COMP

DIVISION OF COMPUTERS IN CHEMISTRY

Program Not Yet Complete -- Run Data Integrity Report to Identify Errors

Times, days, and paper numbers may not be final. W. D. Cornell and J. D. Madura, Program Chairs

SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory

Michael's Amusements: MO Theory, Aromaticity, Pericyclic Reactions, Semiempirical Methods and Enzyme Catalysis

K. M. Merz Jr., Organizer

9:00 — Introductory Remarks.


9:45 — 2. Rejuvenating Michael's legacy. P. V. R. Schleyer

10:45 — Intermission.

11:00 — 3. Potentially pericyclic reactions involving para-intermediates. K. N. Houk

Section B

Unknown Site -- Unknown Room

Structure-Based Design & Development of Estrogen Receptor Modulators

Cosponsored with MEDI
V. Shanmugasundaram and N. Raheja, Organizers

9:00 — Introductory Remarks.

9:05 — 4. Estrogen receptor structure. R. E. Hubbard


10:15 — 6. Binding mode switching between ERalpha and ERbeta as the basis of subtype selectivity. Y.
Wang, S. Y. Guo, J. D. Durbin, A. Boodhoo, D. B. Baldwin, Y -W. Qian, B. H. Norman, T. I. Richardson, G. Durst, V. Krishnan, J. Dodge

10:50 — 7. Structural insights into SERM design. F. F. Vajdos


Section C

Unknown Site -- Unknown Room

Careers for Computational Chemists in Pharma, Biotech, Patent Law, Software Vendors, and the National Institutes of Health

Cosponsored with CINF, and PROF
W. D. Cornell, Organizer

9:00 — Introductory Remarks.

9:05 — 10. Peer review at the National Institutes of Health. G. Chacko


9:55 — 12. Intramural research at the National Center for Biotechnology Information. E. Bolton

10:20 — Intermission.


11:00 — 14. Long and winding road as a computational chemist in biotech. E. K. Bradley

11:25 — 15. Putting science skills to work in the legal profession. M. Shuster


12:15 — Panel Discussion.

Section D

Unknown Site -- Unknown Room

General Oral - Drug Discovery
Data Extraction, Analysis, Classification

M. Torrent, T. L. Johnson, and E. X. Esposito, Organizers

8:30 — Introductory Remarks.


9:00 — 18. Data mining for kinase gene family selectivity. T. L. Johnson, D. Caffrey, R. V. Stanton, S. Xi


9:50 — Intermission.

10:05 — 20. An on-line on-demand application framework for computational chemistry. T. N. Truong


10:55 — Intermission.

11:10 — 22. Understanding 2D and 3D asymmetry in similarity searching and clustering analysis. J. D. MacCuish, N. E. MacCuish

11:35 — 23. 2D visualization and constraint-driven enumeration of chemical fragment spaces. J. Paern, M. Rarey

Section E

Unknown Site -- Unknown Room

General Oral - Molecular Mechanics and Simulation

J. D. Madura, Organizer

8:30 — 24. Solvent-induced attraction between repulsive ions. S. J. Keasler, B. Chen, R. B. Nellas

8:55 — 25. How well does Poisson-Boltzmann solvent compare with explicit solvent? C. Tan, R. Luo


10:10 — Intermission.

10:50 — 29. Generalized coarse-grained model based on Gay-Berne and point multipole potentials. P. A. Golubkov, P. Ren

11:15 — 30. Structure and dynamics of the full-length lipid-modified H-ras protein in a DMPC bilayer. A. A. Gorfe, J. A. McCammon


**Advances in Virtual High-Throughput Screening**

**Applications**

*Sponsored by CINF, Cosponsored with COMP, and MEDI*

**SUNDAY AFTERNOON**

Section A

Unknown Site -- Unknown Room

**Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory**

**Michael's Amusements: MO Theory, Aromaticity, Pericyclic Reactions, Semiempirical Methods and Enzyme Catalysis**

K. M. Merz Jr., Organizer

1:30 — 32. Dewar-type semiempirical methods: Development, impact, perspectives. W. Thiel


3:30 — Intermission.

3:45 — 34. Impact of enzyme motion on activity. S. Hammes-Schiffer

4:15 — 35. Perspective on biological catalysis. S. J. Benkovic, S. Hammes-Schiffer

Section B

Unknown Site -- Unknown Room

**Structure-Based Design & Development of Estrogen Receptor Modulators**

*Cosponsored with MEDI*
V. Shanmugasundaram and N. Raheja, Organizers

1:00 — Introductory Remarks.


1:40 — 37. Structure-based design of estrogen receptor-beta selective compounds. M. S. Malamas, H. A. Harris, J. Keith, B. McDevitt, I. Gunawan, E. Manas, C. P. Miller, R. E. Mewshaw

2:15 — 38. Ligand flipping within the estrogen receptor hormone binding domain. M. Wang, Y. Wang, T. B. Burris, J. A. Dodge, O. Wallace


Section D

Unknown Site -- Unknown Room

General Oral - Molecular Mechanics and Simulation

J. D. Madura, Organizer

1:30 — 42. Locating α-helices and α-strands using recently-developed protocols. T. H. Click, R. A. Wheeler


2:45 — 45. Electronic polarization in the enzymatic pocket of ODCase through first principles molecular dynamics simulation. I-F. W. Kuo, C. J. Mundy

3:10 — Intermission.

3:50 — 47. Surface phenomenon at the liquid/vapor interface of water and methanol from first principles simulation. **I-F. W. Kuo**, C. J. Mundy, M. J. McGrath, J. I. Siepmann


**Section E**

Unknown Site -- Unknown Room

**General Oral - Quantum Chemistry**

J. D. Madura, *Organizer*

1:00 — 49. Does nature use the variational theorem? A comparative study of enzyme active site geometry from crystal structures and quantum mechanics. **J. DeChancie**, F. Clemente, H. Gunaydin, A. Smith, K. N. Houk, D. Baker

1:25 — 50. Enzyme binding specificity and catalytic mechanisms in both wild-type mAChE and H447I mutant: A combined QM/MM-FE and thermodynamic integration study. **Y. Cheng**, X. Cheng, J. A. McCammon


2:15 — 52. The nature of high energy phosphoryl bonds: An anomeric effect. **J. D. Evanseck**, E. A. Ruben, M. S. Chapman

2:40 — Intermission.


4:35 — 57. Quadratic scaling multireference correlation in polyenes and long molecules with the local density matrix renormalization group. **J. Hachmann**, W. R. Cardoen, G. K-L. Chan

**Advances in Virtual High-Throughput Screening**
New Approaches

*Sponsored by CINF, Cosponsored with COMP, and MEDI*

**MONDAY MORNING**

Unknown Site -- Unknown Room

**DFTB, An Approximate DFT Method: Theory and Applications, Sponsored by Elsevier**

*Introducing SCC-DFTB: Comparisons with Traditional Semiempirical Methods*

M. Elstner and T. Frauenheim, *Organizers*
J. McKelvey, *Organizer, Presiding*

9:00 — Introductory Remarks. **J. McKelvey.**

9:10 — 58. An approximate DFT-method to understand complex materials structures, properties and functions. **T. Frauenheim**


10:10 — 60. The SCC-DFTB method applied to biological systems: Successes, problems and extensions. **M. Elstner**

10:40 — Intermission.

10:55 — 61. A practical parameter optimization technique for semiempirical methods. **J. J. P. Stewart**

11:25 — 62. Looking at DFTB from a semiempirical perspective. **W. Thiel**

11:55 — 63. Recent developments and applications of the DFTB (Density Functional Tight Binding) method. **K. Morokuma**

Section B

Unknown Site -- Unknown Room

**Molecular Similarity and Indexing Methods**

A. N. Jain and A. Nicholls, *Organizers*

9:00 — 64. Molecular similarity: Effective methodological testing for practical utilization. **A. N. Jain**

10:00 —66. Ligand-based design at GSK via pFPs and SCOPE. G. P. Brady, C. Duraiswami, Z. P. Yang, X. Hong, M. S. Head

10:30 —67. Molecular equivalence index searching. V. Shanmugasundaram, M. Hall, M. Chang, J. Raymond

11:00 —68. Validating topomer shape similarity as a predictor of biological similarity. R. Jilek, R. D. Cramer

11:30 —69. Cluster representation using reduced graphs. E. J. Gardiner, D. A. Cosgrove, P. Willett, V. J. Gillet

Unknown Site -- Unknown Room

General Oral - Drug Discovery

Exploiting Ligand Knowledge

E. X. Esposito and T. L. Johnson, Organizers
M. Torrent, Organizer, Presiding


9:50 — Intermission.

10:00 —72. Identification of novel bioisosteric replacements from molecular docking. P. Beroza, K. Damadoran, T. Macke, S. Putta

10:25 —73. Super fast conformer search algorithm based on recursive conformer build-up with local rotational symmetry consideration. J. Li, J. Sutter, S. Toba, C. M. Venkatachalam

10:50 — Intermission.

11:00 —74. Quantifying kinase-likeness. A. Filikov, M. A. Ashwell

11:25 —75. Probing the source of the exceptional role played by chlorine in the FXa S1 pocket. D. Sitkoff

Unknown Site -- Unknown Room

Section C

Section D

http://oasys.acs.org/acs/232nm/comp/staff/program.cgi?format=expa...
General Oral - Molecular Mechanics and Simulation

J. D. Madura, Organizer

8:30 — 76. VB/MM: A valence bond ride through classical landscapes. A. Shurki

8:55 — 77. Multi-state empirical valence bond MD simulation of hydroxyl ion transfer in liquid water. I. S. Ufimtsev, A. G. Kalinichev, T. J. Martinez, R. J. Kirkpatrick


10:10 — Intermission.

10:25 — 80. Peptide hydrolysis in thermolysin: Reactant structure and reaction mechanism studied with classical and QM/MM molecular dynamics. G. Lamoureux, J. Blumberger, M. L. Klein

10:50 — 81. QM/MM study of the 1H and 205Tl NMR spectra of the thallium bound G-quadruplex from Oxytricha nova. C. M. Ragain, J. A. Gascon, J. P. Loria, V. S. Batista

11:15 — 82. Simulation of long-range electron transfer in proteins using a combined QM/MM-classical molecular dynamics approach. J. Blumberger, M. L. Klein

11:40 — 83. Understanding enzymes, the Nature's catalysts, from QM (SCC-DFTB)/MM MD and free energy simulations. H. Guo, H. Guo, Q. Xu, N. Rao

Section E

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

J. D. Madura, Organizer

8:30 — 84. A novel linear/exponential hybrid force field scaling scheme. S. Yang, M. Kertesz

8:50 — 85. Ab initio modeling of the interaction of mercury with aromatic molecules. J. A. Steckel

9:10 — 86. Ab initio molecular dynamics studies of proton transport mechanisms in the superprotonic phase of CsH₂PO₄. H-S. Lee, M. E. Tuckerman


9:50 — 88. Inclusion of long-range exchange in TD-DFT: Towards a quantitative charge-transfer model. A. D. Dutoi, A. Drevu, M. Head-Gordon
10:10 — Intermission.

10:25 — 89. Quantum Monte Carlo study on the proton affinities of the 3D-block transition metals. A. A. Gibson, F. Fayton Jr., J. A. Harkless


11:25 — 92. Quantum Monte Carlo studies of ozone dissociation and excited states. J. A. Harkless

MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

DFTB, An Approximate DFT Method: Theory and Applications, Sponsored by Elsevier

Application to Biological Problems: Peptides, DNA and Weak Interactions

M. Elstner and T. Frauenheim, Organizers
J. Hermans, Presiding

2:00 — 93. Development and application of QM/MM methods based on the SCC-DFTB approach. Q. Cui

2:30 — 94. Simulations of biological systems with DFTB and the divide-and-conquer linear scaling method. W. Yang

3:00 — 95. Next-generation DFT-based quantum models for simulations of biocatalysis. D. M. York

3:30 — Intermission.

3:45 — 96. Stabilization energies of DNA base pairs and aminoacid pairs: WFT, DFT and DFTB calculations. P. Hobza

4:15 — 97. SCCDFTB as a bridge between MM and high-level QM. J. Hermans

4:45 — 98. An implementation of DFTB in amber9. A. E. Roitberg


Section B

Unknown Site -- Unknown Room
Molecular Similarity and Indexing Methods

A. N. Jain and A. Nicholls, *Organizers*

1:00 — 100. Implementing a text based method (Lingo) using Finite State Machines for fast similarity searching. J. A. Grant, J. Haigh, **R. Sayle**

1:30 — 101. What is a property-based similarity? **I. V. Tetko**

2:00 — 102. Methods to enhance the performance of similarity searching. **J. Hert**, D. J. Wilton, P. Willett

2:30 — 103. Quantitating similarity between molecular ensembles. **E. Metwally**, E. Abrahamian, R. D. Clark

3:00 — 104. Shape-based screening using multiple structures: Why might it work? **P. C. D. Hawkins**

3:30 — 105. Panel Discussion. A. N. Jain, **A. Nicholls**

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Emerging Technologies in Computational Chemistry, sponsored by Schrodinger, Inc

C. M. Breneman, *Organizer*

1:00 — Introductory Remarks.


1:50 — 107. Accelerating computations to order N for electrostatic interactions of biomolecular systems. **B. Lu**, X. Cheng, J. Huang, J. A. McCammon


3:10 — Intermission.


4:05 — 110. QM/MM geometry optimization. **T. Vreven**, M. J. Frisch

4:45 — 111. Applications of the charge patching approach to individually heterostructured semiconductor nanocrystals. **J. Schrier**, D. Demchenko, L -W. Wang

5:25 — Award Presentation.
Unknown Site -- Unknown Room

General Oral - Molecular Mechanics and Simulation

J. D. Madura, Organizer

1:30 — 112. Applying molecular dynamics to understand signal transduction: Recognition of TRPC6 by FKBP12. P. Tao, J. C. Hackett, C. M. Hadad


2:45 — Intermission.

3:00 — 115. Molecular dynamics simulations on AmtB of Escherichia coli: Mechanism of ammonia transport. Y. Mo, Y. Lin


Section E

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

J. D. Madura, Organizer

1:00 — 118. Raman spectroscopy: New challenges for theory. L. Jensen, G. C. Schatz


1:50 — 120. Methyl rotations in crystals: Quantum mechanical calculations, nuclear magnetic relaxometry and neutron diffraction crystallography. X. Wang, F. B. Mallory, P. Beckmann, M. M. Francl

2:15 — 121. Frozen-density embedding as an efficient method for modeling solvent effects on molecular properties. C. R. Jacob, J. Neugebauer, E. J. Baerends, L. Visscher

2:40 — 122. Quadratic String Method for determining the minimum energy path based on multiobjective optimization. S. K. Burger, W. Yang

3:05 — Intermission.
3:10 — 123. Benchmark study of noncovalent interactions in the zeolite model complexes and their use for validation of density functionals and force fields. **Y. Zhao, D. G. Truhlar**


4:00 — 125. Theoretical investigations of atmospheric species relevant for the search of high-energy density materials. **M. Rosi, G. de Petris, A. Troiani**


**MONDAY EVENING**

Section A

Unknown Site -- Unknown Room

Sci-Mix

W. D. Cornell, Organizer

8:00 - 10:00


**TUESDAY MORNING**

Section A

Unknown Site -- Unknown Room

DFTB, An Approximate DFT Method: Theory and Applications, Sponsored by Elsevier

Application to Biological Problems

M. Elstner and T. Frauenheim, Organizers

W. Yang, Presiding

9:00 — 127. Calculation of the reduction potential of Flavin Adenine dinucleotide in medium chain acyl-CoA dehydrogenase using combined DFTB/MM simulations. **S. Bhattacharyya, M. T. Stankovich, J. Gao**

10:00 — 129. Quantum-mechanical simulations of inclusion compounds: Cyclodextrine and polypeptides in aqueous solution. H. A. Duarte, S. Patchkovskii, H. F. Dos Santos, T. Heine

10:30 — Intermission.

10:45 — 130. Effective application of SCCDFTB in simulating structural and thermodynamic properties of molecular systems. H. Hu, W. Yang, J. Hermans


11:45 — 132. Proton transfer in bacteriorhodopsin studied with SCC-DFTB QM/MM. N. Bondar, M. Elstner, S. Fischer, S. Suhai, J. C. Smith

Section B

Unknown Site -- Unknown Room

Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory

New Semiempirical and Linear Scaling Methods

K. M. Merz Jr., Organizer

9:00 — 133. New semiempirical density functionals. D. G. Truhlar, Y. Zhao, N. E. Schultz, E. E. Dahlke, M. Iron

9:30 — 134. Possible modifications to the NDDO approximations. J. J. P. Stewart

10:00 — 135. Chemically accurate DFT via empirical localized orbital corrections. R. Friesner

10:30 — Intermission.

10:45 — 136. All electron calculations of FK506 binding protein complexes. K. Kitaura


11:45 — 138. Modulating transition metal reactivity in metalloenzymes. N. Richards

Section C

Unknown Site -- Unknown Room

ADME and Physical Property Prediction

Physical Properties - Methodology

D. R. McMasters and M. J. Walker, Organizers


10:00 — 141. Using relational databases for physical property prediction. T. O'Donnell

10:30 — Intermission.


11:45 — 144. Active algorithm training: A key to accurate physicochemical predictions applied to lead optimization. K. Kassam, E. Kolovanov, S. Bhal, G. Pearl

Section D

Unknown Site -- Unknown Room

Current Trends in Molecular Docking and Virtual Screening

D. L. Cheney and R. Farid, Organizers

9:00 — 145. MM-GBSA scoring in docking applications. M. P. Jacobson, N. Huang, C. Kalyanaraman, K. Bernacki

9:20 — 146. Use of the Glide extra precision methodology for docking and scoring. R. A. Friesner, R. B. Murphy, M. P. Repasky, B. W. Sherman

9:40 — 147. Computational assessment of nuclear hormone receptor selectivity. S. R. Krystek Jr., A. Nayeem, D. Schnur

10:00 — 148. Structural descriptors, similarity search, bioisosteric search, and virtual screening. G. Liang, I. Morize, A. Laoui


Section E

Unknown Site -- Unknown Room

Teaching Medicinal Chemistry to B.S. Undergraduate Chemistry Majors
Cosponsored with CHED
J. P. Bowen, Organizer

9:00 —151. Medicinal chemistry: Attracting students to an upper level chemistry course. A. G. Glenn

9:25 —152. Introduction to biomedical chemistry: A senior undergraduate course for chemistry, biochemistry and biology majors. R. S. Hosmane

9:50 —153. Medicinal chemistry for undergraduates at UNC-Greensboro: From organic structures and mechanisms to drug action. R. B. Banks

10:15 —154. Molecular modeling in the medicinal chemistry curriculum. W. J. Hehre


11:05 —156. More than organic: An experiment in medicinal chemistry. T. A. Newton

11:30 —157. Undergraduate medicinal chemistry at Vanderbilt University. T. P. Lybrand

TUESDAY AFTERNOON

Section A
Unknown Site -- Unknown Room

DFTB, An Approximate DFT Method: Theory and Applications, Sponsored by Elsevier

Solids and Clusters

T. Frauenheim, Organizer
W. Thiel, Presiding

2:00 —158. Simulation of processes on the nanometer scale using the DFTB method. T. Heine

2:30 —159. DFTB-based QM/MD simulations of nanostructure formation processes far from thermodynamic equilibrium. S. Irle, Z. Wang, G. Zheng, K. Morokuma


3:30 — Intermission.

3:45 —161. CMx charges for SCC-DFTB and some GaN vignettes. C. J. Cramer

4:15 —162. Wafers, platelets, rods and spheres: Using DFTB to determine the structural minima of atomic clusters. K. A. Jackson

4:45 —163. Application of SCC-tight-binding to reactive systems at extreme conditions. M. R. Manaa, E. Reed, K. Glaesemann, L. Fried

5:15 —164. Equilibrium chemical order and segregation at alloy surfaces and nanoclusters computed
using tight-binding derived coordination-dependent bond energies. **M. Polak, L. Rubinovich**

Section B

**Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory**

**Applications of Semiempirical Methods: Solvation, Spectroscopy and QSAR**

K. M. Merz Jr., *Organizer*

1:30 — 165. Continuum solvation models in the 21st century. **C. J. Cramer**

2:00 — 166. Solvation energies of amides and peptides obtained from hybrid DFT/ONIOM/AM1 calculations and the Cramer/Truhlar (SMx) solvation methods. **J. J. Dannenberg**, P. Salvador, A. Asensio, R. Wieczorek


3:00 — Intermission.


Section C

**ADME and Physical Property Prediction**

**General**

D. R. McMasters and M. J. Walker, *Organizers*

1:30 — Introductory Remarks.


3:05 — Intermission.


3:50 — 175. Metabolism and toxicity modeling: Models and examples. **M. J. de Groot**

4:20 — Panel Discussion.

Section D

Unknown Site -- Unknown Room

**Current Trends in Molecular Docking and Virtual Screening**

D. L. Cheney and R. Farid, *Organizers*

1:00 — 176. Inhibitor based refinement of homology modeled protein structures for molecular docking. **I. Antes**, T. Lengauer


1:40 — 178. Recent developments in the FlexX family. **H. Claußen**


Section E

Unknown Site -- Unknown Room

**Teaching Medicinal Chemistry to B.S. Undergraduate Chemistry Majors**

*Cosponsored with CHED*

J. P. Bowen, *Organizer*

1:30 — 182. Perspectives in developing and teaching courses in medicinal chemistry. **J. P. Bowen**

1:50 — 183. SMC Pharmaceuticals: A quadraginta duoque month report. **J. P. Bays**

2:10 — 184. Synergy in the chemistry curriculum: Outcomes and benefits from the teaching of
medicinal chemistry. **E. Gooch**

2:30 — **185.** Teaching a biochemistry based medicinal chemistry course. **G. A. Olsen**

2:50 — **186.** Teaching drug design at the University of Minnesota. **C. R. Wagner**

3:10 — **187.** Teaching medicinal chemistry at a small liberal arts college. **N. S. Green**

3:30 — **188.** Chem 316: The organic chemistry of drug design and drug action. **R. B. Silverman**

**Cyber Science, Chemistry**

**Interfacing Multiple Computational Approaches and Cyber Education**

*Sponsored by PHYS, Cosponsored with COMP*

**TUESDAY EVENING**

Unknown Site -- Unknown Room

**Poster Session**

W. D. Cornell, *Organizer*

6:00 - 8:00

189. Genetic algorithms for developing odor-structure relationships. **B. K. Lavine**, N. Mirjankar


192. A protocol to evaluate the potency of HIV-1 protease drugs to combat resistance. **T. Hou**

193. A QSPR study on melting points of high-energy molecules. **M. K. Park**, S. G. Cho, Y. S. Kim

194. A QSPR study on sublimation energies of high-energy molecules. **S. G. Cho**, J. R. Cho

195. Ab initio modeling of the A(2A) adenosine receptor and prediction of its ligand binding sites. **M. W. Liu**, J. H. Lin

196. Ab initio QM/MM studies of histone lysine methyltransferase. **P. Hu**, S. Wang, Y. Zhang

197. Accounting for loop rearrangements in docking calculations. **S. E. Wong**, M. P. Jacobson

198. Hydrolysis of B-lactam via ab initio and QM/MM simulations. **A. N. Alexandrova**, W. L.
Jorgensen


200. An efficient parallel coupled cluster program for distributed memory computers. T. Janowski, P. Pulay

201. An efficient search protocol for mapping potential energy landscapes and conformations of an amphiphilic octadecapeptide. R. A. Wheeler, Z. Huang, Z. Guo

202. An investigation of the structures, vibrational spectra, and relative energetics of CH$_3$COBrO$_3$ isomers. S. Guha, J. S. Francisco


207. Binding affinity and mechanism of HEPT analogs with HIV-1 reverse transcriptase using the Linear Interaction Energy Approximation. A. Tavlarakis, R. Zhou

208. Binding affinity prediction of metalloprotein ligands: QM/MM Linear Response approach. A. Khandelwal, S. Balaz


213. Comparison of charge models for fixed-charge forcefields: Small molecule hydration free energies in explicit solvent. É. Dumont, D. L. Mobley, J. D. Chodera, K. A. Dill

214. Computational investigation of pressure profiles in lipid bilayers with embedded proteins. J. Gullingsrud, A. Babakhani, J. A. McCammon

215. Computational modeling of methane hydrates at NETL. C. E. Taylor


218. Configurational-bias sampling technique for predicting side-chain conformations in proteins. **T. S. Jain**, D. Cerutti, J. A. McCammon


220. Conformational search of Antifreeze protein type I. **P. Dalal**


222. Density functional calculations on 3-hydroxykynurenine. **B. C. Dutmer**, T. M. Gilbert


225. Design, development and evaluation of novel protein property-encoded surface translator (PPEST) descriptors for protein similarity comparison. Q. Luo, **C. M. Sundling**, C. M. Breneman

226. Developing "class-optimized" scoring functions for drug design. Z. W. Zhang, **J. H. Lin**


228. DFT calculations on titanium dioxide and titinate clusters. **J. L. Martin**, P. Pulay

229. DFT Study for rational design of internal donor: Correlation between structure of internal donor and its stereoregulating ability in heterogeneous Ziegler-Natta catalyst. **J. W. Lee**, W. H. Jo, J. Huh


232. Evaluation of descriptors used to mine a drug metabolism database. **J. H. Block**, D. Henry

233. Exploring structure, dynamics and assembly of the 30S ribosomal subunit by coarse-grained molecular dynamics simulations. **Q. Cui**, D. A. Case


236. Free energy vs. potential energy landscapes of drug-like molecules. Y. Abraham, A. George, R. Harris, P. S. Hammond, **J. D. Schmitt**

237. Grid methods for free energy calculations and ligand scoring. **V. Hornak**, R. Geney, R. C. Rizzo,
C. L. Simmerling


239. Highly selective prediction of catalytic sites in proteins using electrostatics and sequence conservation. **H. Yang**, M. J. Ondrechen

240. In silico ADME: ”Predicting lipophilicity vs. pH”. L. Quéré, E. Hanon, R. Taylor, G. Longfils, I. Ortmans, **F. Lebon**


243. Integer sequences related to chemistry. N. J. A. Sloane, **P. Nambi**


245. Investigating bias in docking screens with target, ligand and decoy benchmarking sets. **N. Huang**, J. J. Irwin, B. Shöichet

246. KNOBLE: KNOwledge-Based Ligand Enumeration. C. Gerlach, C. Sohn, T. Craan, **W. E. Diederich**, G. Klebe


248. MD simulation study of ABAD/ligand complexes. **X. Ge**

249. Mechanism of gating in a ClC channel at atomistic level. **Y. J. Ko**, J. Huh, W. H. Jo


251. Mechanistic and kinetic study of naphthalene formation. **N. Kungwan**, T. N. Truong


253. Membrane assembly of simple helix homo-oligomers studied via molecular dynamics simulations. **L. Bu**, W. Im, C. L. Brooks III


257. Molecular modeling and simulation: A better understanding of the porphyrin stacks. Z. H. Tang, B. A. Yang

258. Molecular modeling of a readily available polymer having biological activity against HIV-1. N. Nidhi, D. B. Boyd


262. Neural network based QSAR models of Tipranavir analogs: HIV protease inhibitors. C. R. Bernier, B. Bhattacharai, S. Kumar, R. Garg

263. Neural network-based Particle Swarm Optimization (PSO): A novel approach for optimizing experimental conditions. Z. Liu, W. Qi, Z. He


265. New termination mechanism for olefin polymerization catalyzed by n-alkyl (R) substituted 3-R indenyl zirconocenes as determined by DFT calculations. V. L. Cruz, S. Martinez, J. Martinez-Salazar, J. Sancho

266. Nonpolar implicit solvation: An analysis of the cavity-dispersion decomposition scheme. C. Tan, R. Luo


268. On the application of accelerated molecular dynamics to liquid water simulations. C. A. F. de Oliveira, D. Hamelberg, J. A. McCammon


270. Predicting cardiovascular safety: The importance of using the appropriate high quality datasets. W. Sanderson, L. Fenu, T. Thielemans, C. Buyck, M. Engels, A. Teisman, T. Howe

271. Prediction of conformational polymorphism for molecular crystal. S. Obata, N. Nakayama, H. Goto

272. Protein long loop structure prediction: Advances in sampling method and implicit solvent model. K. Zhu, D. L. Pincus, S. Zhao, R. A. Friesner

273. Pushing the boundaries of molecular docking with decoys and model systems. A. P. Graves, B. K. Shoichet

274. Q-Chem 3.0: More chemistry, faster. J. Kong

275. QM(SCC-DFTB)/MM molecular dynamics and free energy simulations of histone
methyltransferases. H. Guo, H. Guo


277. QSAR studies of anti-HIV-1 Ritonavir analogs. R. C. Kasara, B. Bhattarai, R. Garg

278. Quantum mechanical investigation of stacked DNA bases. I. R. Gould

279. Quasiclassical trajectory study of the vibrational quenching of hydroxyl radicals through collision with O atoms. R. Viswanathan, M. Dolgos, R. J. Hinde

280. Rationalizing the observed trends in ring opening polymerizations of several lactones using 1,5,7–Triazabicyclo[4.4.0]dec–5–ene (TBD) as catalyst: Towards establishing a reaction mechanism. A. M. Chuma

281. Recognition and dynamic gating in DNA intercalation. S-H. Yeh, J-H. Lin


283. RI-CIS(D): Efficient perturbative correction on CIS. Y. M. Rhee, M. Head-Gordon

284. RNA Loop prediction. L. Dominguez, M. P. Jacobson


287. Structure development of compressible block copolymer systems. J. Cho


290. The CHECKIN program: Design and implementation of an automated process for submitting open-access NMR data for compound validation and registration. J. F. Mattes, A. C. Bach, W. Massefski

291. Theoretical investigation of the low energy structures of Si$_x$L$_y$ clusters. J. D. Head, Y. Ge


293. Theoretical study to investigate HHR3/HHR4 selectivity: Receptor modeling and molecular docking of histamine ligand. J. Xiao

294. Thermal unfolding of polyalanine in water by molecular dynamics simulations and theoretical prediction of infrared spectra: Helix-coil transition kinetics. S. Yang, M. Cho

295. Time-domain ab initio simulation of electron and hole relaxation dynamics in a single-wall semiconductor carbon nanotube. B. F. Habenicht, C. F. Craig, O. V. Prezhdo

297. Valence selectivity of the gramicidin A channel. J. W. Park, Y. J. Ko, W. H. Jo

298. Variational transition state theory with multidimensional tunneling with Block Hessians. Y.-Y. Chuang


300. Calculating the conductivity of single molecules: Going beyond coherent transport. A. Gagliardi, T. Frauenheim, A. Pecchia, A. Di Carlo

301. Docking of novel reversible monoamine oxidase-B inhibitors: Efficient prediction of ligand binding sites and estimation of inhibitors thermodynamic properties. K. Yelekci, M. Toprakci

302. DFTB/MM studies on wetting behavior and adsorption reactions on technical surfaces. J. M. Knaup, C. Köhler, T. Frauenheim, M. Amkreutz, P. Schiffels, O.-D. Hennemann

303. Modeling long-range proton transfer: New methods and application to the Bacterial Reaction Center. P. H. König, M. Hoffmann, Q. Cui, T. Frauenheim

304. Rare Earth defects in GaN. S. Sanna, B. Hourahine, U. Gerstmann, T. Frauenheim


WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

DFTB, An Approximate DFT Method: Theory and Applications, Sponsored by Elsevier

Excited States and Optical Properties; Single Molecule Conduction

M. Elstner and J. M. McKelvey, Organizers
J. J. P. Stewart, Presiding

9:00 — 306. Computing optical properties of conformationally flexible molecules. F. Furche


10:30 — Intermission.
10:45 — 309. A comparison of ground and excited state properties using SCC-DFTB and semiempirical methods. J. M. McKelvey, S. Tretiak

11:15 — 310. The gDFTB method applied to transport in Si nanowires and carbon nanotubes. A. Pecchia, L. Latessa, T. Frauenheim, A. Di Carlo


Section B

Unknown Site -- Unknown Room

Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory

Biological Applications

K. M. Merz Jr., Organizer

9:00 — 312. “Amusing” tales of modeling in drug discovery. C. H. Reynolds, B. A. Tounge, J. Li

9:30 — 313. AM1* and beyond: Aspects of modern semiempirical methods. T. Clark

10:00 — 314. QM/MM calculations of proton transfer reactions and excited states properties in biological systems using semi-empirical methods. M. Elstner

10:30 — Intermission.


Section C

Unknown Site -- Unknown Room

ADME and Physical Property Prediction

Physical Properties - Applications

D. R. McMasters and M. J. Walker, Organizers

9:00 — 318. Estimation of the total entropy of fusion from molecular structure using SPARC. T. S.
Whiteside, L. A. Carreira


10:00 — 320. Solvation of drug-protein complexes. T. R. Stouch, M. E. Davis

10:30 — Intermission.

10:45 — 321. Computational models for the prediction of aqueous solubility that include crystal packing, solvation, and ionization. S. R. Johnson, X-Q. Chen, D. Murphy, O. Gudmundsson

11:15 — 322. Interfacial logP in structural fragment-based QSAR models. J. F. Rathman, C. Yang

Section D

Unknown Site -- Unknown Room

Current Trends in Molecular Docking and Virtual Screening

D. L. Cheney and R. Farid, Organizers


10:00 — 326. PROLICSS: Analysis and applications. C. M. Sundling, M. D. Ryan, C. M. Breneman

10:20 — 327. Use of metal coordination geometry to improve FlexX docking. A. Kämper, S. Pfeifer, T. Lengauer


Section E

Unknown Site -- Unknown Room

General Oral - Molecular Mechanics and Simulation

J. D. Madura, Organizer


9:20 — 331. DNA-Binding of ruthenium-arene anticancer drugs. C. Gossens, I. Tavernelli, U. Rothlisberger


10:10 — Intermission.


Chemical Information and Organic Chemistry: The Road Ahead

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Computational Chemistry Investigations for Undergraduates

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Cyber Science, Chemistry

Data Bases and Remote Instrumentation

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WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room
DFTB, An Approximate DFT Method: Theory and Applications, Sponsored by Elsevier

Methods: Spin, LDA+U, and Relativistic Implementation;

T. Frauenheim and M. Elstner, Organizers
P. Hobza, Presiding

2:00 — 337. Spinpolarization in the SCC-DFTB formalism. C. Köhler, G. Seifert, T. Frauenheim

2:30 — 338. DFTB and modern DFT. B. Hourahine, B. Aradi, S. Sanna, T. A. Niehaus, T. Frauenheim

3:00 — 339. Relativistic parameterization of the SCC-DFTB method. H. A. Witek

3:30 — Intermission.

3:45 — 340. SIPs: Tailored parallelization of the generalized symmetric eigenproblem. M. Sternberg, H. Zhang, B. Smith, P. Zapol

4:15 — 341. Sparse matrix based implementation of the DFTB method. B. Aradi, B. Hourahine, C. Köhler, T. Frauenheim


Section B

Unknown Site -- Unknown Room

Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory

Semiempirical Applications and Parmeterization

K. M. Merz Jr., Organizer

1:30 — 343. Double and higher-twist Mobius-Listing aromaticity. H. S. Rzepa

2:00 — 344. Computational study of carbon atom reaction with formaldehyde: Theoretical evaluation of $^1B_1$ methylene production. M. L. McKee


3:00 — Intermission.

3:15 — 346. Semiempirical quantum chemical models of the excited states of conjugated polymers. D. Yaron

http://oasys.acs.org/acs/232nm/comp/staff/program.cgi?format=expa...
3:45 — 347. Adapted ab initio theory. **J. McClellan**, R. J. Bartlett

4:15 — 348. NO-MNDO: Reintroduction of the overlap matrix into MNDO. **K. W. Sattelmeyer**, I. Tubert-Brohman, W. L. Jorgensen

Section C

Unknown Site -- Unknown Room

ADME and Physical Property Prediction

Metabolism

D. R. McMasters and M. J. Walker, *Organizers*

1:30 — 349. Computational approaches that predict metabolic intermediate complex formation with CYP3A4. **S. Ekins**, D. R. Jones, L. Li, S. D. Hall


2:30 — 351. Automated regional assignment of metabolic modification using cross correlation algorithms, maximum common substructure analysis, and MS/MS spectral libraries. **S. R. Johnson**, J. L. Josephs, B. Claus, R. A. Langish

3:00 — Intermission.

3:15 — 352. Fuzzy pharmacophore triplets: New descriptors for the construction of QSAR models and application to Cyp2D6 inhibition. **F. Barbosa**


4:15 — 354. Parallel pharmacophoric profiling as lead optimization tool for the prediction of interactions via the cytochrome P450 enzyme family. **D. Schuster**, T. Langer

Section D

Unknown Site -- Unknown Room

Current Trends in Molecular Docking and Virtual Screening

D. L. Cheney and R. Farid, *Organizers*

1:00 — 355. Combining docking and pharmacophore filtering methods for improved virtual screening. **M. L. Peach**, M. C. Nicklaus

1:20 — 356. “Surrogate docking” with AUTOSHIM ensembles: Using PLS/MAGNET to customize scoring functions for an ensemble of diverse kinases to predict the activity of new kinases, even without
crystal structures or homology models. **E. Martin, D. Sullivan**

**1:40 — 357.** Using multiobjective optimization to study the strengths of different interaction energies in protein-ligand complexes. **S. Mardikian, V. J. Gillet, R. M. Jackson, D. R. Westhead**

**2:00 — 358.** Docking high energy intermediates/transition states to enzymes. **J. C. Hermann, J. J. Irwin, B. K. Shoichet**

**2:20 — 359.** Using pharmacophoric and pharmacosteric multiplets to characterize binding sites. **R. D. Clark, E. Abrahamian**

Section E

Unknown Site -- Unknown Room

**General Oral - Molecular Mechanics and Simulation**

J. D. Madura, **Organizer**

**1:30 — 360.** Free energy calculations of a bacterial CLC chloride channel homologue. **U. Mahankali, Z. Kuang, G. Feng, T. L. Beck**

**1:55 — 361.** Homology modeling and molecular dynamics simulations of BRCA1 BRCT domain bound to p53. **J. Liu, R. Nussinov**

**2:20 — 362.** Monte Carlo simulations of model proteins: Free energy computations for (a) confined systems and (b) synthetic peptides. **N. Rathore, T. A. Knotts IV, J. J. de Pablo**

**2:45 — 363.** Novel computational method for predicting minimum RNA binding sequences. **P. C. Anderson, S. Mecozzi**

**3:10 —** Intermission.

**3:25 — 364.** Protein binding mechanism: Fast induced-fit conformational transitions of neurotoxin Fasciculin-2 in complex with acetylcholinesterase. **J. M. Bui, J. A. McCammon**

**3:50 — 365.** Protein folding kinetics and thermodynamics from atomistic simulation. **D. van der Spoel, M. M. Seibert**

**4:15 — 366.** Role of histone tails and linker histone in chromatin folding as revealed by computer simulations. **G. Arya, T. Schlick**

**4:40 — 367.** Winding and unwinding helices: A precursor to folding through residue selection. **T. Chun, J. Ren, C. M. McCallum**

**Computational Chemistry Investigations for Undergraduates**

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Cyber Science, Chemistry

Cyber Science - Materials

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THURSDAY MORNING

Unknown Site -- Unknown Room

Free Energy Computations in Drug Discovery

M. Clark and F. P. Hollinger, Organizers

9:00 — Introductory Remarks.

9:20 — 368. Potential of mean force approach for calculating absolute binding affinities of protein-ligand complexes. M. S. Lee, M. Olson

9:40 — 369. The calculation of free energies of solvation as functions of temperature. A. Chamberlin

10:00 — 370. Evaluation of rigorous and approximate free energy methods in lead optimization. M. P. Repasky, B. W. Sherman


10:40 — Intermission.

11:00 — 372. A multistep approach to structure based drug design: Studying ligand binding at the human neutrophil elastase. T. Steinbrecher, D. A. Case, A. Labahn

11:20 — 373. On avoiding sampling and convergence problems in alchemical binding free energy calculations. D. L. Mobley, J. D. Chodera, K. A. Dill

11:40 — 374. Grand canonical and systematic sampling for free energy computations. M. Clark, S. Meshkat, G. Talbot

12:00 — 375. Extension of the coupled reference interaction site model (RISM)/simulation methodology to the determination of relative solvation free energies of biological complexes. H. Freedman, L. Le, L. Huynh, D. Tikhonov, T. N. Truong

12:20 — Concluding Remarks.

Unknown Site -- Unknown Room
ADME and Physical Property Prediction

General

D. R. McMasters and M. J. Walker, Organizers

9:00 — 376. Efficient prediction of ADME properties and drug similarity based on the COSMO-RS model. M. Diedenhofen, A. Klamt, K. Wichmann

9:30 — 377. Internal hydrogen bonding and passive membrane permeability: Successful in silico prediction of the relative permeabilities of cyclic peptides. T. Rezai, R. S. Lokey, M. P. Jacobson


10:30 — Intermission.


11:15 — 380. Improved naive Bayesian modeling of numerical data for ADME property prediction. A. E. Klon, J. Lowrie, D. J. Diller

11:45 — 381. Survey of the in silico ADME/Tox landscape. O. O. Clement, M. D'Souza, G. M. Banik

12:15 — Concluding Remarks.

Section C

Unknown Site -- Unknown Room

General Oral - Drug Discovery

Protein Structure/Binding Site Prediction

T. L. Johnson and M. Torrent, Organizers
E. X. Esposito, Organizer, Presiding


9:20 — 384. High-recall, high-precision prediction of protein binding sites from 3D structure. Y. Wei, L. F. Murga, M. J. Ondrechen

9:45 — Intermission.
10:00 — 385. Macromolecular crowding destabilizes ordered oligomers of an amyloidogenic peptide. E. P. O'Brien Jr., B. R. Brooks, D. Thirumalai

10:25 — 386. Structure prediction and ligand binding in serotonin 2b and 2c receptors. J. Bray, N. Vaidehi, W. A. Goddard III

10:50 — Intermission.

11:05 — 387. Protein family-based homology modeling and its application to lead optimization. S -B. Rong, J. H. van Drie

11:30 — 388. Analysis of ligand structures in the Protein Data Bank. M. Stahl

Section D

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

J. D. Madura, Organizer

8:30 — 389. DFT Studies on electron attachment to DNA/RNA subunits. D. J. Zhang, H. F. Schaefer III


9:10 — 391. Key stereoelectronic forces along the reaction coordinate that regulate rate and selectivity enhancements of Lewis acid catalyzed Diels-Alder reactions. J. D. Evanseck, J. A. Plumley


9:50 — Intermission.

10:05 — 393. Competition between protein ligands and cytoplasmic inorganic anions for the metal cation. C. Lim, T. Dudev


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Cyber Science - Biological and Environmental

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THURSDAY AFTERNOON

Unknown Site -- Unknown Room

Free Energy Computations in Drug Discovery

M. Clark and F. P. Hollinger, Organizers

1:00 — Introductory Remarks.


2:00 — 399. Use of free energy methods and structure-based drug design in the discovery of a potential new class of drugs for diabetes. M. R. Reddy, M. D. Erion, Q. Dang, P. D. van Poelje, W. N. Lipscomb

2:30 — 400. Water binding free energy: A critical component of successful structure based drug design. F. P. Hollinger, T. T. Fujimoto

3:00 — 401. Quorum-quenching proteins as therapeutic targets: Binding and reaction mechanism. K. Spiegel, M. De Vivo, M. Dal Peraro, M. L. Klein

3:30 — Intermission.

4:00 — 402. Free energy surfaces for binding of COX-2 inhibitors: A combined computational study of Shape Signatures, docking and metadynamics. Z. Liu, M. Kumar, P. B. Moore, R. J. Zauhar

4:30 — 403. Binding free energy calculations in the polar and nonpolar T4 lysozyme mutants. Y. Deng, B. Roux

5:00 — 404. What is the statistical-thermodynamic cost of binding entropy in protein-ligand docking and virtual screening? A. M. Ruvinsky

5:30 — Concluding Remarks.

Section A

Section B

Unknown Site -- Unknown Room

General Oral - Drug Discovery

Structure-based Approaches
E. X. Esposito and M. Torrent, Organizers
T. L. Johnson, Organizer, Presiding


1:10 — 406. Looking for isozyme specificity of histone deacetylase class I isozymes. **E. X. Esposito**, G. R. Cook


2:00 — Intermission.


3:00 — Intermission.


Section C

Unknown Site -- Unknown Room

**General Oral - Molecular Mechanics and Simulation**

J. D. Madura, Organizer

1:00 — 412. Efficient and precise solvation free energies via adiabatic dynamics. **J. B. Abrams**, L. Rosso, M. E. Tuckerman


2:40 — Intermission.


Section D

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

J. D. Madura, Organizer

1:00 — 420. A justification for the nonadiabatic surface hopping Herman-Kluk semiclassical initial value representation method. Y. Wu, M. F. Herman

1:20 — 421. DFT and TDDFT studies of the conformational dependence of the optical properties of perylene aggregates. A. Clark

1:40 — 422. Local fitting of integrals for efficient electronic structure calculations. A. J. Sodt, M. Head-Gordon


2:20 — Intermission.

2:35 — 424. Oxidative addition of methane, silane and heavier AH4 congeners to palladium. J. N. van Stralen, F. M. Bickelhaupt


Cyber Science, Chemistry

Cyber Science – Electronic Structure

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