dynamics. **M. Müller**, K. C. Daoulas

**2:45 —110.** Percolation in networks of nano-rods. **T. Schilling**, M. A. Miller, S. Jungblut

**3:20 —** Intermission.

**3:35 —111.** Self-organized dispersion in a multi-component nano-clay composite by a coarse-grained Monte Carlo simulation. **R. B. Pandey**, B. L. Farmer

**4:10 —112.** Modeling of polymer-attached metal complexes for energy-dissipative materials. **B. C. Rinderspacher**, J. W. Andzelm, A. M. Rawlett, R. H. Lambeth III

**4:30 —113.** Combined ab initio/continuum mechanics approach for calculation of mechanical properties of polystyrene grafted nanotubes. **D. Kosenkov**, J. Leszczynski

**4:50 —114.** Self-Adaptive Surface: Atomistic Modeling Approach to Structural Reorganization of Self-Assembled Monolayer on H-Si (111) Surface. **S. S. Jang**

Section E

Unknown Site -- Unknown Room

**Emerging Technologies**

**Award Symposium Sponsored by COMP and Schrodinger, Inc**

C. M. Breneman, *Organizer, Presiding*

**1:00 —** Introductory Remarks.

**1:05 —115.** Implementation of coarse-grained models for molecular simulation on GPU architecture. I. Tunbridge, R. B. Best, **M. M. Kuttel**

**1:35 —116.** A catchment basin self-avoiding simulated annealing algorithm. **M. Li**, X. Lin

**2:05 —117.** Just add water: the prediction of the water content of binding sites. **J. Michel**, J. Tirado-Rives, W. L. Jorgensen

**2:35 —118.** Role of the active-site solvent in assessing feasibility of small-molecule lead discovery programs. **Y. Che**, V. Shanmugasundaram

**3:05 —** Intermission.

**3:20 —119.** Simultaneous discrete optimization of color and electronic hyperpolarizabilities in a chemical subspace. **B. C. Rinderspacher**, J. W. Andzelm, A. M. Rawlett, J. Dougherty, D. N. Beratan, W. Yang

**3:50 —120.** Quantum-Mechanical Simulation of Biological Macromolecules and its Application in Structure-Based Drug Design. **V. M. Anisimov**, V. L. Bugaenko, C. N. Cavasotto

**4:20 —121.** Combining self-guided Langevin dynamics with temperature-based replica exchange enhances thermodynamic sampling of protein folding. **M. S. Lee**, M. Olson

**4:50 —** Award Presentation.

**Federated Search**

**Beyond Traditional A&I Services**

*Sponsored by CINF, Cosponsored by COMP*

## MONDAY EVENING

Section A

Unknown Site -- Unknown Room

**Leaving the Nest: Life After Post-Doc'ing**

*Cosponsored by CPT, CEPA, YCC, PROF, and WCC*
L. M. Balbes, J. D. Madura, and E. X. Esposito, *Organizers*

**5:00 —122.** Leaving the nest: Life after post-docing. **L. M. Balbes**

Section B

Unknown Site -- Unknown Room

**Sci-Mix**

E. X. Esposito, *Organizer*

**8:00 - 10:00**

**189, 197, 206-207, 209, 212, 214, 216, 229, 236-237.** See subsequent listings.

## TUESDAY MORNING

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Methodology I**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**8:20 —123.** An Emerging Perspective in Free Energy Simulation of Protein Interactions. **W. Yang**

**9:00 —124.** Simulation of pH-dependent conformational changes in biomolecules. N. Di Russo, Y. Meng, M. A. Martí, D. A. Estrin, **A. Roitberg**

**9:40 —125.** Molecular dynamics studies on the interactions between cell-penetrating peptides and lipid bilayers. **H -S. Lee**, C. Dunkin, A. Almeida, P. F. Almeida

**10:00 —** Intermission.

**10:20 —126.** New Method for Enhanced Sampling. **J. Ma**

**11:00 —127.** Characterization of intrinsically unstructured p53 peptide conformations using simulations and experiment. **L. T. Chong**

**11:20 —128.** Energy landscapes analysis of disordered proteins: A case study of histone tail dynamics. **G. A. Papoian**, D. Potoyan

**11:40 —129.** Towards a biophysical characterization of enzyme evolution. M. Singh, K. Streu, A. McCrone, **B. N. Dominy**

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Drug Discovery II**

I. Visiers, *Organizer, Presiding*

**8:30 —130.** Computational analysis on NMR Screenings of the Pfizer Fragment Initiative collection. **Q. Hu**, J. Yan, J. M. Withka, P. Sahasrabudhe, C. Moore, J. Na, L. S. Narasimhan

**9:00 —131.** Computational and lipophilicity based studies drive optimisation of g-carbolines as CB1 agonists for analgesic activity. **S. Srivastava**, Y -X. Cheng, Z -Y. Wei, H. Yang, X. Luo, Z. Liu, M. Tremblay, D. Page, E. Lessard, S. St-Onge, W. Brown, M. Tomaszewski, C. Walpole, T. Groblewski

**9:30 —132.** Computational evaluation and development of novel antiarrhythmic agents targeting human ether go-go potassium ion channel. **J. Subbontina**, V. Yarov-Yarovoy, J. Lees-Miller, S. Noskov, H. Duff

**10:00 —** Intermission.

**10:10 —133.** Computer aided design of novel inhibitors of the p53-hDM2(X) interactions. **J. Michel**, A. Ekkati, E. A. Harker, J. Tirado-Rives, A. Schepartz, W. L. Jorgensen

**10:40 —134.** Design of CETP Inhibitors: A Comparison of Structure-Based and Knowledge-Based Library Design Methods. **M. Tu**, D. Perry, R. Garigipati, G. Chang, B. A. Lefker, R. B. Ruggeri, P. H. Dorff, B. Dow, M. Didiuk, C. M. Hayward

**11:10 —135.** Development of a CNS Multi Parameter Optimization (MPO) Design Tool to Increase the Probability of a Compound Survival by Aligning Metabolism, Permeability, and Safety Properties in One Molecule. **X. Hou**, P. R. Verhoest, A. Villalobos, T. Wager

**11:40 —136.** Does ensemble docking improve virtual screening enrichment? **I. R. Craig**

Section C

Unknown Site -- Unknown Room

**Quantum Chemistry**

**Mr. Materials Goes to Washington**

A. E. Roitberg, *Organizer*
S. Pakkala, *Presiding*

**8:30 —137.** Electronic structure of 3d-M(smif)$_2$: A case study for computational investigations of transition metal complexes and their spectroscopic characterization. **J. Hachmann**, P. T. Wolczanski, G. K -L. Chan

**9:00 —138.** First-principles computational study of chemical degradation of polymer materials. **U. T. Novakovski**, S. L. Richardson, S. Christensen

**9:30 —139.** Molten n-Pyrrole systems: An Adaptive Tempering Monte Carlo Study. **Y. Dai**, E.

Blaisten-Barojas

**10:00 —** Intermission.

**10:10 —140.** Recent developments in ab initio composite methodologies. T. G. Williams, G. A. Oyedepo, B. P. Prascher, M. Majkut, N. DeYonker, **A. K. Wilson**

**10:40 —141.** Time evolution of electronic populations from a combined ab initio structure/ reduced density matrix description: Excited metal nano-clusters on silicon. **D. S. Kilin**, D. A. Micha

Section D

Unknown Site -- Unknown Room

**The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry**

**Quantum Biology**

*Cosponsored by St. Jude Children's Research Hospital*
A. M. Ferreira, *Organizer, Presiding*

**8:30 —142.** Hydrogen-catalysis phenomenon as an option in biological fixation of N2: A theoretical view. **R. Asatryan**, J. W. Bozzelli

**9:15 —143.** The role of QM/MM studies in mechanistic analysis of biomolecular motors and ion pumps. **Q. Cui**

**10:00 —144.** Quantum mechanical scoring for protein docking. **A. E. Cho**

**10:45 —** Intermission.

**11:00 —145.** Large-scale *ab initio* Calculations of DNA Oligomers. **N. Labello**, A. M. Ferreira, B. M. Moore

**11:45 —146.** QC in Med Chem. **M. Orozco**

Section E

Unknown Site -- Unknown Room

**Molecular Visualization**

**small molecules. BIG IMPACT!**

*Cosponsored by CINF*
R. E. Amaro and E. X. Esposito, *Organizers, Presiding*

**8:00 —** Introductory Remarks.

**8:05 —147.** Visualization of cyclic and multi-branched molecules with VMD. S. Cross, J. E. Stone, J. E. Gain, **M. M. Kuttel**

**8:40 —148.** PoseView - 2D visualization of protein-ligand complexes. **K. Stierand**, M. Rarey

**9:15 —149.** A general interface to quantum chemistry simulations in VMD. **J. Saam**, J. E. Stone, A. Kohlmeyer, K. Schulten

**9:50 —** Intermission.

**10:00 —150.** Boltzmann 3D simulations for visualizing molecular motion in the classroom and laboratory. **R. B. Shirts**

**10:35 —151.** Visualization of molecular orbitals and the related electron densities. **M. Haranczyk**, G. Weber, M. S. J. Gutowski

**11:10 —152.** Molekel: A program for the visualization of quantum chemistry data. **U. Varetto**, M. G. Giuffreda, Y. Jang

**11:45 —153.** WebMO: Web-based, state-of-the-art, and cost effective computational chemistry. **W. F. Polik**, J. R. Schmidt

**Herman Skolnik Award Symposium**

**Collections and Uses of Data**

*Sponsored by CINF, Cosponsored by COMP*

## TUESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Methodology II**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**1:20 —154.** X-Pol potential: An explicit quantal force field for protein dynamics and function. **J. Gao**

**2:00 —155.** Anton: A specialized machine for millisecond-scale molecular dynamics simulations of proteins. **D. E. Shaw**

**2:40 —156.** Testing and validation of the newly developed drude polarizable force field for charmm. **P. E. M. Lopes**, J. H. Shim, B. Roux, A. D. MacKerell Jr.

**3:00 —** Intermission.

**3:20 —157.** Protein dynamics from atomistic and coarse-grained simulations. **Q. Cui**

**4:00 —158.** Reorganization free energies for electron transfer systems with different protein folds: comparing cytochrome c, cytochrome b5 and a 4-helix bundle. V. Tipmanee, H. Oberhofer, **J. Blumberger**

**4:20 —159.** Theoretical studies of the role of water in interprotein ET between cytochrome b5 and myoglobin. **S. Keinan**, R. Venkatramani, J. M. Nocek, D. N. Beratan, B. M. Hoffman

**4:40 —160.** Protein heat capacity calculated from replica-exchange molecular dynamics simulations with different implicit solvent models. **I -C. Yeh**, M. S. Lee, M. Olson

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Drug Discovery III**

I. Visiers, *Organizer*
J. H. Voigt, *Presiding*

**1:30 —161.** Computation of 3D queries for ROCS based virtual screens. **G. J. Tawa**, J. C. Baber, K. Fan, D. J. Diller, W. S. Somers, C. Humblet

**2:00 —162.** Driving the Discovery of Novel GlyT1 Inhibitors by in silico ADME Modeling. **X. Hou**, J. A. Lowe III, C. J. Schmidt, F. D. Tingley, S. F. McHardy, M. Kalman, S. DeNinno, M. Sanner, K. Ward, L. Lebel, D. Tunucci, J. J. Valentine

**2:30 —163.** FOG: Fragment Optimized Growth algorithm for the de novo generation of molecules

occupying drug-like chemical space. **P. S. Kutchukian**, D. Lou, E. I. Shakhnovich

**3:00 —** Intermission.

**3:10 —164.** Identification of good and bad chemical structural features for microsomal stability. **Y. Hu**, R. J. Unwalla, A. Denny, J. A. Bikker, L. Di, C. Humblet

**3:40 —165.** Induced-fit docking studies of protein tyrosine kinase ihibitors. **H. Zhong**, L. M. Tran, J. Stang

**4:10 —166.** Large scale evaluation of logP predictors: local corrections may compensate insufficient accuracy and need of experimentally testing every other compound. G. Poda, C. Ostermann, R. Mannhold, J. McDonald, **I. V. Tetko**

**4:40 —167.** Lead finding using 2D similarity and QSAR methods: Assessment of method/descriptor combinations. **W. D. Cornell**, R. P. Sheridan, E. Sherer, S. Ha, Y -D. Gao

Section C

Unknown Site -- Unknown Room

**Molecular Mechanics**

**Lipids. The New Water!**

E. X. Esposito, *Organizer*
K. Shahrokh, *Presiding*

**1:30 —168.** Atomistic simulations of lipid bilayer interactions with a carbon nanotube. V. K. Gangupomu, **F. M. Capaldi**

**2:00 —169.** Coarse grain molecular dynamics simulations of membrane proteins. **J. Galan**, Z. Liu, R. DeVane, P. B. Moore

**2:30 —170.** Coarse grain paramaterization of drugs, protiens, and lipids for use in molecular dynamics simulations. R. DeVane, J. Galan, Z. Liu, **P. B. Moore**

**3:00 —** Intermission.

**3:10 —171.** Membrane attachment, allostery and population-shift in Ras GTPases. **A. A. Gorfe**

**3:40 —172.** Reactivity of DFP in water saturated polymer membrane. **J. W. Andzelm**, J. Walker, H. Schreuder-Gibson, P. Gibson

**4:10 —173.** Understanding how flavonoids provide protection to skin cells: A molecular modeling study. **S. Ravichandran**

Section D

Unknown Site -- Unknown Room

**Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches**

**Biological Assembly I**

*Cosponsored by PMSE*
H. Heinz, *Organizer, Presiding*

**1:00 —** Introductory Remarks.

**1:05 —174.** Biological-nanomaterial interactions. **R. R. Naik**

**1:40 —175.** Controlling crystal growth using organic molecules, biomolecules and arrays. **J. H. Harding**, C. L. Freeman, D. Quigley, P. M. Rodger

**2:15 —176.** Generalized-ensemble simulations of bio-nanostructures. **Y. Okamoto**

**2:50 —** Intermission.

**3:05 —177.** Multiscale modelling of bio-inorganic interfaces. **J. A. Elliott**, D. Antypov, Y. Han, D. J. Cooke

**3:40 —178.** Nature of molecular interactions of peptides with gold, palladium, and Pd-Au bimetal surfaces in aqueous solution. **H. Heinz**, B. L. Farmer, R. B. Pandey, J. Slocik, S. S. Patnaik, R. Pachter, R. R. Naik

**4:00 —179.** Theoretical insights into the interaction mechanism between protein and SWCNT. **Y. Wang**, H. Ai

**Experimental and Theoretical Progress In Unraveling The Detailed Energetics of Drug-Receptor Binding**

*Sponsored by MEDI, Cosponsored by COMP*

**Herman Skolnik Award Symposium**

**Cheminformatics and Structure-Activity Analysis**

*Sponsored by CINF, Cosponsored by COMP*

## TUESDAY EVENING

Section A

Unknown Site -- Unknown Room

**Chemical Computing Group Excellence Award**

C. L. Simmerling, *Organizer*

**6:00 - 8:00**

**180.** Binary QSAR study for identifying selective $LPA_3$ antagonists. **J. I. Fells Sr.**, A. L. Parrill

**181.** Drug Pressure Induced Mutations in HIV-1 Protease alter Flap Conformations. **F. Ding**, C. L. Simmerling

**182.** Dynamics of 1,3-dipolar cycloadditions of diazonium betaines to acetylene and ethylene: Bending vibrations facilitate reaction. K. N. Houk, **L. Xu**, C. Doubleday

**183.** Pair-wise property-encoded shape distribution descriptors applied to prediction of protein-ligand binding affinities. **S. Das**, M. Krein, C. M. Breneman

Section B

Unknown Site -- Unknown Room

**Hewlett-Packard Scholar Awards**

C. L. Simmerling, *Organizer*

**6:00 - 8:00**

**184.** Accelerated molecular dynamics in studying long-timescale biomolecular events. **D. Hamelberg**

**185.** Computational predictions of binding affinities. **D. L. Mobley**

**186.** Integrating electronic-embedding QM/MM approaches with implicit electrostatic solvent models. **J. A. Gascon**

**187.** Multi-scale simulation methods for protein dynamics and synergistic regulation of enzyme complexes. **C -E. A. Chang**, M. Q. Fatmi, R. Ai

Section C

Unknown Site -- Unknown Room

**Poster Session**

E. X. Esposito, *Organizer*

**6:00 - 8:00**

**188.** Sequence effects on the charge transfer in DNA. **A. Balaeff**, S. Keinan, R. Venkatramani, D. N. Beratan

**189.** 3D-QSAR of cell-based biological activities: Integration of disposition function with multi-species, multi-mode CoMFA. **S. Natesan**, S. Balaz

**190.** Comparative analysis of the packing topology of structurally important residues in helical membrane and soluble proteins. **V. Pabuwal**, Z. Li

**191.** Designing specific or promiscuous drug molecules: Theory, methods development, and application to the HIV-1 system. **M. L. Radhakrishnan**

**192.** Modeling the sorption dynamics of aluminum hydride using a reactive force field. **J. G. Ojwang**, A. C. van Duin, W. A. Goddard III, G. J. Kramer, R. A. van Santen

**193.** pH-dependent conformational states of AcrA protein: Implications for the assembly of AcrAB-TolC multidrug efflux pump. **J. Wallace**

**194.** Preferences Across Phases: Structural Preferences in Group 2 Dihalide and Dihydride Monomers, Dimers, Trimers and Solids. **K. J. Donald**

**195.** 3D-QSAR Model for Inhibition Requirements for hASBT using glutamyl-Chenodeoxycholate (glu-CDCA) Conjugates of Aniline. **C. Acharya**, R. Rais, J. E. Polli, A. D. MacKerell Jr.

**196.** A Kirkwood-Buff force field for thiols, sulfides, and disulfides. **N. Bentenitis**, P. E. Smith

**197.** A Tight-Binding Study of Ionic Hydrogen-Bond Networks in Ion Solvation. **Y -L. Zhao**, C. A. Gonzalez, M. Meot-Ner

**198.** Ab initio studies of ether-carbene ylides. **J. M. Standard**, R. D. Quinn

**199.** Accelerating DFT calculations with GPU: A hybrid computing approach. **J. Kong**, Z. Gan, Y. Shao, R. Olivares-Amaya, A. Aspuru-Guzik

**200.** Adaptively biased dynamics study of the excited states of TIM. **S. Tang**, D. Case

**201.** A docking model for convulxin and convulxin -like proteins with Human Glycoprotein VI. Y. J. Tseng, **C -C. Tsai**

**202.** AEI Modeling macromolecular structure, dynamics and energetics. **J. L. Knight**, C. L. Brooks III

**203.** AEI Solving problems of biomedical relevance through multi-scale computational methods and high performance computing. **K. Arora**, C. L. Brooks III

**204.** Algorithmic improvements in DOCK6 for enhanced conformational sampling. **S. Mukherjee**, T. E. Balius, R. C. Rizzo

**205.** Analytic density-functional theory optimization with a parallel genetic algorithm. **M. A. Thompson**, B. I. Dunlap

**206.** Large-scale QM/MM calculations of protien-ligand interaction in Thrombin S1 pocket. **M. Freindorf**, J. Kong, B. Baum, M. Mohamed, M. Zayed, G. Klebe, D. G. Hangauer

**207.** Support Vector Machine Classification Model of Pubchem hERG Bioassay data with 4D-fingerprint and MOE descriptors. Y. J. Tseng, **M -Y. Shen**, B -H. Su

**208.** In silico binary QSAR model based on 4D-fingerprints and MOE descriptors for hERG blockage evaluation. Y. J. Tseng, **B -H. Su**, M -Y. Shen

**209.** 2D- and 3D-Similarity based classification systems for substrate prediction of ABCB1. **R. Schwaha**, G. F. Ecker

**210.** Analyzing the robustness of the MM/PBSA free energy calculation method: Application to DNA conformational transitions. **A. Brice**, B. N. Dominy

**211.** Annelated derivatives of cyclooctatetrane in which $\sigma \rightarrow \pi^*$ electron transfer is energetically favorable . **X. Zhou**, D. A. Hrovat, W. T. Borden

**212.** Application of flexible volumetric alignment in ligand based virtual screening. **A. Kalászi**, G. Imre, Ö. Farkas, M. Vargyas, F. Csizmadia

**213.** Automatic and systematic search for routes of chemical reactions in large flexible systems with a

given reaction center by the microiteration technique and the GRRM method. **S. Maeda**, K. Ohno, K. Morokuma

**214.** Biophysical resolution: How tolerant are binding free energy calculations to errors in protein structure? **M. Singh**, B. N. Dominy

**215.** Calculations of the relative energies of the low-lying electronic states of 2-methylenedihydrophenalene-1,3-diyl: Effects of a 1,8-naphtho bridging group on trimethylenemethane and of a vinylidene bridging group on 1,8-naphthoquinodimethane. **H. Dong**, D. A. Hrovat, H. Quast, W. T. Borden

**216.** CHARMM additive all-atom force field for aldopentofuranoside carbohydrates and Fructofuranoside. **E. R. Hatcher**, O. Guvench, A. D. MacKerell Jr.

**217.** Comparison of biomolecular force fields for the peptide group and ionic sidechains. **M. Kang**, P. E. Smith

**218.** Computational analysis of crystal shapes as modified by surrounding microstructure and affect on crystal size distribution. **R. V. Amenta**

**219.** Computational analysis of HIVgp41 mutants in complex with peptide based fusion inhibitors. **B. E. McGillick**, T. E. Balius, S. Mukherjee, R. C. Rizzo

**220.** Computational approaches to understand the interaction of HIV-1 integrase and its inhibitors from natural sources. **Z. Hu**, D. Chen, L. Dong, X. Wang, W. M. Southerland

**221.** Computational studies on carboxyphosphate. **K. W. Reeping**, S. Pakkala, S. M. Firestine, J. D. Evanseck

**222.** Computational study of intramolecular hydrogen bonding in arylamide compunds: Delocalization effect. **D. M. Todd**, J. Galan, Z. Liu, G. Moyna, V. Pophristic

**223.** Computational study of the conformational properties of the amino acid side chains. **X. Zhu**, A. D. MacKerell Jr.

**224.** Continuum electrostatic and free energy perturbation calculations on leucine transporter complexed with tricyclic antidepressants. **K. Immadisetty**, J. D. Gibbons, J. D. Madura

**225.** Correlation between Quantum Mechanical/Molecular Mechanical (QM/MM) Docking Performance and Binding Site Classification. **J. Y. Chung**, J -M. Hah, A. E. Cho

**226.** Coupling Accelerated Molecular Dynamics Methods with Thermodynamic Integration Simulations. **C. A. F. de Oliveira**, D. Hamelberg, J. A. McCammon

**227.** Density functional theoretical study on redox-dependent hydrogen bonding between amide and

arylurea. **Y. S. Cho**, H. Cho, H. Y. Woo, J -M. Kim, S. Hwang

**228.** Density functional theoretical study on the pKa values of bipyridines. **S. Hwang**, S. W. Joo, Y. H. Jang

**229.** Development of serotonin and norepinephrine transporter inhibitor pharmacophore models: Design of selective ligands. **E. M. Collantes**, D. F. Ortwine

**230.** DFT calculations on the stability of 2D covalent organic frameworks. D. Kim, **D. H. Jung**, K -H. Kim, A. Lee, J. Kim, K. Choi, S -H. Choi

**231.** DFT Study of the Effect of Al2O3 Support on Pt Catalytic Activity. **J. Synowczynski**, J. Andzelm, D. G. Vlachos

**232.** Docking simulation on the inhibitor of exo-polygalacturonase. **Y -J. Lee**, E -H. Kim, S. Hwang

**233.** Dynamics of nitrous oxide in lipid bilayers at different hydrations: A molecular dynamics study. **E. Pinnick**, S. Erramilli, F. Wang

**234.** Effect of the nucleotide modification on the conformation and stability of the triple DNA formation. **E. Darian**, A. Semenyuk, M. M. Seidman, A. D. MacKerell Jr.

**235.** Elucidation of binding profile similarities across structurally diverse ligands using a 3D Dopamine transporter model. **S. Manepalli**, J. D. Madura, D. J. Lapinsky, C. K. Surratt

**236.** Enzymatic DNA base flipping mechanism examined via nudged elastic band simulations. **C. Bergonzo**, A. J. Campbell, C. De los Santos, A. P. Grollman, C. Simmerling

**237.** Implementation of a novel coarse-grain model using rhodopsin in a lipid bilayer. **K. Nguyen**, J. Galan, Z. Liu, P. Moore

**238.** Intrinsic Lewis base strength based upon valency. **J. J. Rosmus**, J. A. Plumley, J. D. Evanseck

**239.** Key role of computational CNS penetration studies in selecting and advancing compounds in P2X7 analgesia project. **S. Srivastava**, M. Roumi, R. Panetta, A -K. Gilbert, S. J. Teague

**240.** Ligand-supported homology modeling of the human melanin concentrating hormone receptor 1 (MCH-R1). **M. Helal**, M. A. Avery

**241.** Mechanism of anesthetic binding to lipid bilayer. **N. Chen**, T. H. T. Nguyen, J. Snow, P. B. Moore

**242.** Modeling of pillared covalent organic frameworks as the hydrogen storage material. **D. Kim**, D. H. Jung, K -H. Kim, A. Lee, J. Kim, K. Choi, S -H. Choi

**243.** Models for the nucleation and growth of calcium carbonate. **J. H. Harding**, C. L. Freeman, M. Yang, D. J. Cooke, J. A. Elliott, D. M. Duffy, J. Lardge, D. Quigley, P. M. Rodger

**244.** Molecular dynamics of proteins embedded in a lipid bilayer. **T. H. Nguyen**, P. B. Moore

**245.** Molecular dynamics of second-shell interactions in zinc finger binding sites. **M. L. Peach**, M. C. Nicklaus

**246.** Molecular dynamics simulations of complex mixed lipid bilayers to model yeast membranes. J. B. Lim, **J. B. Klauda**

**247.** Molecular dynamics simulations of the quick micelle formation of Azotab in $D_2O$ solution: Micellar structure and the swing of two benzene rings . **C -Y. Lin**, K. Shing, C. T. Lee

**248.** Molecular modeling of interaction between sAnk157-122 and obscurin6322-6339 in striated muscle. **T. Oashi**, B. Busby, C. D. Willis, R. J. Bloch, A. D. MacKerell Jr.

**249.** Navigating molecular worms inside chemical labyrinths. **M. Haranczyk**, J. A. Sethian

**250.** Novel protocols for modeling flexible loops: Implications for drug design . **K. A. Rossi**, C. A. Weigelt, A. Nayeem, S. R. Krystek Jr.

**251.** Numerical integration of the coupled rate differentials via a discretized Adomian decomposition. **J. M. Younker**, M. T. Green

**252.** On the applicability of homology models of G protein-coupled receptors to computer-aided drug discovery. **S. Vilar**, G. Ferino, S. Costanzi

**253.** Optimal design of paper mill process energy with mathematical programming and three-link modelling. **J. Tao Sr.**, J. Li Sr., H. Liu

**254.** Parameterization of desipramine, imipramine, and clomipramine. **J. D. Gibbons**, J. D. Madura

**255.** Potential of mean force calculations of the free energy of binding of Type I Antifreeze Proteins at water/ice interface. **A. Wierzbicki**, K. Battle, J. D. Madura

**256.** Prediction of fold resistance for inhibitors of EGFR using all-atom molecular dynamics simulations. T. E. Balius, **R. C. Rizzo**

**257.** Probing Protein-ligand Interactions by ab initio NMR Chemical Shift Calculations . **B. Wang**, X. He, K. M. Merz Jr.

**258.** Properties of Alcohol Water Mixtures by Computer Simulation. **Y. Jiao**, **F. Chen**, **P. E. Smith**

**259.** QSAR modeling and knowledge discovery of a large unbalanced dataset of hERG K+ channel

blockers and openers . **K. Wang**, A. Golbraikh, B. L. Roth, A. Tropsha

**260.** Quantitative conformationally sampled pharmacophore for μ opioid ligands . **J. H. Shim**, A. Coop, A. D. MacKerell Jr.

**261.** Representation, searching and enumeration of Markush structures - from molecules towards patents. **S. Csepregi**, N. Máté, R. Wagner, T. Csizmazia, S. Dóránt, E. Biro, F. Csizmadia

**262.** Search for inhibitors of S100B-p53 interaction. **E. P. Raman**, S. Zhong, P. T. Wilder, T. H. Charpentier, D. J. Weber, A. D. MacKerell Jr.

**263.** Simulation study of interprotein electron transfer in Hemoglobin tetramers. **R. Venkatramani**, S. Keinan, D. N. Beratan

**264.** Structure-based drug design against pandemic influenza using all-atom molecular dynamics and docking. **R. Goyal**, R. C. Rizzo

**265.** Surface tension, contact angle and line tension in a liquid nanodroplet. **D. V. Perez**, C -C. Chiu, S. O. Nielsen, P. Moore

**266.** Targeted design of dual kinase inhibitors for breast cancer. **Y. Huang**, R. C. Rizzo

**267.** The development of an affinity evaluation and prediction system by using protein-protein docking simulations and parameter tuning. T. Yoshikawa, **K. Fukui**

**268.** The effects of conformational variations on the packing of cup shaped molecules. **M. Roumanos**, M. Kertesz, K. T. Holman

**269.** The energetics of stop codon recognition on the ribosome. **J. Sund**, M. Andér, J. Åqvist

**270.** The Nature of Intermolecular Interactions in Water-Methanol Complexes. **V. S. Pakkala**, J. A. Plumley, J. Evanseck

**271.** The role of human skin emanation in understanding how a mosquito repellent works. **J. Song**, Z. Wang, J. Chen, T. Yi, G. Fan, S. Chen

**272.** Theoretical studies for the crystal structure prediction: Tests on indenopyrazine. K -H. Kim, D. Kim, A. Lee, S -H. Choi, Y -I. Park, S -K. Kim, C -H. Seok, J -W. Park, J -H. Lee, **D. H. Jung**

**273.** Training pKa and logP Prediction . J. Szegezdi, **F. Csizmadia**

**274.** Vibrational and spin properties of radicals derived from ubiquinol (dihyroubiquinone). **R. A. Wheeler**, S. E. Boesch

**275.** Web services to promote GPCRs peptide mimetics. **W. Nemoto**, K. Fukui, H. Toh

## WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Protein Folding**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**8:20 —276.** Simulating protein folding on experimental timescales in all-atom detail. **V. S. Pande**

**9:00 —277.** Hydration effects on peptide stability in confinement. S. Vaitheeswaran, D. Suvlu, **J. C. Rasaiah**, **D. Thirumalai**

**9:40 —278.** The Kinetics and Structure of Protein Energy Landscape. **M. C. Prentiss**, D. J. Wales, P. G. Wolynes

**10:00 —** Intermission.

**10:20 —279.** Action of Urea: Molecular Picture of Protein Chemical Denaturing from Large Scale Simulations. **R. Zhou**

**11:00 —280.** Folding free-energy landscape of an alpha/beta fold protein from replica exchange molecular dynamics simulations. **C. Wu**, M. T. Bowers, J -E. Shea

**11:20 —281.** Helix formation and helix-helix interactions in protein folding. **R. D. Murphy**, C. T. Leahy, N -V. Buchete

**11:40 —282.** Probing the role of domain cooperativity in the mechanical unfolding of proteins. **R. I. Dima**

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Drug Discovery IV**

I. Visiers, *Organizer, Presiding*

**8:30 —283.** Ligand free energy ranking using Constrained Fragment Annealing (CFA): A step towards a practical analysis of full ligand / protein interactions. **I. S. Cloudsdale**, J. L. Kulp Jr.

**9:00 —284.** Machine learning and drug discovery: Never the twain shall meet? **N. Duffy**, J. Yu, G. Lanza, J. Griffin, P. Boardman, R. McClellan, B. Dolin, P. Linehan, S. Sylvis, B. Allgood

**9:30 —285.** Methods for structure based scaffold replacement. **P. Labute**

**10:00 —** Intermission.

**10:10 —286.** Modeling allosteric regulation in GPCRs: Towards rational structure-based drug design. **I. A. Balabin**, W. Yang, D. N. Beratan

**10:40 —287.** Modeling novel planar BACE1 inhibitors – trying to hit a moving target. **J. Voigt**, J. Caldwell, S. Chackalamannil, X. che, J. Cumming, M. Czarniecki, J. Durkin, M. Kennedy, R. Kuvelkar, R. D. Mazzola, B. McKittrick, T. Nechuta, E. M. Parker, M. Senior, E. Smith, Z -Y. Sun, L. Wang, Y -S. Wang, Y. Wu, D. Wyss, Y. Xia, Y. Ye, Z. Zhu, A. Stamford, W. J. Greenlee, C. Strickland

**11:10 —288.** Modeling of prolyl-leucyl-glycinamide (PLG) analogs that modulate the dopamine D2 receptor: Method evaluation, pharmacophore mapping/database searching and 3D-QSAR. **R. L. Wood**, R. L. Johnson, E. A. Amin

**11:40 —289.** Of things that are rare - Iridium, dinosaur coprolite, and high quality protein-ligand structure databases. **G. L. Warren**, T. Do, S. D. Warren

Section C

Unknown Site -- Unknown Room

**Quantum Chemistry**

**Definitely Flakey Theory? NO! Density Functional Theory!**

A. E. Roitberg, *Organizer*
S. Manepalli, *Presiding*

**8:30 —290.** Assessment of DFT and NDDO models for Zn molecules, clusters and biocenters. **E. A. Amin**, D. G. Truhlar, A. Sorkin

**9:00 —291.** Computation of interaction energies via density functional theory with empirical van der Waals corrections. **C. Deligkaris**, J. H. Rodriguez

**9:30 —292.** Density functional molecular dynamics calculation of the dissociation constant of liquid water. M. Sulpizi, **M. Sprik**

**10:00 —** Intermission.

**10:10 —293.** Density functional theory studies of doping in both bulk- and surface-state titania. R. Long, **N. J. English**

**10:40 —294.** Electronic coupling matrix elements from charge constrained DFT calculations: a plane wave basis set implementation. H. Oberhofer, **J. Blumberger**

Section D

Unknown Site -- Unknown Room

**The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry**

**Quantum Medicinal Chemistry**

*Cosponsored by St. Jude Children's Research Hospital*
A. M. Ferreira, *Organizer, Presiding*

**8:30 —295.** Binging Free Energy Calculations of Protein-Ligand Complexes using Fragment Molecular Orbital Method Combined with Continuum Solvent Model. **K. Kitaura**

**9:20 —296.** Electronic properties and intermolecular binding in drug-like molecules. **T. Clark**

**10:10 —297.** Quantum mechanics in drug discovery and design. **K. M. Merz Jr.**, X. He, B. Wang

**11:00 —** Intermission.

**11:15 —** Panel Discussion.

Section E

Unknown Site -- Unknown Room

**Molecular Visualization**

**Giving Your Proteins Appeal! ;)**

*Cosponsored by CINF*
R. E. Amaro and E. X. Esposito, *Organizers, Presiding*

**8:00 —** Introductory Remarks.

**8:05 —298.** Active-site flexibility maps derived from molecular dynamics trajectories. **I. R. Craig**

**8:40 —299.** Use of quaternions in biomolecular structure analysis. **R. M. Hanson**, D. Kohler, S. Braun

**9:15 —300.** Sirius: A versatile desktop visualization environment. **A. Bowen**, O. Buzko, K. Baldridge

**9:50 —** Intermission.

**10:00 —301.** Molecular visualization and animations using PMV. **M. F. Sanner**

**10:35 —302.** UCSF Chimera. C. C. Huang, T. D. Goddard, E. F. Pettersen, G. S. Couch, E. C. Meng, **T. Ferrin**

**11:10 —303.** PyMOL Molecular Viewer: Updates and Refinements. **W. L. DeLano**

**Federated Search**

**Chemical and Biological Databases**

*Sponsored by CINF, Cosponsored by COMP*

## WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Motors and Assemblies**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**1:20 —304.** The energy landscape for folding and molecular motors – the kinesin story. **J. N. Onuchic**

**2:00 —305.** Working principle of biomolecular motors revealed by molecular dynamics simulations. **S. Takada**

**2:40 —306.** Computer simulations of protein unfolding and translocation by Clp ATPase nanomachines. **G. Stan**, A. Kravats

**3:00 —** Intermission.

**3:20 —307.** Viral shell mechanics. **H. Grubmuller**, M. Zink

**4:00 —308.** Molecular simulations of large-size protein assemblies on graphics procesors . **V. Barsegov**, R. Dima, A. Zhmurov

**4:20 —309.** $Cl^-$ channel anti-porter function. **E. W. Knapp**, G. Kieseritzky

**4:40 —310.** Volatile anesthetic modulation of dynamic structure of water in α4β2 nicotinic acetylcholine receptor. **D. Willenbring**, Y. Xu, P. Tang

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Drug Discovery V**

I. Visiers, *Organizer*
M. R. Landon, *Presiding*

**1:30 —311.** Paratope structural optimization during antibody-antigen docking. **A. Sircar**, J. J. Gray

**2:00 —312.** Predicted 3D structure for the histamine H3 receptor and its binding site. **S -K. Kim**, P. Fristrup, R. Abrol, W. A. Goddard III

**2:30 —313.** Predicting druggable binding sites at the protein-protein interface. **J. C. Fuller**, N. J. Burgoyne, R. M. Jackson

**3:00 —** Intermission.

**3:10 —314.** Prioritizing ligand protonation states in docking. **J. C. Shelley**, J. R. Greenwood, M. P. Repasky

**3:40 —315.** Protein-ligand docking based on ant colony optimization. **T. E. Exner**, O. Korb, T. ten Brink, T. Stützle

**4:10 —316.** Screening Rule of Structure Parameters in Quantitative Structure-Activity Relationships Model. **D. Gao**, P. Wang

**4:40 —317.** Self-organizing molecular conformations – from SPE to SOS. **P. Liu**, F. Zhu, H. Xu, D. K. Agrafiotis

Section C

Unknown Site -- Unknown Room

**Molecular Mechanics**

**COMP's Stimulus Package: Free Energy for Everyone!**

E. X. Esposito, *Organizer*
R. E. Amaro, *Presiding*

**1:30 —318.** Alchemical predictions of free energies, from hydration to binding. **D. L. Mobley**

**2:00 —319.** Benchmarks for validating and testing free energy calculations in molecular design. **M. Shirts**

**2:30 —320.** Molecular dynamics simulations and free energy calculations for predictions of siRNA duplex stability. **L. Shen**, T. L. Johnson, S. Sciabola, Q. Cao, R. V. Stanton, S. L. Clugston, Z. Wang

**3:00 —** Intermission.

**3:10 —321.** Structural and mechanistic modeling of the HER3/ErbB3 pseudo-kinase domain. **S. E. Telesco**, F. Jia, Y. Liu, R. Radhakrishnan

**3:40 —322.** Structural Changes and Quantification of Ligand Affinity in Lactose Permease of Escherichia coli. **P. Y. Pendse**, J. B. Klauda

Section D

Unknown Site -- Unknown Room

**Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches**

**Biological Assembly II**

*Cosponsored by PMSE*

H. Heinz, *Organizer, Presiding*

**1:00 —323.** Peptide-based functional nanostructures. **M. Sarikaya**, C. Tamerler

**1:35 —324.** Directed assembly in biomineralization, amyloid fibrils, and viruses. **M. Muthukumar**

**2:10 —325.** Computational modeling of biopolymers on carbon nanotubes. **B. L. Farmer**

**2:45 —** Intermission.

**3:00 —326.** A quantum of common sense in crystallography. **K. M. Merz Jr.**

**3:35 —327.** Quantifying Adsorption of Amino Acids and Surfactants on Au {111} Surfaces in Aqueous Solution. **J. Feng**, B. L. Farmer, R. Naik, H. Heinz

**3:55 —328.** An effective Hamiltonian approach to study Zinc binding to a Zinc-finger. **P. Dixit**, D. Asthagiri

**4:15 —** Concluding Remarks.

## THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

**Protein Dynamics and Function**

**Molecular Motions**

H -X. Zhou and G. Hummer, *Organizers, Presiding*

**8:20 —329.** Effects of cosolvents on protein/polypeptide hydration and dynamics. **Y. Q. Gao**

**9:00 —330.** Reducing the essential side chain degrees of freedom in molecular docking. **S. Vajda**, G -Y. Chuang, D. Beglov, D. Kozakov

**9:40 —331.** Identification of two distinct inactive conformations of the $\beta_2$-adrenergic receptor reconciles structural and biochemical observations. **R. O. Dror**, D. H. Arlow, D. W. Borhani, M. Ø. Jensen, S. Piana, D. E. Shaw

**10:00 —** Intermission.

**10:20 —332.** Probing the principles of dynamics and energy flow in proteins. **J. E. Straub**, Y. Zhang, H. Fujisaki

**11:00 —333.** New methods for connecting protein NMR data to structure and dynamics. **S. Tang**

**11:20 —334.** Non-equilibrium molecular dynamics study of electric and low-frequency microwave fields on hen egg white lysozyme. **N. J. English**, P. O'Brien, G. Y. Solomentsev

**11:40 —335.** Intrinsic Mobility of Rhodopsin Photointermediates Investigated by Molecular Dynamics Simulations. **I. Tikhonova**, S. Costanzi

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Drug Discovery VI**

I. Visiers, *Organizer*
Y. J. Tseng, *Presiding*

**8:30 —336.** A computational workflow to identify and validate the druggable allosteric binding sites. **X. S. Wang**, R. Hajjo, A. Tropsha

**9:00 —337.** SKATE: Decoupling systematic sampling from scoring to achieve more accurate docking. **J. A. Feng**, G. R. Marshall

**9:30 —338.** Staying in the loop: Innovations in loop modeling at ligand binding sites. **C. A. Weigelt**, K. A. Rossi, A. Nayeem, S. R. Krystek Jr.

**10:00 —** Intermission.

**10:10 —339.** Synthetically accessibe compounds from giant virtual chemistry spaces. **C. Lemmen**, C. Detering, M. Gastreich, H. Claußen

**10:40 —340.** Using quantitative high-throughput screening (qHTS) results as biological descriptors to assist quantitative structure activity relationship (QSAR) modeling of rat acute toxicity. **H. Zhu**, A. Sedykh, F. A. Wright, I. Rusyn, A. Tropsha

**11:10 —341.** Utilizing Structure-Based Design to Discover a Potent, Selective, In Vivo Active PDE10A Inhibitor Lead Series for the Treatment of Schizophrenia. **X. Hou**, C. J. Helal, Z. Kang, J. Pandit, E. Marr, K. F. Fennell, L. Chenard, C. Fox, C. J. Schmidt, R. D. Williams, D. Chapin, J. Siuciak, L. Lebel, F. Menniti, J. Cianfrogna, K. Schmidt, F. Nelson, S. Liras

Section C

Unknown Site -- Unknown Room

**Quantum Chemistry**

**Quantum Chemistry + ???. Frankeinsteining Methods**

A. E. Roitberg, *Organizer*
D. R. Roe, *Presiding*

**8:30 —342.** Elucidating the two acidity constant behavior of silica with ab initio molecular dynamics simulations. **K. Leung**, I. M. B. Nielsen, L. J. Criscenti

**9:00 —343.** Formalism and implementation of a continuous surface charge polarizable continuum model of solvation. **G. Scalmani**, M. J. Frisch

**9:30 —344.** Quantum Monte Carlo study of low-lying electronic states and thermo chemsitry of small molecules. **Z. Zhang**, J. Lawson, R. L. Jaffe, C. J. Umrigar, J. Toulouse

**10:00 —** Intermission.

**10:10 —345.** Quantum Monte Carlo study of methylene excited states. **P. Zimmerman**, Z. Zhang, C. Musgrave, J. Toulouse, C. J. Umrigar

**10:40 —346.** The evaluation of QM/MM full hessian and some applications. H. L. Woodcock III, A. Ghysels, **Y. Shao**, J. Kong, B. R. Brooks

**11:10 —347.** Variable-occupation-number perturbation theory. **B. I. Dunlap**

Section D

Unknown Site -- Unknown Room

**Molecular Mechanics**

**Protein Force Fields & CHARMM Goes Together Like Peas & Carrots. Right Forest?**

E. X. Esposito, *Organizer*
C. Bergonzo, *Presiding*

**8:30 —348.** Building a CHARMM polarizable force field for nucleic acids. **C. M. Baker**, V. M. Anisimov, I. Vorobyov, A. D. MacKerell Jr.

**9:00 —349.** Development and Testing of Protein Backbone Torsional Potentials for the Kirkwood Buff Derived Force Field of Peptides and Proteins. **F. Chen**, P. E. Smith

**9:30 —350.** Evaluating CHARMM parameters and the λ-dynamics free energy method for structure-based drug design. **J. L. Knight**, F. Bardinelli, C. L. Brooks III

**10:00 —** Intermission.

**10:10 —351.** Improving the lipid force field of CHARMM: A quantum mechanical and experimental approach. **J. B. Klauda**, R. Venable, A. D. MacKerell Jr., R. W. Pastor

**10:40 —352.** Simulation of cis-trans isomerization of the protein peptide bond. **D. Hamelberg**

**11:10 —353.** Towards an automatic force field parametrization engine: assignment of parameters by analogy for the CHARMM General Force Field (CGenFF). **K. Vanommeslaeghe**, S. Pamidighantam, R. M. Sheetz, J. W. D. Connolly, A. E. Roitberg, A. D. MacKerell Jr.

Submit Final Program