COMP

DIVISION OF COMPUTERS IN CHEMISTRY

Final Program, 235th ACS National Meeting, New Orleans, LA, April 6-10, 2008

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

SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Phase Equilibria

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
J. I. Siepmann and J. K. Johnson, *Organizers*

8:00 —1. Molecular modeling of complex fluids. **C. McCabe**

8:40 —2. Phase diagram calculations of alloys using density functional theory. **V. B. Warshasky**, **X. Song**

9:20 —3. Quantum Statistical Mechanics of rigid and semirigid molecular condesed matter. **E. Curotto**

9:40 — Intermission.

9:50 —4. The non-bulk like phase behavior for nano-cluster systems. **B. Chen**, R. B. Nellas, S. J. Keasler, H. Kim, J. I. Siepmann

10:30 —5. Modeling the kinetics of nanocrystal growth. **S. K. Kumar**, M. Tambasco

11:10 —6. Simulation of pure component phase equilibrium properties using a modified Stockmayer potential. **T. McKnight**, K. Bolton

Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Methods I

S. Rick, *Organizer*

8:00 —7. Replica-Exchange Method and Its Generalizations. **Y. Okamoto**

8:40 —8. Multiplexed Replica Exchange Molecular Dynamics Simulations of Protein Folding with a Physics-based Coarse-grained Force Field. C. Czaplewski, S. Kalinowski, A. Liwo, S. Oldziej, **H. A. Scheraga**

9:20 — Intermission.

9:40 —9. Improving the convergence of replica exchange simulations for complex systems. **C. L. Simmerling**

10:20 —10. Replica exchange with Solute Tempering. **B. J. Berne**, R. Zhou

11:00 —11. Biasing potential replica-exchange to enhance sampling of peptide and protein conformations during molecular dynamics simulations. **M. Zacharias**

Section C

Unknown Site -- Unknown Room

Drug Discovery

Docking and Scoring

Cosponsored by CINF
I. Visiers, *Organizer*
A. Tebben, *Presiding*

8:00 —12. Abandoning the rigid receptor approximation: Side-chain flexibility in GOLD. **P. Carlqvist**, J. W. Liebeschuetz

8:25 —13. Accurate docking and scoring of fragment molecules for lead discovery and optimization. K. Armstrong, **B. W. Sherman**

8:50 —14. Advances in induced-fit docking with applications toward predicting binding energies of diverse molecules. **I. Alberts**, R. B. Murphy, B. W. Sherman, R. Farid, R. Friesner

9:15 —15. Improved water handling in structure-based molecular docking. A. Rumpl, **C. Detering**, H. Claußen

9:40 — Intermission.

9:55 —16. Predicting absolute binding free energies with physics-based methods. **D. L. Mobley**, K. A. Dill

10:20 —17. Protein loop flexibility around ligand binding sites: Implications for drug design. **C. A. Weigelt**, K. A. Rossi, A. Nayeem, S. R. Krystek Jr.

10:45 —18. Role of quantum mechanical energies in binding sites of metalloproteins. **A. E. Cho**, D. Rinaldo

11:10 —19. Structure-based lead optimization of small molecule β-secretase (BACE1) inhibitors. **K. Y.**

Fan, J. Bard, R. Chopra, D. Cole, J. Erdei, W. F. Fobare, I. Gunawan, Y. Hu, C. Humblet, E. S. Manas, A. Olland, N. Pawel, D. A. Quagliato, P. Reinhart, W. R. Solvibile, W. S. Somers, J. Turner, E. Wagner, Y. Yan, P. Zhou, A. J. Robichaud, M. S. Malamas

Section D

Unknown Site -- Unknown Room

Quantum Chemistry

Organic and Biorganic

A. Roitberg, *Organizer*

8:00 —20. Cation binding and quadrupole moments of substituted cyclopentadienyl rings. **K. Cormier**, M. Lewis

8:25 —21. Effects of the crystal environment on potential energy surfaces for proton transfer in aspirin. M. M. Francl, **M. Wampole**

8:50 —22. Evaluation of several correlated electronic methods in the context of calculations common to drug design. **D. L. Cheney**, K. A. Rossi

9:15 —23. Influence of molecular oxides on transition metal tricarbonyls. **C. W. Earley**

9:40 — Intermission.

9:55 —24. Novel QM/MM Investigations of Enzyme Catalysis. **M. Williamson**, I. R. Gould, D. R. Klug, R. C. Walker

10:20 —25. Minding the gap: Lowering the barrier to the bergman cyclization of enediynes. **C. A. Parish**

10:45 —26. The contribution of electronic and conformational constraints to the selectivity of P450-catalyzed oxygenation versus dehydrogenation reaction mechanisms during tamoxifen metabolism. **K. Shahrokh**, G. Yost, T. E. Cheatham III

SUNDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Computational Catalysis

Zeolites and Homogeneous

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
A. M. Rappe and S. Linic, *Organizers*

1:30 —27. ACE, a virtual screening tool for asymmetric catalysts. **C. R. Corbeil**, J. Schwartzentruber, N. Moitessier

2:00 —28. Assessing the performance of density functional theory for metal-salen catalysis. **J. S. Sears**, C. D. Sherrill

2:30 —29. Born-Oppenheimer molecular dynamics simulations of enzyme catalysis with ab initio QM/MM methods. **Y. Zhang**, S. Wang, P. Hu

3:00 — Intermission.

3:30 —30. Dehydrogenation of ammonia-borane catalyzed by N-heterocyclic carbene nickel complexes: A DFT study. **X. Yang**, M. B. Hall

4:00 —31. Kinetics of oxidation of monosaccharides by protonated N-bromosuccinimide using nano-amount of chloro-complex of Rh(III) as homogeneous catalyst. **A. K. Singh**, R. Srivastava, J. Srivastava, S. Srivastava, P. Singh

Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Computational Efficiency

S. Rick, *Organizer*

1:30 —32. Comparison between regular and replica exchange molecular dynamics simulations and their applications in protein folding. W. Zhang, H. Lei, C. Wu, Z. Wang, **Y. Duan**

2:10 —33. Enhanced Sampling via Replica Methods. **A. E. Roitberg**

2:50 — Intermission.

3:10 —34. Simple continuous and discrete models for simulating replica exchange simulations of protein folding and binding. **R. M. Levy**, M. Andrec, E. Gallicchio, W. Zheng

3:50 —35. Exploring the energy landscape of protein folding using replica-exchange and conventional molecular dynamics simulations. **V. Daggett**

4:30 —36. Limitations of temperature replica exchange (T-REMD) in protein folding simulations. **J. W. Pitera**, W. C. Swope

Section C

Unknown Site -- Unknown Room

Molecular Mechanics

Advancing Methodologies I

E. X. Esposito, *Organizer*

1:30 —37. Ab initio Molecular Dynamics simulations of water under shock compression: Chemistry behind shock fronts. **N. Goldman**, E. J. Reed, L. E. Fried, C. J. Mundy, I. F. W. Kuo, A. Curioni

1:55 —38. Conformational and isomeric free energy differences from cluster-based simulations. **S. J. Keasler**, H. Kim, R. B. Nellas, M. E. McKenzie, B. Chen

2:20 —39. Photoisomerization of azobenzene: A quantitative force field-based implementation and simulation of assemblies with layered silicates in comparison with experiment. **H. Heinz**, R. Vaia, H. Koerner, B. L. Farmer

2:45 — Intermission.

3:00 —40. Using wide-angle x-ray scattering and molecular mechanics to explore the conformational ensemble of a hexameric porphyrin macrocycle: Evaluating charmm's ability to reproduce large amplitude motions. **K. L. Mardis**, H. Sutton, D. M. Tiede

3:25 —41. Ultrafast transformation of graphite to diamond: An ab initio study of graphite under shock compression. **N. Goldman**, C. J. Mundy, E. J. Reed, I. F. W. Kuo, L. E. Fried, A. Curioni

MONDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Phase Equilibria

II

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
J. I. Siepmann and J. K. Johnson, *Organizers*

8:00 —42. Simulations of phase transitions and activity coefficients in ionic systems. **A. Z. Panagiotopoulos**

8:40 —43. Comparing the Gibbs Ensemble and Grand-Canonical Transition-Matrix Monte Carlo Methods in the Determination of Fluid Phase Equilibria. **V. K. Shen**, A. S. Paluch, J. R. Errington

9:20 —44. Free energy calculations of molecular solutes in polymeric microstructures. **N. F. van der Vegt**, B. Hess, T. A. Ozal, C. Peter

9:40 — Intermission.

9:50 —45. Molecular simulation of equilibrium properties of fluids: From understanding toward quantitative predictions. **V. Lachet**

10:30 —46. Predicting phase equilibria using efficient Monte Carlo simulations. **J. I. Siepmann**, M. J. McGrath, J. L. Rafferty, K. E. Anderson, X. S. Zhao

11:10 —47. Discretized transferable Lennard-Jones united atom models for phase equilibria. **J. Elliott**, P. Stuhldreher

Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Methods II

S. Rick, *Organizer*

8:00 —48. Problem Oriented Sampling Design via the Replica Exchange Strategy. **W. Yang**

8:40 —49. Extrapolating to equilibrium from early simulation results of replica exchange calculations on proteins. **W. C. Swope**, J. W. Pitera

9:20 —50. New replica exchange methods for spanning large temperature ranges. **S. Rick**, A. J. Lee, H. Yu

10:00 — Intermission.

10:20 —51. Conformational sampling of peptides in different dielectric environments. **M. Feig**, M. Sayadi, S. Tanizaki

11:00 —52. Advanced sampling in exploring pH-dependent conformational transitions in proteins and peptides. **C. L. Brooks III**

11:40 —53. Temperature intervals with global energy reassignment (TIGER): Algorithm development and application to protein folding. **R. A. Latour**

Section C

Unknown Site -- Unknown Room

Drug Discovery

Finding hits

Cosponsored by CINF
I. Visiers, *Organizer*
J. Woolfrey, *Presiding*

8:00 —54. Identification of Pyk2 FERM ligands by combining protein similarity assessment,

mutagenesis study, pharmacophore prediction, and in silico screening. **L. Wang**, N. Meurice, J. Loftus, Y -P. Pang, B. Clark, C. A. Lipinski

8:25 —55. Improving enrichment rates: A practical solution to an impractical problem. **N. M. O'Boyle**, R. Taylor

8:50 —56. Annotated DB of Chemically Feasible Scaffolds: Key Point for an Efficient Scaffold Hopping. **J. Oyarzabal**, T. Howe, J. I. Andres, J. Alcazar, R. M. Alvarez

9:15 —57. Fragment based de novo design using an existing fragment based docking program, eHiTS. **D. Reid**, Z. Zsoldos, A. P. Johnson

9:40 — Intermission.

9:55 —58. Identification of a potent novel non-steroidal progesterone receptor modulator from a virtual screen. **R. J. Unwalla**, A. Fensome, M. Marella, J. Cross, E. Melenski, J. Wilhelm, A. Olland, S. Wolfrom, H. Elokdah, J. Wrobel, R. C. Winneker, M. Yudt, S. nagpal, J. Cohen

10:20 —59. Virtual screening discovered catechol-containing compounds as STAT3 SH2 domain inhibitors. **Y. Hu**, W. Hao, X. Huang, C -P. B. chang, J. Gibbons, J. Xu, C. Humblet

10:45 —60. Searching for new targets for the inhibition of Acetyl-CoA Carboxylase. **M. E. McKenzie**, G. L. Waldrop, B. Chen

11:10 —61. Computer-aided design of novel Akt inhibitors targeting to the pleckstrin homology domain. **L. Du-Cuny**, G. Powis, E. J. Meuillet, E. Mash, S. Zhang

Section D

Unknown Site -- Unknown Room

Quantum Chemistry

Quantum-Methods I

A. Roitberg, *Organizer*

8:00 —62. Computation of acidity constants in solution from vertical energy gaps. M. Sulpizi, A. Shah, **M. Sprik**

8:25 —63. Dual-Basis Methods: Energies and derivatives with application to non-covalent interactions. **R. P. Steele**, R. A. DiStasio Jr., M. Head-Gordon

8:50 —64. Semiempirical PM6 modeling of organic crystal structures. **J. J. P. Stewart**

9:15 — Intermission.

9:40 —65. Evaluating the accuracy of semi-empirical QM/MM methods using replica exchange and AMBER 10: Phi/Psi free energy calculations of peptides in solution. **R. C. Walker**, G. D. M. Seabra, A. Roitberg

10:05 —66. Stacking and hydrogen bonding: Effective fragment potential modeling of DNA bases. **T. Smith**, L. V. Slipchenko, M. S. Gordon

10:30 —67. Multi-centered ONIOM method for weakly bound non-covalent clusters: Recent advances and applications. **G. S. Tschumper**

MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Computational Catalysis

Nano

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
A. M. Rappe, S. Linic, and J. W. Bennett, *Organizers*

1:30 —68. First principles study on the effect of metal and interface identities on thin film surface activity. **V. R. Cooper**, A. M. Kolpak, A. M. Rappe

2:00 —69. Computational study of hydrogenated transition metal clusters on zeolite support. **N. Roesch**, G. P. Petrova, G. N. Vayssilov, E. A. Ivanova Shor, V. A. Nasluzov, A. M. Shor

2:30 —70. Surface chemistry of gold nano-structures deposited on oxides: oxide-specific O2 interactions with supported gold and the oxidation state of gold. S. Laursen, **S. Linic**

3:00 — Intermission.

3:30 —71. Density Functional Theory Study of Pt and Pd-based Pseudomorphic Monolayer Alloy Catalysts for NOx Storage Reduction Applications. J. Jelic, **R. J. Meyer**

4:00 —72. First principle calculations of supported catalysts: CO binding on MgO supported gold clusters and nanoparticles. **G. Mpourmpakis**, D. G. Vlachos

Section B

Unknown Site -- Unknown Room

Thomas Kuhn Paradigm Shift Award Competition

A. Nicholls and A. G. Skillman, *Organizers*

1:00 — Introductory Remarks.

1:05 —73. Believe it or not: Understanding prediction confidence in computational drug discovery. **D. Debe**

1:45 —74. Exploration of Chemical Space for Drug Discovery by Database Generation. **J -L. Reymond**

2:25 — Intermission.

2:40 —75. Considering a treatment of induced electronic polarization based on the Poisson equation. **J -F. Truchon**, A. Nicholls, A. Grant, B. Roux, R. I. Iftimie, C. I. Bayly

3:20 —76. Extracting configurational entropy changes using a mutual-information expansion: Binding in the TSG101/PTAP complex. **B. J. Killian**, J. Y. Kravitz, P. Dasgupta, Y -P. Pang, M. K. Gilson

4:00 — Concluding Remarks.

Section C

Unknown Site -- Unknown Room

Quantum Chemistry

Quantum-Methods II

A. Roitberg, *Organizer*

1:30 —77. Natural linear scaled coupled cluster theory with local transferable triple excitations: Applications to polymers. **T. F. Hughes**, N. Flocke, R. J. Bartlett

1:55 —78. Dispersion in combined ab initio/effective fragment potential systems. **T. Smith**, L. V. Slipchenko, M. S. Gordon

2:20 —79. Statistical correlation approach to improved thermodynamic predictions from DFT. **A. M. Shough**, D. J. Doren, D. M. DiToro

2:45 — Intermission.

3:10 —80. Pushing the limits of MCSCF. **L. Roskop**, M. S. Gordon

3:35 —81. Reaction path analysis: Approximations and applications. **W -J. van Zeist**, A. H. Koers, L. P. Wolters, F. M. Bickelhaupt

ADAPT'ing to Retirement: A Symposium Honoring Peter C. Jurs

Sponsored by CINF, Cosponsored by COMP and PROF
R. Guha, *Organizer*
R. Guha, *Presiding*

1:10 — Introductory Remarks.

1:15 —47. Wavelet based search prefilters for spectral library matching. **B. K. Lavine**, N. Mirjankar, K. Nuguru

1:45 —48. Fragment Activity Comparison Tool. **S. R. Johnson**, B. L. Claus, O. Gudmundsson, P. A. Elzinga, G. Everlof, M. J. Hageman

2:15 —49. Modeling a touch of freshness: Developing a QSPR model for amine-assisted perfume delivery in laundry detergent. **D. T. Stanton**, J. Smets, M. Van de Walle, A. Pintens, S. Van de Velde, R. Trujillo

2:45 — Intermission.

3:00 —50. QSAR at the undergraduate institution and a model of air-to-blood partition coefficients for small organic molecules. **N. R. McElroy**, S. D. Smith

3:30 —51. Adapting in an ABCD world. **E. P. Jaeger**

MONDAY EVENING

Section A

Unknown Site -- Unknown Room

Sci-Mix

E. X. Esposito, *Organizer*

8:00 - 10:00

116, 121, 127, 132, 136, 141, 143-144, 147, 151, 155, 157, 163, 199, 204. See subsequent listings.

TUESDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Phase Equilibria

III

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
J. I. Siepmann and J. K. Johnson, *Organizers*

8:00 —82. Coarse-grain simulations of complex systems. **J. J. de Pablo**

8:40 —83. Optimized expanded ensembles for simulations involving molecular insertions and deletions. **F. A. Escobedo**, F. J. Martínez-Veracoechea

9:20 —84. Use of the AUA intermolecular potential to determine the solubility of hydrogen in oxygenated solvents. **R. Lugo**, N. Ferrando, C. Nieto-Draghi

9:40 — Intermission.

9:50 —85. Monte Carlo simulations for phase equilibria: Polymer solubility and quantum effects. **C. D. Wick**

10:30 —86. Thermodynamics of solvent reorganization in solvent/co-solvent mixtures. **N. F. van der Vegt**, M -E. Lee, T. A. Ozal

11:10 —87. Structure of liquid water from ab initio molecular dynamics at the complete plane wave basis set limit. **O. Isayev**, L. Gorb, J. Leszczynski

11:30 —88. Treatment and importance of conformations in COSMO-RS. **A. Klamt**, M. Diedenhofen

Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Applications to Protein Folding

S. Rick, *Organizer*

8:00 —89. Computing properties determining the stability diagram of a miniprotein in dilute aqueous solution by full atomic detail computer simulation. **D. Paschek**, A. E. Garcia

8:40 —90. Convergence of folding free energy landscapes via application of enhanced sampling methods in a distributed computing environment. **V. S. Pande**, X. Huang, G. Bowman

9:20 — Intermission.

9:40 —91. Structure and dynamics of the Aβ21-30 peptide from the interplay of NMR experiments and molecular simulations. **T. Head-Gordon**, N. L. Fawzi, A. Phillips, J. Z. Ruscio, M. Doucleff, D. Wemmer

10:20 —92. Sampling sequences: Engineering protein structure and function with theoretical protein design. **J. G. Saven**

Section C

Unknown Site -- Unknown Room

Drug Discovery

Mostly about Ligands

Cosponsored by CINF
I. Visiers, *Organizer*
E. Feyfant, *Presiding*

8:00 —93. Applications of target class pharmacophore fingerprint modeling and multi-objective genetic algorithm optimization to large-scale combinatorial library design for corporate compound collection enhancement. **Z. Yang**, G. P. Brady

8:25 —94. Combining clique-detection, MOGUL and MOGA for pharmacophore generation. D. A. Cosgrove, **E. J. Gardiner**, V. J. Gillet, R. Taylor

8:50 —95. Confirm: Connecting fragments in receptor molecules. D. C. Thompson, A. Denny, D. Joseph-McCarthy, C. Humblet, **E. Feyfant**

9:15 —96. Fast and accurate method for flexible ligand superposition and shape-based screening. S. L. Dixon, P. Dalal, J. Gata-Aura, S. N. Rao, J. C. Shelley, **B. W. Sherman**

9:40 — Intermission.

9:55 —97. Pharmacophore fingerprints and application to target class modeling. **G. P. Brady**, Z. P. Yang

10:20 —98. QSAR-based design of novel anti-HRV 2 agents. **A. Artemenko**, E. N. Muratov, V. E. Kuz'min, E. Varlamova, V. Makarov, O. Riabova, M. Schmidtke, P. Wutzler

TUESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Computational Catalysis

Surfaces

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
A. M. Rappe, S. Linic, and V. R. Cooper, *Organizers*

1:30 —99. Modeling the Fischer-Tropsch synthesis catalyzed on a Fe(1,0,0) surface. J. Lo, **T. Ziegler**

2:00 —100. First-principles modeling of $Ba(Ce_{1-x},Pd_x)O_{3-x}$: redox, structure, and chemistry. **J. W. Bennett**, R. Seshadri, S. L. Scott, A. M. Rappe

2:30 —101. First-principles investigations of oxygen vacancies, copper adatoms, and their interactions on TiO_2 (110). **S. Lewis**

3:00 — Intermission.

3:30 —102. Identification of surface intermediates through the combined use of molecular modeling and vibrational spectroscopy. **J. W. Medlin**

4:00 —103. NO oxidation thermodynamics and kinetics at high O coverage on Pt(111). **R. B. Getman**, W. F. Schneider

4:30 —104. Density functional theory study of CO oxidation on Pd alloy surfaces. **M. B. Sullivan**, J. Zhang, F. C. H. Lim, H -M. Jin, P. Wu

Section B

Unknown Site -- Unknown Room

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of J. Andrew McCammon

J. D. Madura, *Organizer*

1:00 — Introductory Remarks.

1:10 —105. Investigating allosteric communication in protein systems with new conformational fluctuation covariance analysis methods. M. J. Bradley, R. L. Rice, P. T. Chivers, E. Di Cera, **N. A. Baker**

1:50 —106. Brownian dynamics with hydrodynamic interactions: Application to lipid bilayers and biomembranes. **F. L. H. Brown**

2:30 —107. Ensemble approaches yeild new scaffolds and new binding sites. **H. A. Carlson**

3:10 — Intermission.

3:30 —108. Molecular simulations of macromolecular behavior in physiological conditions. **A. H. Elcock**

4:10 —109. Adventures in computational chemistry. **J. A. McCammon**

Section C

Unknown Site -- Unknown Room

Molecular Mechanics

Advancing Methodologies II

E. X. Esposito, *Organizer*

1:30 —110. The generalized Born model: Past, present, future? **A. V. Onufriev**

1:55 —111. Salt Effects and explicit ions in continuum representations of water. **S. A. Hassan**

2:20 —112. Charge asymmetries in hydration of polar solutes. **D. L. Mobley**, A. Barber II, C. J. Fennell, K. A. Dill

2:45 — Intermission.

3:00 —113. Molecular dynamics with generalized effective fragment potentials. **J. M. Mullin**, M. S. Gordon

3:25 —114. Novel algorithms enabling practical microsecond-scale molecular dynamics simulations. K. J. Bowers, E. Chow, **R. O. Dror**, M. P. Eastwood, B. A. Gregersen, J. Gullingsrud, M. Ø. Jensen, J. L. Klepeis, I. Kolossváry, R. A. Lippert, C. A. Rendleman, Y. Shan, H. Xu, D. E. Shaw

3:50 —115. Programming generalized Born models for a SIMD architecture. **I. C. Lagerstedt**

Careers in Chemical Information

Sponsored by CINF, Cosponsored by CHAL, PROF, COMP, CEPA, and WCC
L. M. Balbes, *Organizer*

1:30 — Introductory Remarks.

1:35 —81. Chemist-librarian: The best of both worlds. **F. B. Culp**

2:00 —82. You know you're a Chemical Information Searcher if. **B. M. Bridgewater**

2:25 —83. Information highway to drug discovery. **L. P. Greenblatt**

2:50 — Intermission.

3:00 —84. Path less traveled: From the periodic table to public relations. **J. E. Mears**

3:25 —85. Breaking news: Chemistry is everywhere. **I. Amato**

3:50 —86. Careers in patent law: Going beyond the bench with your chemistry degree. **J. J. Hasford**

4:15 — Networking Discussion.

TUESDAY EVENING

Section A

Unknown Site -- Unknown Room

Poster Session

E. X. Esposito, *Organizer*

7:00 - 9:00

116. On the applicability of GPCR homology modeling to drug discovery: A comparison between crystal structure and in silico model of the β2 adrenergic receptor complexed with carazolol. **S. Costanzi**

117. Decomposition of high-energy density materials using high-level coupled-cluster theory. **A. G. Taube**, R. J. Bartlett

118. building aromatic oligoamide foldamers. **J. A. Geer**, Z. Liu, V. Pophristic

119. Salt effects on the conformational preferences of alanine peptides. **E. Asciutto**, J. D. Madura

120. Molecular dynamics of the RNA-binding domain of Influenza A NS1. **C. Young**, R. Manetsch, E. Rivera, A. van Olphen, A. E. Cardenas

121. TAE augmented scoring functions: Application to enzymatic and non-enzymatic proteins. **S. Das**, C. M. Breneman, N. Sukumar, M. D. Ryan

122. A novel computational strategy for identifying peptides that bind pancreatic lipase. J. Audie, **A. Spock**

123. Hypothesis-driven computational biophysics: a possible explanation for trypsin-BPTI binding. J. Audie, **K. Hannigan**, **K. Naik**

124. Theoretical Study of the Glutamate Receptor Ligand Binding Domain Flexibility and Conformational Reorganization. **T. Mamonova**, M. Kurnikova

125. A New Strategy to Drug Discovery - Systems-Based Drug Discovery. **Z. Hu**

126. ab initio calculation of reaction between series of gilman cuprates and CH3I. **J. Liu**, J. P. Snyder

127. Acute toxicity of polynitroaromatics and products of their biotransformation on *Vibrio fischeri*: 2D QSAR study. **A. Artemenko**, A. V. Lyahovskij, V. E. Kuz'min, E. N. Muratov, L. Gorb, M. Quasim, J. Leszczynski

128. Amyloidogenic intermediates: A computational study of the conversion of the β-sheet to α-sheet structure. **A. M. Canfield**, S. Huo, H. Wu

129. Analysis of polarization effects in protein-water simulations. **S. Urahata**, J. W. Ponder

130. Analysis of torsional effects and ring flipping in heavily substituted oxazolidine rings. **P. M. Spoutz**, M. C. Milletti

131. Application of the fault-injection system algorithm for chips coated with silsesquioxanes. **Q. Pan**, B. Hong, Q. Pan, L. Hu

132. Artificial neural network prediction of metal hydride properties with experimental and/or computational data. **W. O. Griffin**, J. A. Darsey

133. Atomic level computational identification of ligand migration pathways between solvent and binding site in myoglobin. J. Z. Ruscio, M. G. Prisant, T. Murali, **A. V. Onufriev**

134. Axial bonding in alkylcobalamins: DFT analysis of the inverse trans influence. **J. Kuta**, J. Wuerges, L. Randaccio, P. M. Kozlowski

135. Binding energies in dimers of N-methyl methyl carbamate, N-methyl S-methyl thiocarbamate, and N-methyl methyl dithiocarbamate. **H. McAlexander**, D. H. Magers

136. Calculation of adsorption free energy for peptide interactions with a crystalline polylactide polymer surface. **C. O'Brien**, D. A. Bruce, R. A. Latour Jr.

137. Calculation of rotational barriers for two iminium cation stereoisomers. **L. A. Lello**, M. C. Milletti

138. Calculations of the acidities of n-butylbenzene protons in aqueous media under normal and supercritical conditions. **P. R. Alburquerque**, T. Junk, B. Ramachandran

139. CCl_4 adsorption and dissociation on Si(111)- $\sqrt{3}x\sqrt{3}$- Ag surface from first principles. **X. Liu**, H. Guo, C. Meng

140. Combinatorial QSAR analysis of histone deacetylase inhibitors and QSAR-based virtual screening. **H. Tang**, X. S. Wang, X -P. Huang, B. L. Roth, A. P. Kozikowski, A. Tropsha

141. Comparing the thermodynamic stability of skipped diene radicals: A model for the peroxidation of arachidonic acid. **C. E. Tornow**, M. C. Milletti

142. Comparison of density functionals and semiempirical methods for protonated creatinine. **N. Settergren**, E. A. Amin, P. Buhlmann

143. Comparison of DFT and MP2-based electronic models in the estimation of relative conformational and tautomeric energies and torsional potentials of drug-like moieties. **D. L. Cheney**, K. A. Rossi

144. Comparison of pose generation and virtual screening accuracy for several molecular docking programs. **J. B. Cross**, D. C. Thompson, B. K. Rai, J. C. Baber, K. Y. Fan, Y. Hu, C. Humblet

145. Computational studies of gas phase and heterogeneous sulfur oxide reactions. **J. M. Standard**, P. Gorczynski, R. D. Quinn, M. T. Van der Hoven

146. Structure-activity relationships in FF neuropeptide sudied with computational simulations. **G. Leonis**, M. Arrar, A. E. Roitberg

147. Computational study of the interaction of sulfoindocyanine dye Cy3 with single- and double-stranded DNA. **E. Dolghih**, J. Krause, A. E. Roitberg

148. Density functional study on the reductive elimination at an (NCN)Pt(IV) center. **S. Hwang**, H. Y. Woo, H. Cho, J. Jang

149. Density functional theoretical study on the proton migration in radical cations of substituted cytosine:guanine pair. **Y. S. Cho**, S. Hwang, Y. H. Jang

150. Density functional theory calculations on Ti and Li decoration in MOF-5. **D. H. Jung**, D. Kim, J. Kim, S -H. Choi

151. Design of peptidomimetic ligands using core hopping. **M. Shelley**

152. Deterioration of popular DFT model chemistries for electron affinities. **D. Bates**, G. S. Tschumper

153. Development of a QSPR method for the prediction of chemicals explosibility. **G. Fayet**, P. Rotureau, L. Joubert, C. Adamo

154. Direct dynamics study of [1,3]-sigmatropic shift of bicyclo[3.2.0]hept-2-ene to norbornene. **L. Xu**, C. E. Doubleday, K. N. Houk

155. Docking based pharmacophore modeling of combined AT1-PPAR gamma ligands. **F. Shah**, P. Mukherjee, M. A. Avery

156. Doublet-quartet gaps of substituted carbynes. **K. A. Daniel**, E. V. Patterson

157. Effects of salt concentration on the HIV Rev-RRE complex using molecular dynamics simulations. **B. R. Miller III**, J. A. Chenault, A. K. Sezhiyan, M. C. Nagan

158. Efficient extrapolation to the CCSD(T)/CBS limit using pair natural orbitals. **E. C. Barnes**, G. A. Petersson

159. Enhanced stacking interactions between nucleic acid base pairs upon hydrogenation. **M. Mandziuk**, J. Landers, F. Duffy

160. Enthalpies of formation of TNT derivatives by homodesmotic reactions. **A. Sood**, D. H. Magers

161. Establishing a balance between prediction accuracy and applicability domain of QSAR models. **L. Ye**, H. Zhu, A. Golbraikh, A. Tropsha

162. Evaluation of density functionals, semiempirical methods, SCC-DFTB and molecular mechanics force fields for prolyl-leucyl-glycinamide (PLG) analogs designed as dopamine D2 receptor modulators. E. A. Amin, **R. L. Wood**, R. L. Johnson, B. J. Young-Dixon

163. Exploring pharmacophore generation programs. **K. Y. Fan**, G. J. Tawa, C. Humblet

164. Fast folding of peptides and small proteins using the “temperature intervals with global energy reassignment” (TIGER) method. **X. Li**, S. J. Stuart, R. A. Latour

165. Finding the right path: Computational approach to DNA base eversion. **C. Bergonzo**, C. L. Simmerling

166. FITTED: A docking-based virtual screening tool for flexible and complex systems. **C. R. Corbeil**, J. Schwartzentruber, N. Moitessier

167. Formic acid tetramer: Hydrogen-bonding versus π-stacking. **G. Tipton**, G. S. Tschumper

168. HiT QSAR analysis of chiral AchE inhibitors. **V. Kuz'min**, E. N. Muratov, A. G. Artemenko, L. Gorb, J. Wang, M. Quasim, J. Leszczynski

169. Homology modeling: Studying conformationally flexible loops near ligand binding sites. **K. A. Rossi**, C. A. Weigelt, A. Nayeem, S. R. Krystek Jr.

170. How do SET-domain Protein Lysine Methyltransferases Achieve the Methylation State Specificity? An ab initio QM/MM Molecular Dynamics Study. **P. Hu**, S. Wang, Y. Zhang

171. Identification of Inhibitors for Blocking S100B-P53 Interaction using Virtual Database Screening. **S. Zhong**, P. T. Wilder, T. H. Charpentier, M. Liriano, D. J. Weber, A. D. MacKerell Jr.

172. Interplay of π-stacking and hydrogen bonding: An *ab intio* study of diacetylene/water and cyanogen/water clusters. **K. Copeland**, G. S. Tschumper

173. Iterative refinement of parameters for computer simulation of peptides and proteins. **P. J. Steinbach**

174. Kinetic aspects of the oxygenation reaction mechanism in COX-1. **M. A. Lukowski**, M. C. Milletti

175. Kirkwood-Buff derived force fields for mixtures of thiols in water. **N. Bentenitis**, **M. Mullins**

176. Mechanism of hydrogen production by [Fe-Fe]-hydrogenase in DdH and CpI: A QM/MM study. **S. Trohalaki**, R. Pachter

177. Mechanistic study of inosine monophosphate dehydrogenase. **D. E. Mendes**, A. Cook, S. Braun-Sand

178. Mixed Quantum/Classical studies of Trypanosoma Cruzi's Trans-sialidase. **J. M. Swails**, Ö. Demir, G. D. M. Seabra, A. Roitberg

179. Molecular dynamics studies of human immunodeficiency virus RSG-1.2-RRE recognition. **L. A. Michael**, B. R. Miller III, M. C. Nagan

180. Molecular modeling of nonpeptidic agonists of glucagon-like peptide 1 (GLP-1) receptors. **Z. Hu**, W. M. Southerland

181. Novel derivatives of bicyclo[2.2.2]octane and their strain energies. **E. C. Garrett III**, E. J. Valente, D. H. Magers

182. ONIOM investigation of nucleotide selectivity in phosphodiesterases 3, 4, and 5. E. A. Salter, K. A. O'Brien, R. W. Edmunds, **A. Wierzbicki**

183. Predicting ligand binding affinity to the rat α4β2 neuronal nicotinic receptor : Lessons from bayesian categorization modeling. **D. C. Kombo**, J -P. Strachan, J. Chewning, M. Lanning, P. S. Hammond, D. Yohannes, C. Woodward, D. F. Frey, S. R. Breining, C. H. Miller, G. J. Gatto

184. QSPR predictions of an aqueous solubility for military compounds using SiRMS. **E. N. Muratov**, V. E. Kuz'min, A. G. Artemenko, L. Gorb, M. Quasim, J. Leszczynski

185. Quantitative method for computational investigations of enzyme and antibody catalysis: The Kemp Elimination. **G. Kiss**, K. N. Houk, D. Baker, D. Hilvert

186. Quantitative structure-activity relationship modeling of the A_{2B} adenosine receptor agonists. **A. A. Ivanov**, K. A. Jacobson

187. RankScore2: A novel scoring function for ligand-protein binding affinities. **P. Englebienne**, N. Moitessier

188. Reduced point charge approximation for speeding up the computation of electrostatic potential in biomolecular systems. **R. Anandakrishnan**, A. V. Onufriev

189. Relative stability of isomers of 2,3-disubstituted 1-aminoindenes. **A. K. Magers**, D. H. Magers

190. Relative stability of isomers of a dipseudoacid. **P. J. Huwe**, D. V. Liskin, E. J. Valente, D. H. Magers

191. Relativity aromaticity in pentacene derivatives. **B. Cao**, D. H. Magers

192. Significance of electrostatics at hydrogen bond donor and polarization at hydrogen bond acceptor: Insight through QM/MM simulation. **V. S. Pakkala**, J. A. Plumley, J. D. Evanseck

193. Simulated interactions between structured peptides and functionalized surfaces. **G. Collier**, S. J. Stuart, B. R. Brooks, R. A. Latour Jr.

194. Simulations of polypeptide folding using new efficient replica exchange methods. **A. J. Lee**, S. Rick

195. Strain energies in isomers of 1,3-cycloheptadiene and bicyclo[3.2.0]hept-6-ene. **B. Magers**, S. R. Davis, D. H. Magers

196. Structural Effects of Interstrand Crosslinks on DNA through Molecular Dynamic Simulations. **A. J. Campbell**, K. Song, A. Guainazzi, O. D. Scharer, C. L. Simmerling

197. Surflex-Docking into the minor groove of DNA. **L. Wang**, T. E. Mansley

198. Targeting the protein-protein interaction of Bcl-xL for drug discovery. **P. Mukherjee**, P. V. Desai, Y -D. Zhou, M. A. Avery

199. Temperature dependent structural dynamics of the Villin Headpiece Helical Subdomain: An ultrafast folding protein. **L. Wickstrom**, S. Brewer, R. B. Dyer, D. P. Raleigh, C. L. Simmerling

200. The free energy and entropy of a water molecule in hydrophobic cavities. **H. Yu**, S. Rick

201. The radical enhanced nucleation of water. **S. J. Keasler**, B. Chen, J. S. Francisco, R. B. Nellas

202. The role of the active site solvent in the thermodynamics of factor Xa-ligand binding. **R. Abel**, T. Young, R. Farid, B. Berne, R. A. Friesner

203. Unusual participation of the counterion in charge transfer copper(I) complexes. **L. M. Matosziuk**, T. Pintauer, J. D. Evanseck

204. Virtual screening with pharmacophore model: application in search of novel CB1 antagonists. **H. Wang**, R. A. Duffy, G. Boykow, S. Chackalamannil, V. S. Madison

Section B

Unknown Site -- Unknown Room

Chemical Computing Group Excellence Award

A. Good, *Organizer*

7:00 - 9:00

205. Considering a treatment of induced electronic polarization based on the Poisson equation. **J -F. Truchon**, A. Nicholls, A. Grant, B. Roux, R. I. Iftimie, C. I. Bayly

206. Coupled-cluster theory on supercomputers. **J. R. Hammond**, K. Kowalski

207. FORECASTER: A new platform for drug discovery. **P. Englebienne**, C. R. Corbeil, N. Moitessier

208. Hydrophobic interaction in acidic aqueous solutions. **H. Chen**, G. A. Voth

209. Using computer simulations to explore pressure effects on proteins. **S. Sarupria**, S. Garde

Section C

Unknown Site -- Unknown Room

HP Scholar Award Poster Session

C. M. Breneman, *Organizer*

7:00 - 9:00

210. Determination of absolute configuration in solution. **M. L. Abrams**

211. Predictive electronic and vibrational many-body methods. **S. Hirata**

212. Advances in potentials of mean force methodology for organic and biological simulations. **O. Acevedo**

213. Integration of a bioinformatics approach to high-throughput docking and its dpplication to the discovery of novel TNF receptor-associated factor 6 (TRAF6) inhibitors. **S. Zhang**, B. Darnay, L. Du-Cuny

WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Evaluation of Rate Constants

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
T. N. Truong and H. DaCosta, *Organizers*

8:00 — Introductory Remarks.

8:05 —214. A Fast Semi-Empirical Approach to Accurate Rate Constants. **N. S. Ostlund**, J. R. Barker

8:50 —215. Rates of quantum states population and coherence relaxation during optical excitation of surfaces: A density matrix computational approach. **D. A. Micha**, A. S. Leathers, D. S. Kilin

9:35 — Intermission.

9:50 —216. Efficient estimators for quantum instanton evaluation of the kinetic isotope effects. **J. Vanicek**, W. H. Miller

10:20 —217. Kinetic analysis of the pyrolysis of phenethyl phenyl ether with different substituents: Computational prediction of α/β-selectivities. **A. Beste**, A. C. Buchanan III, R. J. Harrison

10:50 —218. Transition state theory rate constants for intramolecular hydrogen transfer reactions in oxygenated radicals. **K. T. Kuwata**, T. S. Dibble, E. Sliz, E. B. Petersen

11:20 —219. Two transition state model for radical-molecule reactions. **S. J. Klippenstein**, Y. Georgievskii, H. Sabbah, L. Biennier, I. R. Sims, I. W. M. Smith

Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Methods III

S. Rick, *Organizer*

8:00 —220. Parallel tempering techniques for simulation of proteins. **U. H. Hansmann**, W. Nadler

8:40 —221. Extracting averages and distributions from replica-exchange simulations of large systems: a new version of WHAM. **J -E. Shea**, A. Jewett

9:20 —222. Mechanisms of protein (un)folding and signaling state formation revealed with replica exchange. J. Juraszek, J. Vreede, M. Wolf, **P. G. Bolhuis**

10:00 — Intermission.

10:40 —223. A different architecture for expanded ensemble simulation: Adaptive AIS. **E. Lyman**, D. M. Zuckerman

11:20 —224. Protein folding network, and energy landscape, studied by parallel Wang-Landau sampling. **S. Takada**

12:00 —225. Protein folding using replica exchange and mechanism-based conformational searching. **M. S. Shell**, B. Ozkan, V. Voelz, A. Wu, K. A. Dill

Section C

Unknown Site -- Unknown Room

Drug Discovery

Drug Discovery

Cosponsored by CINF
I. Visiers, *Organizer*
P. Carlqvist, *Presiding*

8:00 —226. Binding Response: A Method for the Prediction of Ligand Binding Sites on Proteins. **S. Zhong**, A. D. MacKerell Jr.

8:25 —227. Giving the Rule-of-5 a more accurate twist. **G. Pearl**, S. Bhal, I. G. Peirson, K. Kassam

8:50 —228. Virtual screening for superior R-groups. **R. D. Cramer**

9:15 —229. Histone deacetylase inhibitors: Reasons for isoform selectivity. **G. Estiu**, O. Wiest, E. Greenberg, R. Mazitschek, J. Bradner

9:40 —230. Modeling the metabolic space in drug discovery. L. Terfloth, B. B. Bienfait, J. Gasteiger, **C. H. Schwab**

WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Computational Catalysis

Electro-catalysis and the Impact of Environment

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
A. M. Rappe and S. Linic, *Organizers*

1:30 —231. Surface segregation in nanoalloys under reaction conditions. **P. B. Balbuena**, Y. Ma, G. Ramirez-Caballero, J. R. Callejas-Tovar

2:00 —232. First principles studies of electrochemical oxidation reactions at model solid oxide fuel cell (SOFC) anodes. D. Ingram, J. Mukherjee, **S. Linic**

2:30 —233. Why PtVFe nanoparticles are better catalysts for oxygen reduction. **T. Lin**, J. Williams, L. Wang

3:00 — Intermission.

3:30 —234. Configurational correlations in the adsorption properties of atomic adsorbates on transition metal surfaces. **J. R. Kitchin**

4:00 —235. First-principles prediction of switchable stoichiometry at interfaces. **S. V. Levchenko**, A. M. Rappe

4:30 —236. Thermochemistry and kinetics of steam methane reforming on Ni(111) under realistic conditions. **T. Ogura**, D. W. Blaylock, G. J. O. Beran, W. H. Green Jr.

Section B

Unknown Site -- Unknown Room

Model Applicability Domains: When Can I Use my Model?

Cosponsored by CINF
C. M. Breneman and D. F. Ortwine, *Organizers*

1:00 — Introductory Remarks.

1:10 —237. Domain applicability of ligand and structure-based virtual screening. **A. Nicholls**, M. McGann, P. Hawkins

1:35 —238. Testing the limits of a QSAR model: How many cases are actually needed to develop a reliable predictive model? **C. M. Sundling**, C. M. Breneman, M. J. Embrechts, C. Huang, X. Wu, N. Sukumar

2:00 —239. Automatic detection of outliers prior to QSAR studies. **A. Golbraikh**, H. Zhu, L. Ye, M. Wang-Bell, H. Tang, A. Tropsha

2:25 — Intermission.

2:40 —240. Combining global and local approaches to model domain applicability. **R. Guha**, D. T. Stanton

3:05 —241. QSAR model stability: How much information is in the data? **D. Ryan**, M. McLellan, C. M. Breneman

3:30 —242. Domain applicability: How far are ideal and reality? **E. N. Muratov**, V. E. Kuz'min, A. G. Artemenko

Section C

Unknown Site -- Unknown Room

Molecular Mechanics

Biomolecular Simulations

E. X. Esposito, *Organizer*

1:30 —243. Solvation of carbon nanotubes using de-novo peptide helices: A molecular dynamics approach. **C -C. Chiu**, G. R. Dieckmann, S. O. Nielsen

1:55 —244. Examination of proposed intercalation models for imidazoacridone related compounds. **I. E. Weidlich**, S. G. Tarasov, I. V. Filippov, M. C. Nicklaus

2:20 —245. Computational studies of structure-activity relationships in FF neuropeptide. **G. Leonis**, M. Arrar, A. E. Roitberg

2:45 — Intermission.

3:00 —246. Computational study of the interaction of sulfoindocyanine dye Cy3 with single- and double-stranded DNA. **E. Dolghih**, J. L. Krause, A. E. Roitberg

3:25 —247. Role of ligand-receptor flexibility in the design of apoptosis targeting agents: Insight from molecular dynamics. **G. Krilov**, Q. Wang, W. J. Novak, H. Wang

THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Evaluation of Rate Constants

Computational Evaluation of Rate Constants

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
T. N. Truong and H. DaCosta, *Organizers*

8:00 — Introductory Remarks.

8:05 —248. Improved software user interfaces for computational prediction of kinetic rate constants. **R. M. Shroll**, G. D. Black, B. J. Palmer, W. L. Hase, T. L. Windus, S. Baidya, Y. Zhuang

8:50 —249. The Determination of Reaction Rate Constants for H-atom Abstraction from N2H4 by H, NH2, CH3, C2H5 and NO2. **C. Chiung-Chu**, M. Michael

9:35 — Intermission.

9:50 —250. Rate constants from biased and unbiased reactive path ensembles. **B. M. Dickson**, G. Henkelman, D. E. Makarov

10:20 —251. Rate estimation rules for H abstraction reactions by H and CH3 from pure and oxygenated hydrocarbons. **H -H. Carstensen**, A. M. Dean

10:50 —252. Theoretical study of serially coupled chlorite-iodide oscillators. **D. A. Long**, L. Chodroff, T. M. O'Neal, S. Hemkin

11:20 —253. An ab initio molecular dynamics study of the initial chemical events in nitramines: Thermal decomposition of CL-20. **O. Isayev**, L. Gorb, M. Qasim, J. Leszczynski

Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Applications

S. Rick, *Organizer*

8:00 —254. Simulations of hydrogen clathrate hydrates. **D. L. Freeman**, W. Cardoen, E. Curotto, J. D. Doll

8:40 —255. Calculation of the Folding/Unfolding Thermodynamics of an RNA Tetraloop by Replica Exchange Molecular Dynamics. **A. E. Garcia**, D. Paschek

9:20 — Intermission.

9:40 —256. Thermodynamic and transport properties of DNA from Monte Carlo simulations of a coarse-grained model. **E. J. Sambriski**, A. B. Oldham, T. A. Knotts IV, J. J. de Pablo

10:20 —257. Calculation of adsorption free energy for peptide-surface interactions using biased-REMD simulations. **N. A. Vellore**, B. R. Brooks, D. A. Bruce, S. J. Stuart, R. A. Latour

10:40 —258. Novel Ligand-induced Survivin Dimer Conformation via Replica Exchange Molecular Dynamics (REMD) and Receptor-Based Reverse Virtual Screening. **I. H. Park**, C. Li

Section C

Unknown Site -- Unknown Room

Quantum Chemistry

Quantum-Materials

A. Roitberg, *Organizer*

8:00 —259. Testing, validation, and parameterization of density functionals and molecular orbital theory for zinc bio- and nanocenter coordination chemistry. **E. A. Amin**, D. G. Truhlar, A. Sorkin

8:25 —260. Methane and silane dimer potentials from quantum chemistry calculations. **S. D. Chao**, A.

H -T. Li

8:50 —261. Nonequilibrium DFT properties of intramolecular hydrogen bonding in malonaldehyde, aminoacrolein, iminopropenylamine and derivatives. **J. N. Woodford**

9:15 — Intermission.

9:30 —262. Origin of Lewis acid strength within mixed boron halides. **J. A. Plumley**, J. D. Evanseck

9:55 —263. Quantum chemical calculations of surface photovoltages: Applications to adsorbates on Si (111). **D. S. Kilin**, D. A. Micha

10:20 —264. Solid Memory: Structural Preferences in Group 2 Dihalide Monomers, Dimers, and Solids. **K. J. Donald**, R. Hoffmann

THURSDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Molecular Modeling Applied on DPP-4 Inhibitor Programs

Y -D. Gao, *Presiding*

1:00 —265. 3D structural insights for DPP-IV inhibition with Abbott compounds. **K. Longenecker**

1:30 —266. Structural biology and molecular modeling in the design of novel DPP-4 inhibitors. **G. Scapin**

2:00 —267. Lessons about molecular recognition from structure-guided targeting of DPP-IV. **B. Kuhn**, M. Hennig, T. Luebbers, P. Mattei, J. U. Peters, M. Stahl

2:30 —268. Structure, function and inhibitors of prolyl dipeptidase DPP8. **X. Chen**

3:00 —269. Homology models of Dipeptidyl Peptidases 8 and 9. **C. Rummey**, G. Metz

Section B

Unknown Site -- Unknown Room

Model Applicability Domains: When Can I Use my Model?

Part II

Cosponsored by CINF
C. M. Breneman and D. F. Ortwine, *Organizers*

1:00 — Introductory Remarks.

1:05 —270. Applicability domains, space coverage, and predictive power of QSAR models. **A. Tropsha**, A. Golbraikh, H. Zhu

1:30 —271. Testing the validity range of QSAR models using one-class support vector machines. **M. J. Embrechts**, C. M. Breneman, C. Huang, N. Sukumar

1:55 —272. Assessment of Additive/Non-Additive Effects in SAR: Implications in the Drug Discovery Iterative Process. Y. Patel, V. J. Gillet, P. Willet, J. Pastor, T. Howe, **J. Oyarzabal**

2:20 — Intermission.

2:35 —273. Similarity based assessment of model applicability domain and quantitative evaluation of the reliability of the prediction. **P. Japertas**, A. Sazonovas, R. Didziapetris, A. Petrauskas

3:00 —274. Localizing uncertainty in PLS predictivity. **R. D. Clark**, G. Stahl, T. E. Mansley

3:25 —275. Ensemble QSAR. **G. D. Purvis III**

Section C

Unknown Site -- Unknown Room

Molecular Mechanics

Advancing Methodolgies III

E. X. Esposito, *Organizer*

1:00 —276. Advanced multicanonical replica exchange simulations. **D. J. Sindhikara**, A. Roitberg

1:25 —277. Force field evaluation based on NMR experiments and molecular dynamics simulations involving folded proteins. **P. Maragakis**, K. Lindorff-Larsen, M. P. Eastwood, R. O. Dror, J. L. Klepeis, D. E. Shaw

1:50 —278. Multiscale Monte Carlo sampling of proteins. **J. P. Nilmeier**, E. A. Coutsias, M. P. Jacobson

2:15 — Intermission.

2:40 —279. Predicting protein structure using inter-residue distances. **C. R. Crecca**, A. E. Roitberg

3:05 —280. The Coordination Environments of Cu(I) in Proteins: Cu(I) Parameter Development for CHARMM. **M. Harrison**, A. Loccisano, C. T. Dameron, J. D. Evanseck

Submit Final Program