MOLECULAR MODELING & COMPUTATIONAL CHEMISTRY

Editorial and News

In the first half of this volume of the newsletter, we have been trying an experiment with journal reviews. Because of a new offering, the *Journal of Chemical Theory and Computation*, and an increasing number of computatational articles in *JACS and JPhysChemB,* we wrote comprehensive journal reviews covering most of the QM literature, while retaining our usual reviews of macromolecular MD literature in the body of the newsletter.

Without going into the details, I will just say that the new journal is mostly QM, and I have decided to maintain our standard selection criteria, which do not include that literature.

The real topic of this newsletter will remain as it has always been, *macromolecular modeling*, with somewhat of an emphasis on biomolecular modeling. Thus we tend to include large-scale QM work on biomacromolecules or when it is part of QM/MM, but otherwise, we expect you to look elsewhere for information on advances in QM. We also exlude articles that are mainly experimental with computational support, articles about LJ systems, DFT or MC studies in chemical physics, or QSAR studies that do not have a substantial computational chemistry or biomolecular component. On the other hand, we include combined-atom approaches when applied to biomolecular modeling, and we try to be comprehensive in our coverage of atomistic empirical force field simulations.

In the past, we have always included *J. Comput. Chem.* in the Journal Reviews section, but it has become so QM oriented, that I have also decided to treat it like other journals from now on.

Although I suspect many of our readers would appreciate a QM newsletter, this is beyond our ken and would require as much again effort and space as the macromolecular modeling requires. Therefore, we will return, after this issue, to a more moderately sized *Journal Reviews* section.

David D. Busath, Editor

1. <u>APPLICATIONS</u>

1.1.   *Small Molecules*

Water and Solvation

A molecular-dynamics study of a model SN1 dissociation reaction at the water liquid/vapor interface.

N. Winter and I. Benjamin* [U Calif Santa Cruz]

J. Chem. Phys. **122,** 18471701-18471710 (2005)

The removal of Cl- from tert-butylchloride, leaving behind a butyl+, has a transmission coefficient of 0.49 in bulk and 0.05 above the Gibbs surface at the liquid-vapor interface. The 10x reduction "despite the lower friction is shown to be due to slow vibrational relaxation."

Organic Solvents

Rheological and structural studies of liquid decane, hexadecane, and tetracosane under planar elongational flow using nonequilibrium molecular-dynamics simulations.

C. Baig, B.J. Edwards* [U Tennessee], D.J. Keffer, and H.D. Cochran

J. Chem. Phys. **122,** 184906101-184906111 (2005)

MD simulations explore the structural behaviors of the four title alkanes, identifying two types of elongation viscosity that converge in Newtonian flow. Nematic (aligned elongated) structure is observed at high elongation rates.

Medicinal Chemistry and Drug Design

Comparative molecular dynamics simulations of HIV-1 integrase and the T66I/M154I mutant: binding modes and drug resistance to a diketo acid inhibitor.

A. Brigo, K.W. Lee, F. Fogolari, G.I. Mustata, and J.M. Briggs* [U Houston]

Proteins **59,** 723-741 (2005)

Detailed analysis of MD simulations and MM/PBSA calculations on HIV integrase and one of its double mutants in complex with several inhibitors reveals new insights in modes of binding and possible mechanisms of inhibition.

Medicinal Chemistry and Drug Design (cont'd)

Protonation-induced stereoisomerism in nicotine: Conformational studies using classical (AMBER) and ab initio (Car–Parrinello) molecular dynamics.

P.S. Hammond* [Targacept], Y. Wu, R. Harris,
T.J. Minehardt, R. Car, and J.D. Schmitt

J. Comput.-Aid. Molec. Design **19**, 1-15 (2004)

A detailed comparison between MM and QM MD simulations of *trans* and *cis* protonated nicotine is presented. Striking similarities as well as differences are reported.

Antimycobacterial activity of new 3-substituted 5-(pyridin-4-yl)-3*H*-1,3,4-oxadiazol-2-one and 2-thione derivatives: Preliminary molecular modeling investigations.

M.G. Mamolo* [U Trieste], D. Zampieri, L. Vio,
M. Fermeglia, M. Ferrone, S. Pric, G. Scialino, and E. Banfi

Bioorg. Med. Chem. **13**, 3797-3809 (2005)

Oxadiazolone derivatives showed antimycobacterial activity against the tested strain of Mycobacterium tuberculosis H37Rv. Molecular modeling investigations showed that the active compounds interact at the active site of the mycobacterial cytochrome P450-dependent sterol 14α-demethylase in the sterol biosynthesis pathway. The binding free energy values of these compounds are in good agreement with their MIC values.

Quantitative Structure-Activity Relations

Predictive three-dimensional quantitative structure-activity relationship of cytochrome P450 1A2 inhibitors.

L.E. Korhonen* [U Kuopio], M. Rahnasto, N.J. Mähönen,
C. Wittekindt, A. Poso, R.O. Juvonen, and H. Raunio

J. Med. Chem. **48**, 3808-3815 (2005)

Fifty-two compounds assayed to inhibit CYP1A2 at between 2.3uM and 40mM were used to derive CoMFA and GRID/GOLPE models of CYP1A2.

T

AFMoC enhances predictivity of 3D QSAR: A case study with DOXP-reductoisomerase.

K. Silber, P. Heidler, T. Kurz, and G. Klebe* [Philipps U]

J. Med. Chem. **48**, 3547 –3563 (2005)

The new AFMoC (adaptation of fields for molecular comparison) allows inclusion of protein binding site 3D structure into 3D QSAR modeling.

T

Proteins Markovian 3D-QSAR with spherically-truncated average electrostatic potentials.

L. Saíz-Urra, H. González-Díaz*
[U Santiago de Compostela], and E. Uriarte

Bioorg. Med. Chem. **13,** 3641-3647 (2005)

The Markov chain model approach was used to evaluate the electrostatic potentials from spatial distribution of charges within the protein backbone. The average electrostatic potentials are used to predict protein properties. The effects of abrupt, shifting, force shifting, and switching truncation functions on 3D-QSAR models in classifying 26 proteins were studied. MC results were fairly robust for different truncation schemes and r_{off} values.

Quantitative Structure-Activity Relationships (cont'd)

The role of hydrophobic properties of chemicals in promoting allosteric reactions.

M.B. Suresh, A. Kurup, R.P. Verma, and
C. Hansch* [Pomona College]

Bioorg. Med. Chem. **13**, 3737-3762 (2005)

The role of hydrophobic properties of chemicals in promoting allosteric reactions was explored via log *P* with 50 QSAR equations. The best QSAR model was found to be $\log(1/C) = -a \cdot \log(P) + b \cdot \log(P^2) + \text{constant}$.

1.2.   *Biopolymers*

Bioinformatics

Incorporating hidden Markov models for identifying protein kinase-specific phosphorylation sites.

H.-D. Huang* [Natl Chiao Tung U], T.-Y. Lee, S.-W. Tzeng, L.-C. Wu, J.-T. Horng* [Natl Central U], A.-P. Tsou, and K.-T. Huang

J. Comput. Chem. **26,** 1032-1041 (2005)

Based on currently known phosphorylation sites and their kinases, a Web-based tool was constructed to identify unknown sites and the kinases that would phosphorylate them.

Application of InChI to curate, index, and query 3-D structures.

M.D. Prasanna, J. Vondrasek, A. Wlodawer, and
T.N. Bhat* [NIST]

Proteins **60***,* 1-4 (2005)

The indexation of the HIV structural database using the UIPAC International Chemical Identifier and an example query are described.

Universal biases in protein composition of model prokaryotes.

G. Pascal* [Genoscope], C. Médigue, and
A. Danchin* [Pasteur]

Proteins **60***,* 27-35 (2005)

Correspondence analysis of three microbial genomes (*E. coli*, *B. subtilis* and *M. jannaschii*) and shows hydropathy is linked to membrane integration and orphan proteins are relatively high in aromatic content.

Protein Sequence Analysis and Alignment

Structure alignment via Delaunay tetrahedralization.

J. Roach* [U N Carol], S. Sharma, M. Kapustina, and
J. Charles W. Carter

Proteins **60***,* 66-81 (2005)

Tessellation-based geometric descriptor strings form the basis for a new structural alignment method that largely eliminates the need for rigid-body transformations and fitting. Application to aminoacyl-tRNA synthases, separate known structural classes, sub-classes, and free and bound structures. Possibilities for general structure analysis, *e.g.* simulations, are discussed.

Protein Sequence Analysis and Alignment (cont'd)

Molecular dynamics simulations of evolved collective motions of atoms in the myosin motor domain upon perturbation of the ATPase pocket.

T. Kawakubo* [Toin U Yokohama], O. Okada, and T. Minami

J. Biophys. Chem. **115,** 77-85 (2005)

Does an ATP hydrolysis cause atomic vibration from the nucleotide-binding site to be transmitted throughout the myosin head? MD simulations indicate that the disturbance signal extends over the motor domain in 150 ps and induces slowly varying collective motions of atoms at the actin-binding site.

Threading and Fold Recognition

Recognizing protein folds by cluster distance geometry.

G.M. Crippen* [U Michigan]

Proteins **60***,* 82-89 (2005)

Using distance geometries from residue clusters, contact potentials are derived on a 211 protein test-set selected from 262 structures, and used for threading. For 698 PDB structures, the native fold was correctly identified.

Protein Structure Prediction

High accuracy prediction of beta-turns and their types using propensities and multiple alignments.

P.F. Fuchs* [U Paris] and A.J. Alix

Proteins **59***,* 828-839 (2005)

A novel method for b-turn prediction based on residue conservations in multiple alignments and weighted PSI-BLAST predictions is described. An MCC of 0.42 and accuracy of 75% are comparable to neural net-based methods, but at much lower computational cost.

Crystal packing effects on protein loops.

C.S. Rapp* [Yeshiva U] and R.M. Pollack

Proteins **60***,* 103-109 (2005)

A loop prediction method that explicitly includes crystal-packing effects is tested on sets of alternate symmetries. From simulations of loops with and without packing, predictions are made if a loop with packing contacts is in its most stable conformation.

A structural alphabet for local protein structures: Improved prediction methods.

C. Etchebest, C. Benros, S. Hazout, and A.G. de Brevern* [U Paris]

Proteins **59***,* 810-827 (2005)

!

An update of a 'structural alphabet' is presented. Increased database sizes are shown to preserve essential and overall features of the previous model. More rigorous relations with sequence could be derived, yielding increased prediction rates (up to 49%). Some implications for classification of structural motifs are discussed.

Comparative or Homology Modeling

A three-dimensional structure of *Plasmodium falciparum* serine hydroxymethyltransferase in complex with glycine and 5-formyl-tetrahydrofolate. Homology modeling and molecular dynamics.

T.C.C. França, P.G. Pascutti, T.C. Ramalho, and J.D. Figueroa-Villar* [Inst Militar de Engenharia]

J. Biophys. Chem. **115,** 1-10 (2005)

A 3D-model of *Plasmodium falciparum* serine hydroxymethyltransferase (pfSHMT) in complex with glycine and 5-formyl tetrahydrofolate was developed based on homology modeling. The active sites of this model were compared with that of crystallographic Human SHMT (hSHMT) and reveal key differences useful for the design of new selective inhibitors of pfSHMT.

Protein Structure Analysis

!

Geometric cooperativity and anticooperativity of three-body interactions in native proteins.

X. Li and J. Liang* [U IL]

Proteins **60***, 46-65 (2005)*

From a geometric definition of 3-body interactions, thorough comparisons with pairwise interactions in protein structures are made. Generally, protein interior hydrophobic interactions are anti-cooperative, interior ionic and H-bonding interactions are cooperative, while on the protein surface this is reversed.

!

Comparison of x-ray and NMR structures: Is there a systematic difference in residue contacts between x-ray and NMR-resolved protein structures?

S.O. Garbuzynskiy, B.S. Melnik, M.Y. Lobanov, A.V. Finkelstein, and O.V. Galzitskaya* [Russ Ac Sci]

Proteins **60***, 139-147 (2005)*

A thorough and detailed analysis of contact densities for internal and external residues and backbone and sidechain atoms is presented. NMR structures differ more from X-ray structures than X-ray structures, and NMR structures, from themselves. More interesting small-scale but significant differences are identified and discussed.

Progress of structural genomics initiatives: An analysis of solved target structures.

A.E. Todd* [U College London], R.L. Marsdena, J.M. Thornton, and C.A. Orengo

J. Mol. Biol. **348**, 1235-1260 (2005)

The 316 non-redundant entries to the PDB represent an addition of 459 and 393 domains to the CATH and SCOP structure classification compendiums, respectively.

Influence of protein flexibility on the electrostatic energy landscape in gramicidin A.

B. Corry* [U Western Australia Crawley] and S.-H. Chung

Europ.Biophys. J. **34,** 208-216 (2005)

MD simulations are used to determine an electrostatic model of the gramicidin A channel that allows protein atoms to move in response to the presence of a permeating ion. When protein atoms are allowed to move, the dielectric model used in electrostatic calculations breaks down when modeling the gramicidin channel.

Protein Folding

Folding pathways for initiator and effector procaspases from computer simulations.

S. Piana* [Curtin U], Z. Taylor, and U. Rothlisberger

Proteins **59***, 765-772 (2005)*

Folding pathways for procaspases 3, 7 and 8 analyzed based on MD simulations with GROMACS. A Go-type potential derived from contact maps of mature caspases is used. Procaspase 8 showed markedly different folding pathways, notably on the linker region.

Protein folding rates estimated from contact predictions.

M. Punta and B. Rost* [Columbia U]

J. Mol. Biol. **348**, 507-512 (2005)

Two-state folding rates are estimated from predicted internal residue-residue contacts in proteins with unknown structure, and shown to be, on average, as accurate as folding rates predicted from those estimated from known contacts as well as secondary structure predictions.

Protein Folding (cont'd)

Complex stability of single proteins explored by forced unfolding experiments.

H. Janovjak* [U Tech], K.T. Sapra, and D.J. Müller

Biophys. J. **88,** L37-L39 (2005)

MC simulations of forced unfolding of the bacteriorhodopsin trimer shows three energetically distinct states for the D and E helices that don't occur with the monomer. Relative forces are robustly measurable, whereas the force spectrum is very sensitive to calibration of the scanning probe instrument.

Comparison of sequence-based and structure-based energy functions for the reversible folding of a peptide.

A. Cavalli, M. Vendruscolo, and E. Paci* [U Zurich]

Biophys. J. **88,** 3158-3166 (2005)

With MD, atomistic and Gō-like force fields yield similar folding pathways and kinetics for a 20-residue peptide, but the apparent free energy topology differed greatly for the two.

Molecular mechanism for stabilizing a short helical peptide studied by generalized-ensemble simulations with explicit solvent.

Y. Sugita* [U Tokyo] and Y. Okamoto

Biophys. J. **88,** 3180-3190 (2005)

Folding of the C-peptide of ribonuclease A is studied with replica-exchange multicanonical MD.

Rapid assessment of contact-dependent secondary structure propensity: Relevance to amyloidogenic sequences.

S. Yoon and W.J. Welsh* [U New Jersey]

Proteins **60***,* 110-117 (2005)

A neural network method identifies the importance of non-local (tertiary) contacts for secondary structure propensities for acylphosphatase and hIAPP. Application to 6390 domains from SCOP shows DNA-binding proteins in the top 10, and high scores for known amyloidogenic proteins.

Denatured-state ensemble and the early-stage folding of the G29A mutant of the B-domain of protein A.

S. Chowdhury, H. Lei, and Y. Duan* [U Calif Davis]

J. Phys. Chem. B **109**, 9073-9081 (2005)

A three-helix bundle protein (the G29A mutant of BdpA) is explored in a series of MD simulations started from an extended state. In one (out of 16 400ns trajectories), folding to within 2.9 Å is observed. Fast hydrophobic collapse appeared to be the driving force.

Protein Hydration

Hydration of protein–protein interfaces.

F. Rodier, R.P. Bahadur, P. Chakrabarti, and J. Janin* [CNRS]

Proteins **60***,* 36-45 (2005)

A comparison of 161 protein-protein dimers *vs.* 173 crystal-packing interfaces in X-ray structures is presented. Although some are 'dry', most interfaces are 'wet' and packing interfaces 'wettest' on average. Specific hydration patterns and the importance of stabilizing water-mediated interactions are discussed.

Protein Dynamics

What contributions to protein side-chain dynamics are probed by NMR experiments? A molecular dynamics simulation analysis.

R. Best, J. Clarke and M. Karplus* [U Louis Pasteur]

J. Mol. Biol. **349**, 185-203 (2005)

A method for calculating converged NMR side-chain order parameters uses replica exchange molecular dynamics in conjunction with an implicit solvent model. "These simulations allow the influence of various factors, such as the flexibility of side-chains and their free volume, on the mobility to be tested by perturbing the system."

Molecular dynamics and protein function.

M. Karplus* [Harvard U] and J. Kuriyan

PNAS **102,** 6679-6685 (2005)

MD simulations are useful for the exploration of the conformational energy landscape accessible to macromolecules. MD simulations have contributed to understanding the mechanism in protein folding and enzymatic catalysis. The results with the F_1 ATPase molecular motor and the Src family of signaling proteins are examples.

Free Energy

Free energies of ligand binding for structurally diverse compounds.

C. Oostenbrink and W.F. van Gunsteren*
[Swiss Fed Inst Tech]

PNAS **102,** 6750-6754 (2005)

Depending on the choice of reference compound, relative free energies of binding rigid ligands to the ligand-binding domain is in good agreement with experimental values. The present approach is easily applied to many rigid ligands, and it is relatively easy to extend the method to account for ligand flexibility.

Ligand Binding

Decoys for docking.

A.P. Graves, R. Brenk, and B.K. Shoichet*
[U Calif San Francisco]

J. Med. Chem. **48**, 3714-3728 (2005)

Two sets of docking decoys are presented: (1) 20 geometric decoys that have subtly incorrect bound conformations, and (2) 166 hit-list decoys that are predicted to be false positives by DOCK. A comparison of other scoring functions is made using these decoys.

The molecular basis of resilience to the effect of the Lys103Asn mutation in non-nucleoside HIV-1 reverse transcriptase inhibitors studied by targeted molecular dynamics simulations.

F. Rodriguez-Barrios, J. Balzarini, and F. Gago* [U Alcala]

J. Amer. Chem. Soc. **127**, 7570-7578 (2005)

Nevirapine, efavirenz, and etravirine (all non-nucleoside HIV-1 RT inhibitors) each were steered in MD simulation into the binding pocket of reverse transcriptase, and the conformation steered from the apo to holo form, to better understand the effects of specific active site mutation.

Enzyme Catalysis

Comparison of multiple molecular dynamics trajectories calculated for the drug-resistant HIV-1 integrase T66I/M154I catalytic domain.

A. Brigo, K.W. Lee, G.I. Mustata, and J.M. Briggs*
[U Houston]

Biophys. J. **88,** 3072-3082 (2005)

How three point mutants interfere with catalysis is explored with MD simulations from four different starting configurations. The different simulations converge in the timescale studied.

Large-scale conformational dynamics of the HIV-1 integrase core domain and its catalytic loop mutants.

M.C. Lee, J. Deng, J.M. Briggs, and
Y. Duan* [U Calif Davis]

Biophys. J. **88,** 3133-3146 (2005)

Over 480 ns of simulation show a large-scale change involving >20-Å motions gating the catalytic domain. At least seven conformations for the catalytic domain were identified.

Protein-Protein Interactions

How does nitrous oxide reductase interact with its electron donors? - A docking study.

K. Mattila* [CSC] and T. Haltia

Proteins **59***, 708-722 (2005)

Rigid body docking and selection of complexes by CHARMM forcefield energies with the ACE solvation model, produces a variety of NOR-c555 and NOR-pseudoazurin complexes. Many of those are rotationally related, and most share important features that could be linked to the electron-transfer mechanism and pathways.

Following the aggregation of amyloid-forming peptides by computer simulations.

A. Melquiond* [U Paris 7], G. Boucher, N. Mousseau, and
P. Derreumaux

J. Chem. Phys. **122,** 17490401-17490408 (2005)

With the "activation-relaxation technique coupled with a coarse-grained energy model," the amyloidogenic KFFE peptide was found to have complex intermediate structure formations with numerous dead ends. As a control, simulations with KPGE showed only disordered structures.

Membrane Proteins and Lipid-Peptide Interactions

Folding is not required for bilayer insertion: replica exchange simulations of an alpha-helical peptide with an explicit lipid bilayer.

H. Nymeyer, T.B. Woolf, and A.E. García* [LANL]

Proteins **59***, 783-790 (2005)

Replica exchange simulations in explicit solvent with CHARMM show a marked preference for an 'insertion/folding' pathway of WALP-16 membrane insertion. A detailed analysis of the enthalpic/entropic balance that shifts throughout the insertion process is provided.

Electrostatic recognition and induced fit in the κ-PVIIA toxin binding to *Shaker* potassium channel.

X. Huang, F. Dong, and H.-X. Zhou* [FSU]

J. Amer. Chem. Soc. **127**, 6836-6849 (2005)

Brownian and MD simulations and electrostatic calculations investigater the binding process of a conotoxin to a potassium ion channel. Significant induced fit was evident after initially electrostatically driven attraction.

Membrane Proteins and Lipid-Peptide Interactions (cont'd)

Role of ions on structure and stability of a synthetic gramicidin ion channel in solution. A molecular dynamics study.

G. Morra, U. Koert, and E.-W. Knapp* [Freie U Berlin]

J. Phys. Chem. B **109**, 10441-10448 (2005)

MD simulations with an implicit solvent (GB) model investigate cesium ions in a synthetic gramicidin-like ion channel under various (explicit) salt conditions.

Perturbation of a lipid membrane by amphipathic peptides and its role in pore formation.

A. Zemel, A. Ben-Shaul* [Hebrew U], and S. May

Europ.Biophys. J. **34,** 230-242 (2005)

The membrane perturbation free energy depends critically on peptide orientation: In the transmembrane pore state, the lipid perturbation energy, per peptide, is smaller than in the adsorbed state. The gain in conformational freedom of the lipid chains is a central driving force for pore formation. A weak, lipid-mediated, gain in membrane perturbation free energy occurs upon dimerization of interfacially adsorbed peptides.

Structure and dynamics of model pore insertion into a membrane

C.F. Lopez, S.O. Nielsen, B. Ensing, P.B. Moore, and M.L. Klein* [U Pennsylvania]

Biophys. J. **88,** 3083-3094 (2005)

A course-grained nanotube with hydrophobic surface, without or with hydrophilic caps at the ends of the nanotube, was simulated inserting into a planar lipid bilayer. The peptide entered the bilayer horizontally, was pulled to the center, and then rotated to span the membrane. The hydrophilic-capped tube behaved similarly, but carried three lipid molecules with it.

Spontaneous formation of detergent micelles around the outer membrane protein OmpX

R.A. Böckmann* [U Zurich] and A. Caflisch* [U Zurich]

Biophys. J. **88,** 3191-3204 (2005)

100-ns MD simulations of Omp X with dihexanoylphosphatidylcholine in water shows that ~18 detergent molecules combine to form micelles, that ~100 molecules are needed to coat the protein, that charged groups on the protein surface seed micelle formation, and that polar groups retain water contact. The protein appears to have a fishing pole structure rather than forming a membrane channel.

The α-helical propensity of the cytoplasmic domain of phospholamban: A molecular dynamics simulation of the effect of phosphorylation and mutation.

M.G. Paterlini* [Certusoft] and D.D. Thomas

Biophys. J. **88,** 3243-3251 (2005)

Phosphorylation of Ser16 results in a salt bridge to Arg13, which distorts the helix. Arg9Cys leads to helix reduction through increased water access to the backbone. These results may help explain how these changes relieve calcium-pump inhibition by phospholamban.

Water molecules and hydrogen-bonded networks in bacteriorhodopsin - molecular dynamics simulations of the ground state and the M-intermediate.

S. Grudinin, G. Büldt, V. Gordeliy, and A. Baumgaertner* [Forsch Jülich]

Biophys. J. **88,** 3252-3261 (2005)

A large-scale simulation of the bacteriorhodopsin trimer focuses on the extent of water in the protein in G and M states and the possible Grotthus pathways for proton transport through the more hydrated M state.

Membrane Proteins and Lipid-Peptide Interactions (cont'd)

Homology model of the GABA$_A$ receptor examined using Brownian dynamics.

M. O'Mara, B. Cromer, M. Parker, and S.-H. Chung* [Australian Natl U]

Biophys. J. **88,** 3286-3299 (2005)

The homology model is based on the transmembrane structure of the nicotinic acetylcholine receptor channel and the acetylcholine binding protein. There are strong anion absorbing regions in the channel and external vestibules, which together hold 10 Cl$^-$ ions.

Conformational dynamics of the ligand-binding domain of inward rectifier K channels as revealed by molecular dynamics simulations: Toward an understanding of K$_{ir}$ channel gating.

S. Haider, A. Grottesi, B.A. Hall, F.M. Ashcroft, and M.S.P. Sansom* [U Oxford]

Biophys. J. **88,** 3310-3320 (2005)

Simulations of the C-terminal domains for the two-helix K$^+$ channels, one a crystal structure and the other a homology model, reveals that ATP binding to the latter causes the four-fold symmetry of the homotetramer to shift to a dimer-of-dimers symmetry, probably responsible for gating the channel.

Molecular dynamics simulation of the M2 helices within the nicotinic acetylcholine receptor transmembrane domain: Structure and collective motions.

A. Hung, K. Tai, and M.S.P. Sansom* [U Oxford]

Biophys. J. **88,** 3321-3333 (2005)

The effects of bending of the M2 helix from the NAChR embedded in an octane bilayer were analyzed and proposed to be responsible for gating events.

Protein-Nucleic Acid Interactions

Recognition complex between the HMG domain of LEF-1 and its cognate DNA studied by molecular dynamics simulations with explicit solvation.

M. Drumm, S. Tetechea, and J. Kozelka* [CNRS]

J. Biomol. Struct. Dyn. **23**, 1-11 (2005)

MD simulations based on the NMR structures investigate the LEF-1 protein DNA complex. An "induced fit" mechanism is demonstrated upon DNA binding along with a key role of water in the interaction.

Molecular dynamics simulations of a nucleosome and free DNA.

T. C. Bishop* [Tulane U]

J. Biomol. Struct. Dyn. **22**, 673-685 (2005)

MD simulations are performed on the 146 base pair free DNA and also bound to the nucleosome. The DNA appears to be less flexible when bound. As part of the analysis, a Fourier method is developed that allows de- and re-construction of the structure and dynamics.

Towards an understanding of DNA recognition by the methyl-CpG binding domain 1.

C. Rauch, M. Trieb, F. R. Wibowo, B. Wellenzohn, W. Mayer, and K. R. Liedl* [U Innsbruck]

J. Biomol. Struct. Dyn. **22**, 695-706 (2005)

MD simulations probe the symmetric recognition of methylated CpG steps by a monomeric (asymmetric binding) protein domain. The calculations suggest that only one of the methyl groups contributes to the binding and hypothesize that there is a direct interaction between particular residues in the protein and the DNA.

Protein-Nucleic Acid Interactions (cont'd)

Induced fit and the entropy of structural adaptation in the complexation of CAP and λ-repressor with cognate DNA sequences.

S.B. Dixit, D.Q. Andrews, and D.L. Beveridge* [Wesleyan U]

Biophys. J. **88,** 3147-3157 (2005)

Catabolite-activator protein causes pronounced bending of DNA when bound, whereas λ-repressor does not. Part of the entropy change upon binding is due to constraint of the protein, and part due to constraint of the DNA. In addition, a surprisingly large part of the entropy change comes from DNA-protein cross-correlation.

Nucleic Acids

The B- to A-DNA transition and the reorganization of solvent at the DNA surface.

N. Pastor* [U Autónoma del Estado de Morelos]

Biophys. J. **88,** 3262-3275 (2005)

An 11-ns MD simulation of a forced transition from B- to A-DNA for a 24-basepair double helix shows that it follows the slide-first, roll-later mechanism. Hydrogen bonds to waters don't change much, but counterion contacts and water bridges do.

Free energy landscape of A-DNA to B-DNA conversion in aqueous solution.

N.K. Banavali* [Cornell U] and B. Roux

J. Amer. Chem. Soc. **127**, 6866-6876 (2005)

Using RMSd as a reaction coordinate, the PMF for the conversion of A-DNA to B-DNA within the CHARMM all27 force field is performed. The extensive sampling (in explicit solvent) gives insight into the backbone and sugar substates and suggest there is no other minima on the A-B pathway.

Molecular dynamics study on the interaction of a mithramycin dimer with a decanucleotide duplex.

S.-Y. Chen, and T.-H. Lin* [Natl Tsing Hua U]

J. Phys. Chem. B **109**, 9764-9772 (2005)

MD and binding free energy estimations are applied to the 1:1 and 2:1 binding of the minor groove binding drug mithramycin to 10-mer DNA duplex.

Comparison of positively charged DNG with DNA duplexes: A computational approach.

J.W. Toporowski* [UCSB], Y.S. Reddy and T.C. Bruice

Bioorg. Med. Chem. **13**, 3691-3698 (2005)

MD simulations are used to investigate the structural properties of the cationic DNA analogue deoxynucleic guanidine (DNG) and the DNG duplex dodecamers $d(Ag)_{12} \cdot d(Tg)_{12}$ and $d(Gg)_{12} \cdot d(Cg)_{12}$ and their counterparts. The major and minor groove widths of DNG are narrower than those of the respective DNA counterparts.

How sequence defines structure: A crystallographic map of DNA structure and conformation.

F.A. Hays, A. Teegarden, Z.J.R. Jones, M. Harms, D. Raup, J. Watson, E. Cavaliere, and P.S. Ho* [Oregon State U]

PNAS **102**, 7175-7162 (2005)

A data set of 37 single-crystal structures from 29 of the sequences in this motif is assembled, representing three structural classes of DNA. The resulting data set allows dissecting in detail the stabilization and conformational variations within structural classes and identifying significant conformational deviations within a particular structural class that result from sequence rather than crystal or crystallization effects.

Nucleic Acids (cont'd)

Hinge-like motions in RNA kink-turns: The role of the second A-minor motif and nominally unpaired bases.

F. Rázga, J. Koca, J. Sponer* [Acad Sci Czech Rep], and N.B. Leontis* [Bowling Green State U]

Biophys. J. **88,** 3466-3485 (2005)

Hinge-like K-turn motions occur on the ns timescale according explicit solvent MD simulations but do not affect tertiary interactions or fold. They may be important for large-scale motions during ribosome function.

Lipids and Surfactants

Examination of membrane fusion by dissipative particle dynamics simulation and comparison with continuum elastic models.

D.-W. Li and X.Y. Liu* [Natl U Singapore]

J. Chem. Phys. **122,** 17490401-17490408 (2005)

Dissipative particle dynamics simulations indicate that the stalk model needs to be modified. Lipid tilt is modified during stock formation. Transmembrane contact involves asymmetric expansion of the stalk. A bent stalk with a pore or inverted micelle structure is more likely to occur with negative-curvature lipids.

Protons may leak through pure lipid bilayers via a concerted mechanism.

H.L. Tepper and G.A. Voth* [U Utah]

Biophys. J. **88,** 3095-3108 (2005)

With an improved empirical valence bond model for a proton in water, it is now found that water forms a networked strand through a bilayer, rather than a single-file column. The strands are stable for hundreds of ps and help explain high proton conductance.

Influence of DPH on the structure and dynamics of a DPPC Bilayer

J. Repáková, J.M. Holopainen, M.R. Morrow, M.C. McDonald, P. Capková, and I. Vattulainen* [Helsinki Tech U]

Biophys. J. **88,** 3398-3410 (2005)

The dye, DPH, has little influence on the headgroups and affects lipid tails locally, but not globally, according to MD simulations in conjunction with DSC and NMR studies.

Carbohydrates

Conformational dynamics of sialyl lewis^X in aqueous solution and its interaction with selectin E. A study by molecular dynamics.

K. Veluraga, and C. J. Margulis* [U Iowa]

J. Biomol. Struct. Dyn. **23**, 101-111 (2005)

MD simulations investigate the dynamics of free and bound sugar to selectin E. The AMBER parm99 force field is applied along with the GAFF force field for the sugar. In order to properly represent the binding to protein, the charges on the sugar had to be modified (via a Gaussian run with calcium).

1.3.   *Polymers*

Molecular dynamics simulation of the polymer electrolyte poly(ethylene oxide)/LiClO4. I. Structural properties.

L.J.A. Siqueira and M.C.C. Ribeiro* [U São Paulo]

J. Chem. Phys. **122,** 19491101-19491108 (2005)

The lithium chloride salt causes elongation of the polymer in MD simulations at 373 K, but not at 500 K. There is no mention of water being used in the united atom simulations. Ion contact pairing increases with temperature. Static structure factor results are consistent with neutron scattering spectroscopy.

Atomistic molecular-dynamics simulations of the size and shape of polyethylene in hexane at infinite dilution.

G. Zifferer* [U Wien] and A. Kornherr

J. Chem. Phys. **122,** 20490601- 20490607 (2005)

Simulations with 15-60 monomer units begin to reveal characteristics of polymer coils.

---

2. <u>**METHODOLOGY**</u>

Potentials and Parameters

Helix-coil transition of alanine peptides in water: force field dependence on the folded and unfolded structures.

S. Gnanakaran and A.E. Garcia* [LANL]

Proteins **59***, 773-782 (2005)

A modified Amber96 and the Opls/AA/L forcefields both reproduce the temperature dependent folding characteristics of $(Ala)_{21}$ peptides in replica exchange MD with Amber 4.1, but with significantly different intermediate states.

Smooth solvation method for d-orbital semiempirical calculations of biological reactions. 2. Implementation.

J. Khandogin, B.A. Gregersen, W. Thiel, and D.M. York* [U Minnesota]

J. Phys. Chem. B **109**, 9799-9809 (2005)

The smooth conductor-like screening model for solvation is extended to a d-orbital semi-empirical framework (MNDO/d-SCOSMO).

Solvation Energy

Comparative study of generalized Born models: Protein dynamics.

H. Fan, A.E. Mark* [U Groningen], J. Zhu, and B. Honig

PNAS **102,** 6760-6754 (2005)

MD simulations involving the application of three generalized Born (GB) models, the Still, HCT, and modified analytical generalized Born models are applied to 10 proteins in the computationally efficient GROMACS package. The results suggested that the modified analytical generalized Born model gives the best agreement between calculated and experimentally derived structures.

Normal Modes Analysis

Quantifying allosteric effects in proteins.

D. Ming and M.E. Wall* [Los Alamos Natl Lab]

Proteins **59**, 697-707 (2005)

Detailed analysis of normal mode calculations in CHARMM of turkey lysozyme with and without NAG bound, expressed as contributions from the eigenvalue spectrum, mean conformation and eigenvectors, reveals that large changes in the eigenvector contribution correlate with ligand binding interactions.

Molecular Dynamics

!

!MDSIMAID: Automatic parameter optimization in fast electrostatic algorithms.

M.S. Crocker, S.S. Hampton, T. Matthey, J.A. Izaguirre* [U Notre Dame]

J. Comput. Chem. **26,** 1021-1031 (2005)

MDSimAid recommends particle mesh Ewald parameters for sequential and parallel multigrid summation solvers. It "optimizes the running time or parallel scalability of these methods within a given error tolerance." Optimized configurations "are up to 14 times faster or 17 time more accurate than published recommendations." Available at http://mdsimaid.cse.nd.edu.

Practical conversion from torsion space to Cartesian space for *in silico* protein synthesis.

J. Parsons, J.B. Holmes, J.M. Rojas, J. Tsai, and C.E.M. Strauss* [Los Alamos Natl Labs]

J. Comput. Chem. **26,** 1063-1068 (2005)

The Natural Extension Reference Frame method for computing Cartesian coordinates from internal coordinates appears to be minimal in floating point calculations, offers good parallelization, and outperforms traditional two-step rotations, vector algebra, and Quaternion product algorithms.

Artifacts in dynamical simulations of coarse-grained model lipid bilayers.

A.F. Jakobsen* [U Southern Denmark], O.G. Mouritsen, and G. Besold

J. Chem. Phys. **122**, 20490101-20490111 (2005)

A fingerprint of simulation pressure and bead temperature artifacts due to time step, integration technique, and thermostat algorithm is developed for use with coarse-grained lipid bilayers.

Selection of temperature intervals for parallel-tempering simulations.

A. Kone and D.A. Kofke* [U Buffalo]

J. Chem. Phys. **122**, 20610101- 20610102 (2005)

Equally spaced steps in parallel tempering simulations are shown to optimally efficient. Although the prediction is based on the assumption of piecewise constant heat capacity, the result seems to be independent of heat capacity. "Temperatures in replica-exchange simulations should be spaced such that about 20% of the phase-swap attempts are accepted."

Normal-modes-based prediction of protein conformational changes guided by distance constraints.

W. Zheng* [NIH] and B.R. Brooks

Biophys. J. **88,** 3109-3117 (2005)

5-10 NOE constraints for the end state added to the Hamiltonian are enough to guide the transformation from the crystal structure via the elastic network model.

Molecular Dynamics (cont'd)

Molecular dynamics integration and molecular vibrational theory. I. New symplectic integrators.

D. Janežič* [Natl Inst Chem], M. Praprotnik, and F. Merzel

J. Chem. Phys. **122**, 17410101-17410114 (2005)

This and two following application papers describe a new integrator that combines standard time integration with calculated molecular vibrations (i.e. normal modes analysis for each molecule individually). The approach allows a long integration time step. It is applicable for molecules with a single equilibrium configuration.

Free Energy Methods

Calculation of absolute protein-ligand binding free energy from computer simulations.

H.-J. Woo and B. Roux* [Weill Med Coll Cornell U]

PNAS **102**, 6825-6830 (2005)

The equilibrium binding constant of a flexible ligand to a protein receptor can be decomposed into three stages. The free ligand in the bulk is first restrained into the configuration it adopts in the bound state with biasing potentials. Then it is translated into the binding site, where it is released completely.

Peptide conformational equilibria computed via a single-stage shifting protocol.

F.M. Ytreberg* [U Pitt] and D.M. Zuckerman

J. Phys. Chem. B **109**, 9096-9103 (2005)

Extending Voter's method to shift potential energy functions, a generalization involving shifting of internal coordinates and use of Bennett's iterative method is applied to provide overlap in two-state free energy calculations aimed at elucidating the conformational equilibria of peptides.

Rosenbluth-sampled nonequilibrium work method for calculation of free energies in molecular simulation.

D. Wu* [State U New York] and D.A. Kofke

J. Chem. Phys. **122,** 20410401-20410413 (2005)

In Rosebluth (1955) sampling, steps are selected from alternatives with a bias for low-work steps. The Jarzinski definition of work is modified to account for the bias. Accuracy is improved by an order of magnitude over unbiased sampling, allowing equivalent accuracy with 100-fold less sampling. λ- and configuration-bias sampling methods are compared, the first being most valuable in entropy-limited processes and the second most valuable in energy-limited processes.

QM/MM

A combined freeze-and-cut strategy for the description of large molecular systems using a localized orbitals approach.

S. Borini* [U Ferrara], D. Maynau, and S. Evangelisti

J. Comput. Chem. **12,** 1042-1051 (2005)

A methodology that has potential applications in QM/MM simulations is described in which localized orbitals are used to evaluate part of a macromolecular system in QM detail. "By exploiting freeze strategy at the self-consistent field (SCF) level and a cut of the unneeded atomic orbitals, it is possible to perform a localized complete active space (CAS-SCF) calculation on a reduced system."

Multiple –steering QM-MM calculation of the free energy profile in chorismate mutase.

A. Crespo, M. A. Marti, D. A. Estrin* [U Buenos Aires], and A. E. Roitberg* [U Florida]

J. Amer. Chem. Soc. **127**, 6940-6941 (2005)

The Jarzynski multiple steering molecular dynamics approached is developed and applied in the context of DFT/MM calculations on the enzyme chorismate mutase.

QM/MM (cont'd)

A critical evaluation of different QM/MM frontier treatments with SCC-DFTB as the QM method.

P. H. Konig, M. Hoffmann, T. Frauenheim* [U Paderborn], and Q. Cui* [U Wisc]

J. Phys. Chem. B **109**, 9082-9095 (2005)

Different link-atom based frontier treatments in QM/MM are evaluated. In general, some results (such as proton affinities and deprotonation energies) are very sensitive to the link-atom method applied. However, if charge is conserved, the methods appear to be not too sensitive to the approach and in most cases it is more important to worry about details of long-range electrostatics and other technical details.

Protein/ligand binding free energies calculated with quantum mechanics/molecular mechanics.

F. Grater, S. M. Schwarz, A. Dejaegere, S. Fischer* [U Heidelberg], and J. C. Smith* [U Heidelberg]

J. Phys. Chem. B **109**, 10474-10483 (2005)

QM/MM is used to estimate binding free energies of 47 benzamidine derivatives bound to trypsin. The authors suggest that such simulations could be a useful tool in automated docking and scoring of flexible ligands.

***Ab initio* quantum chemistry: Methodology and applications.**

R.A. Friesner* [Columbia U]

PNAS **102,** 6648-6653 (2005)

An overview of state-of-the-art *ab initio* quantum chemical methodology and applications are presented. The accuracy of each approach for key chemical properties is summarized, and the computational performance is analyzed with significant advances in algorithms and implementation. Combined QM/MM or self-consistent reaction field techniques are presented for condensed-phase environment.

***Ab initio* molecular dynamics: Concepts, recent developments, and future trends.**

R. Iftimie, P. Minary, and M.E. Tuckerman* [Stanford U]

PNAS **102**, 6654-6659 (2005)

Ab initio molecular dynamics is leading to new paradigms in the elucidation of microscopic mechanisms, rationalization of experimental data, and testable predictions of new phenomena.

Protein Folding

Estimation of protein folding probability from equilibrium simulations.

F. Rao, G. Settanni, E. Guarnera, and A. Caflisch* [U Zurich]

J. Chem. Phys. **122,** 18490101-18490105 (2005)

The probability of folding to a native state, P, (vs. unfolding) should be 0.5 for transition state configurations. From a single trajectory containing multiple folding and unfolding events, it is helpful to determine the probability of folding based on a given cutoff criterion called the commitment time, which is long compared to local fluctuations, but long compared to average folding time.

An independent method for the analysis of protein folding kinetics from all-atom molecular dynamics simulations.

N.J. Marianayagam* [U Cambridge], A.G. Brown, and S.E. Jackson

J. Biomol. Struct. Dyn. **23**, 73-76 (2005)

Time correlation functions of various structural properties are proposed which can determine the endpoint of folding and its mechanism in this "hypothesis" paper.

Protein Folding (cont'd)

Energy landscape paving simulations of the trp-cage protein.

A. Schug* [Forsch Karlsruhe], W. Wenzel, and U.H.E. Hansmann

J. Chem. Phys. **122,** 19471101-19471107 (2005)

The efficiencies of energy-paving algorithms, in which MD or MC simulations utilize a self-avoiding energy function, are compared. These algorithms demonstrate the funnel shaped energy landscape for trp-cage protein.

A directed essential dynamics simulation of peptide folding.

C. Chen, Y. Xiao* [Huazhong U Sci Tech], and L. Zhang

Biophys. J. **88,** 3276-3285 (2005)

In directed essential dynamics, principle components analysis is used to determine the most active collective motions. Then motions are simulated using these active modes, with a directing force to encourage motions towards the folded state to avoid nonproductive paths. The method is illustrated with S-peptide folding.

Energy landscape distortions and the mechanical unfolding of proteins.

D.J. Lacks* [Case Western Reserve U]

Biophys. J. **88,** 3494-3501 (2005)

The energy surface changes during stretching, according to molecular simulations and energy landscape analysis. If thermalization is faster than stretching, new minima can appear that modify mechanical unfolding rates.

Ligand Docking

Influence of external vibration on tether chain in ligand-receptor binding.

B. Xue and W. Wang* [Nanjing U]

J. Chem. Phys. **122,** 19491201-19491208 (2005)

A tether extends more when exposed to low frequency vibrations in the environment, which should strongly affects tethered ligand binding.

Structure Determination

RECOORD: a recalculated coordinate database of 500+ proteins from the PDB using restraints from the BioMagResBank.

A.J. Nederveen, J.F. Doreleijers, W. Vranken, Z. Miller, C.A. Spronk, S.B. Nabuurs, P. Guntert, M. Livny, J.L. Markley, M. Nilges, E.L. Ulrich, R. Kaptein, and A.M. Bonvin* [Utrecht U]

Proteins **59***, 662-672 (2005)

545 protein structures are recalculated from the NMR distance restraints (BioMagResBank FRED data) using CNS and CYANA. In most cases models could be refined to significantly higher quality (*e.g.* packing and Ramachandran distribution) and less violations than the deposited (PDB) models. Significance and inter-correlation of various NMR structure quality indicators is discussed at length.

Clustering algorithms for identifying core atom sets and for assessing the precision of protein structure ensembles.

D.A. Snyder and G.T. Montelione* [Rutgers U]

Proteins **59***, 673-686 (2005)

A method for defining structural cores, and for deciding whether a single or multiple cores are necessary, in structural ensembles is presented. Some of the controversies and difficulties in assessing NMR structure quality are discussed.

3. J O U R N A L   R E V I E W S

Journal of the American Chemical Society 127(14-22), 2005

5204-5211 **Reactions of d^0 group 4 amides with dioxygen. Preparation of unusual oxo aminoxy complexes and theoretical studies of their formation**, R. Wang, X.-H. Zhang, S.-J. Chen, X. Yu, C.-S. Wang, D. B. Beach, Y.-D. Wu* [Hong Kong U], and Z.-L. Xue* [U TN] [DFT calculations look at Zn and Hf oxo aminoxide complexes]

5449-5462 **Spectroscopic and computational studies of Ni superoxide dismutase: Electronic structure contributions to enzymatic function**, A. T. Fiedler, P. A. Bryngelson, M. J. Maroney, and T. C. Brunold* [U Wisc] [DFT and spectroscopy applied to nickel superoxide dismutase]

5794-5795 **Factors controlled the barriers to degenerate hydrogen atom transfters**, C. Isborn, D. A. Hrovat, W. T. Borden* [U WA], J. M. Mayer* [U WA], and B. K. Carpenter* [Cornell U] [Bond dissociation energies are estimated in high level calculation]

6048-6051 **A computational analysis of the ring-opening polymerization of *rac*-Lactide initiated by single-site *b*-diketiminate metal complexes: Defining the mechanistic pathway and the origin of stereocontrol**, E. L. Marshall, V. C. Gibson, and H. S. Rzepa* [Imperial College] [DFT simulations ranging from STO-3G to 6-311G(3d) probe ring-opening polymerization at a magnesium center]

6077-6086 **Photoinduced charge generation and recombination dynamics in model donor/acceptor pairs for organic solar cell applications**, V. Lemaur, M. Steel, D. Beljonne, J.-L. Bredas, and J. Cornil* [U Mons-Hainaut] [QM gives insight into organic solar cells exciton dissociation and charge recombination]

6116-6122 **The enthalpies of formation of *o*-, *m*-, and *p*-benzoquinone: Gas-phase ion energetics, combustion calorimetry, and quantum chemical computations combined**, A. Fattahi, S. R. Kass* [U Mn], J. F. Liebman* [U Md], M. A. R. Matos* [U Porto], M. S. Maranda, and V. M. F. Morais [DFT complements mass spectrometry]

6257-6265 **Ab initio studies on the radiationless decay mechanisms of the lowest excited singlet states of 9H-adenine**, S. Perun, A. L. Sobolewski* [Polish Acad Sci], and W. Domche [Multireference ab initio methods at CASSCF level and above probe photochemical pathways of adenine]

6443-6450 **AT base pair anions versus (9-methyl-A)(1-methyl-T) base pair anions**, D. Radisic, K. H. Bowen, Jr* [Johns Hopkins], I. Dabkowska, P. Storoniak, J. Rak, and M. Gutowski [Czech Acad Sci] [DFT simulation complement anion photoelectron spectroscopy]

6541-6458 **Solid-state NMR and quantum chemical investigations of $^{13}C^{\alpha}$ shielding tensor magnitudes and orientations in peptides: Determining ϕ and ψ torsion angles**, S. Wi, H. Sun, E. Oldfield* [UIUC], and M. Hong* [Iowa State U] [Calculations of shielding tensors on dipeptide models]

6583-6594 **Pairwise decomposition of residue interaction energies using semiempirical quantum mechanical methods in studies of protein-ligand interaction**, K. Raha, A. J. van der Vaart, K. E. Riley, M. B. Peters, L. M. Westerhoff, H. Kim, and K. M. Merz, Jr.*[PSU], [Off-diagonal Fock matrix elements highlight the interaction of the ionic core and valence electrons between the protein and bound ligand]

6802-6813 **Electric field induced switching behaviors of monolayer-modified silicon surfaces: Surface designs and molecular dynamics simulations**, Y. Pei, and J. Ma* [Nanjung U], [Surfaqce tethered carboxylated alkyl chains are probed in MD under electric fields]

6830-6835 **Water at a hydrophilic solid surface probed by ab initio molecular dynamics: Inhomogeneous thin layers of dense fluid**, G. Cicero* [LLNL], J. C. Grossman, A. Catellani, and G. Galli, [Car-Parrinello on cubic SiC with water]

6902-6909 **Theoretical study of the suicide inhibition mechanism of the enzyme pyruvate formate lyase by methacrylate**, M. de Fatima Lucas, and M. J. Ramos* [U Porto] [DFT on model systems]

7215-7226 **An efficient fragment-based approach for predicting the ground-state energiesand structures of large molecules**, S. Li* [Nanjing U], W. Li, and T. Fang ["Quantum locality" allows a fragment based HF approach to large molecules]

7721-7728 **Nitric oxide interaction with cytochrome *c'* and its relevance to guanylate cyclase. Why does the iron histidine bond break?**, M. A. Marti, L. Capece, A. Crespo, F. Doctorovich, and D. A. Estrin* [U Beunos Aires] [Hybrid quantum-classical simulations are applied to the enzyme]

7924-7931 **Design of C_2-chiral diamines that are computationally predicted to be a million-fold more basic than the original proton sponges**, R. W. Alder* [U Bristol] [DFT predicts pKa values in the range of 23-26 in water]

8026-8027 **Theoretical investigation of C-H hydroxylation by $(N4Py)FE^{IV}=O^{2+}$: An oxidant more powerful than P450?**, D. Kumar, H. Hirao, L. Que, Jr., and S. Shaik* [Hebrew U] [High level QM calculations are applied]

Journal of Physical Chemistry B 109(14-18), 2005

6457-6460 **David Chandler Tribute** [Issue 14 is a special issue devoted to David Chandler and includes many interesting articles only a few of which are listed here]

7482-7487 **All-atom molecular dynamic simulations and relative NMR spectra study of weak C-H¨O contacts in amide-water systems**, R. Zhang, H. Li* [Zhejiang U], Y. Lei, and S. Han [NMR and all atom MD investigate CHO contacts]

7488-7499 **Mosaic energy landscapes of liquids and the control of protein conformational dynamics by glass-forming solvents**, V. Lubchenko* [UCSD], P. G. Wolynes, and H. Frauenfelder [Random first-order transition theory is used to explain protein conformational motions]

7529-7534 **Simulation of electron transfer between cytochrome c_2 and the bacterial photosynthetic reaction center: Brownian dynamics analysis of the native proteins and double mutants**, J. Lin, and D. N. Beratan* [Duke U] [BD with a exponential distance-dependent electron-transfer rate model]

7614-7616 **Molecular dynamics study of the hydration of lanthanum(III) and europium(III) including many-body effects**, C. Clavaguera, R. Pollet, J. M. Soudan, V. Brenner, and J. P. Dognon* [CNRS] [The first set of MD simulations on lanthanides including many-body effects]

7671-7685 **Computational study of the structure, dynamics, and photophysical properties of conjugated polymers and oligomers under nanoscale confinement**, B. G. Sumpter* [ORNL], P. Kumar, A. Mehta, M. D. Barnes, W. A. Shelton, and R. J. Harrison [MD, MC and experiment look at various confined polymers]

7749-7757 **Electronic structure of the nucleobases**, J. MacNaughton* [U Saskatchewan], A. Moewes, and E. Z. Kurmaev [Ab initio and DFT calculations of bases compared to X-ray absorption and emission spectroscopy]

7903-7914 **Conformation dependence of electronic structures of poly(ethylene oxide)**, B. Brena, G. V. Zhuang, A. Augustsson, G. Liu, J. Nordgren, J.-H. Guo, P. N. Ross, and Y. Luo* [Royal Inst Tech] [Ab initio and DFT calculations are performed on four different polymeric chain conformations]

7948-7951 **Density function theory study of NO adsorbed on A-zeolite**, Y.-J. Liu, A. Lund, P. Persson, and S. Lunell* [Uppsala U] [B3LYP at 6-31g and 6-31g(d)]

7952-7960 **DFT investigation of alkoxide vs alkylammonium formation in amine-substituted zeolites**, D. Lesthaeghe, V. Van Speybroeck, G. B. Marin, and M. Waroquier* [Ghent U] [Double zeta 6-31g(d) B3LYP]

8091-8096 **Supercooled water in PVA matrixes. II. A molecular dynamics simulation study and comparison with QENS results**, E. Chiessi* [U Roma], F. Cavalieri, and G. Paradossi [MD of water in hydrogels]

8097-8102 **Calculation of the hydration free energy difference between pyridine and its methyl-substituted derivatives by computer simulation methods**, L. Partay, P. Jedlovsky* [Eotvos Lorand U], and G. Jancso* [KFKI Atomic Ener Res Inst] [FEP simulation]

8125-8131 **Atomistic molecular dynamics simulation of benzene as a solute in a columnar discotic liquid crystal**, G. Cinacchi* [U Pisa] [MD of a binary LQ in benzene]

8164-8170 **Influence of confinement on the electrostatic interaction between charged colloids: a (N,V,T) Monte Carlo study within hyperspherical geometry**, A. Delville* [CNRS] [MC to look at ionic distributions]

8185-8194 **Thermodynamic characterization of fluids confined in heterogeneous pores by Monte Carlo simulations in the grand canonical and the isobaric-isothermal ensembles**, J. Puibasset* [CNRS] [MC and thermodynamic integration are applied]

8216-8219 **Methyl transfer in glycine *N*-methyltransferase. A theoretical study**, P. Velichkova, and F. Himo* [Albanova U] [DFT calculations of GNMT methyl transfer step]

8605-8612 **Investigation of possible structures of silicon nanotubes via density-functional tight-binding molecular dynamics simulations and ab initio calculations**, R. Q. Zhang, H.-L. Lee, W.-K. Li, and B. K. Teo* [U Ill Chicago] [Gearlike structures with alternating sp2 and sp3 like local silicon configurations are found in single walled silicon nanotubes]

8663-8672 **Dynamics and thermodynamics of water in PAMAM dendrimers at subnanosecond time scales**, S.-T. Lin, P. K. Maiti, and W. A. Goddard, III* [Cal Tech] [MD of generation 5 polyamidoamine dendrimers in water]

9119-9131 **Toward a full characterization of nucleic acid components in aqueous solution: Simulations of nucleosides,** N. Foloppe, and L. Nilsson* [Karolinska Inst] [MD assesses the performance of CHARMM and other nucleic acid force fields on nucleosides in water]

9810-9817 **Smooth solvation method for d-orbital semiempirical calculations of biological reactions. 2. Application to transphosphorylation thio effects in solution**, B. A. Gregersen, J. Khandogin, W. Thiel, and D. M. York* [U Mn], [Application of a new semi-empirical method to phosphorous and sulfur]

9818-9829 **How to model solvation of peptides? Insights from a quantum mechanical and molecular dynamics study of *N*-methylacetamide. 1. Geometries, infrared, and ultraviolet spectra in water**, B. Mennucci* [U Pisa], and J. M. Martinez, [QM and classical calculation at the continuum, solute-solvent cluster and clusters embedded in a continuum are applied to a solvated alanine dipeptide]

9830-9838 **How to model solvation of peptides? Insights from a quantum mechanical and molecular dynamics study of *N*-methylacetamide. 2. ^{15}N and ^{17}o nuclear shielding in water and in acetone**, B. Mennucci* [U Pisa], and J. M. Martinez, [Continuation of the previous study looking at shifts of O and N shieldings]

10484-10492 **Role of hydrogen bonds in protein-DNA recognition: Effect of nonplanar amino groups**, S. Mukherjee, S. Majumdar, and D. Bhattacharyya* [Saha Inst], [Ab initio and database analysis of protein-DNA complexes]

10493-1004 **Excitation dynamics in the LHCII complex of higher plants: Modeling based on the 2.72 Å crystal structure**, V. I. Novoderezhkin, M. A. Palacios, H. Van Amerongen, and R. Van Grondelle* [Vrije U], [Based on the crystal structure, steady-state spectra and energy-transfer dynamics are probed]

Current Opinion in Structural Biology, 15(2), April 2005

135-136   **Theory and simulation: pushing the limits**, J.A. McCammon* [UCSD] and R.C. Wade

In this article, an overview on the limitations of theory and simulation are presented.

137-143   **Improving implicit solvent simulations: A Poisson-centric view,** N.A. Baker* [Washington U. in St. Louis]

Recent developments of implicit solvent models are compared with computational efficiency and accuracy. These techniques are converging to a point at which both are suitable for simulating certain types of biomolecular systems over sizable time and length scales.

144 -150   **Coarse-grained models for proteins,** V. Tozzini* [NEST-INFM Scuola Normale Superiore]

The use of more rigorous parameterization techniques and novel algorithms are achieved for sampling configurational space to predict all-atom simulations.

151-156   **Long-timescale simulation methods,** Ron Elber* [Cornell U.]

The basic time-step of atomically detailed simulations is not difficult to find molecular processes in biology that span more than ten orders of magnitude of relevant times. Several techniques are developed in recent years to address these problems.

157-163   **Biomolecular simulations at constant pH**, J. Mongan and D.A. Case* [The Scrips.]

MD simulations are used to calculate the proton transfer between the system and a hypothetical bath of protons at a given pH. The energetics of charge changes upon protonation or deprotonation is accurately modeled.

164-170   **Enhancing the accuracy, the efficiency and the scope of free energy simulations**, T. Rodinger and R. Pomès* [Hospital for Sick Children, Toronto]

Novel methods combining the advantages afforded by various existing approaches of free energy calculations offer promising strategies to elucidate the physical basis of important biological processes.

171-175   **Macromolecular recognition**, C. Deremble and R. Lavery* [Inst. Biol.Phys.Chem.]

Computational speed and refining process is required on search algorithms, molecular representations and interaction potentials to detect the binding surfaces of individual macromolecules and to predict the structure of binary macromolecular complexes.

176-183   **The dynamics and energetics of water permeation and proton exclusion in aquaporins**, B.L. de Groot and H. Grubmüller* [Max-Planck Inst.]

Water molecules and small solutes ability to block proton flux is particularly remarkable across lipid bilayers. Atomistic computer simulation methods are used to study the dynamics of the water molecules and the mobility of protons inside the aquaporin channel.

185-187   **Macromolecular assemblages - from molecules to functional modules,** Patrick Cramer* [Univ. of Munich] and W. Baumeister
    Research Article not available.

188-196   **Nucleosome and chromatin fiber dynamics,** K. Luger* [Colorado State U.] and J.C. Hansen

The inherent dynamics of nucleosomal assemblages at all structural levels are a key link between the condensed domains found in eukaryotic genomes and the functions that take place within them.

197-203   **The dynamic machinery of mRNA elongation**, K. -Jean Armache, H. Kettenberger and P. Cramer* [Univ. of Munich]

This study suggested that how RNA polymerase II unwinds DNA, how it separates the RNA product from the DNA template and how it incorporates nucleoside triphosphate (NTP) substrates into the growing RNA chain.

204-212   **A cradle for new proteins: trigger factor at the ribosome**, T. Maier, L. Ferbitz, E. Deuerling and Nenad Ban* [Swiss Federal Inst. of Tech.]

The structural results provided a comprehensive view of the role of trigger factor during co-transitional protein folding.

213-220   **Targeting proteins to membranes: structure of the signal recognition particle**, P.F. Egea, R.M. Stroud and P. Walter* [UCSF]

The results provided new insights into three essentials steps of the SRP-dependent protein targeting cycle: the assembly and interaction of the SRP ribonucleoprotein core, the GTP-dependent SRP-SR association, and the interaction between SRP and the ribosome.

221-226   **Modularity within the architecture of the nuclear pore complex**, T.U. Schwartz* [Massachusetts Inst. of Tech.]

Recent studies using complementary techniques have significantly enhanced the understanding of the nuclear pore complexe (NPC) structure.

227-236   **Virus maturation: dynamics and mechanism of a stabilizing structural transition that leads to infectivity,** A.C. Steven*, J.B. Heymann, N. Cheng, B.L. Trus and J.F. Conway, T.U. Schwartz* [Massachusetts Inst. of Tech.]

The determination of the folds of the five major proteins - major capsid protein, scaffolding protein, portal, protease and accessory protein - that are typically involved in capsid assembly. These data provide a frame work for detailed mechanistic investigations and elucidation of mutations that affect assembly in various ways.

237-243   **Adenovirus complex structures**, Stephen Cusack* [EMBL Grenoble Outstation]

Capsid architecture identification studies have the importance in engineering adenovirus for use in various gene transfer applications.

Journal of Molecular Graphics and Modeling 23(5), April, 2005

389-394   **Structure analysis of the protein transduction domain of human Period1 and its mutant analogs,**
  X.L. Yang, J. Xie, B. Niu, X.N. Hu, Y. Gao, Q. Xiang, Y.H. Zhang, Y. Guo and Z.G. Zhang* [Chinese
  Acad. of Med.Sci.], See **Applications / Protein Structure Analysis**

395-405   *LigScore:* **a novel scoring function for predicting binding affinities,** A. Krammer* [Accelrys Inc.],
  P.D. Kirchhoff, X. Jiang, C.M. Venkatachalam and M. Waldman, See **Applications / Ligand Binding.**

409-418   **Inhibitor-based validation of a homology model of the active-site of tripeptidyl peptidase II,**
  H. De Winter* [Johnson & Johnson Pharm.], H. Breslin, T. Miskowski, R. Kavash and M. Somers
   See **Applications / Comparative or Homology Modeling.**

419-431   **Modelling of HLA-DQ2 and its interaction with gluten peptides to explain molecular recognition in
  celiac disease.** S. Costantini, M. Rossi, G. Colonna and A.M. Facchiano* [Inst. of Food Sci.],
   See **Applications / Comparative or Homology Modeling**

433-438   **Modeling kinase-substrate specificity: implication of the distance between substrate nucleophilic
  oxygen and attacked phosphorus of ATP analog on binding affinity.** Ming Sun* [Tsinghua U.],
  X. -H. Liu, S. -H. Ji and Y. -F. Zhao, See **Applications / Ligand Binding.**

439-446   **Combining structure-based drug design and pharmacophores.** Renate Griffith* [Univ. of Newcastle],
  Tien T.T. Luu, J. Garner and P.A. Keller, See **Applications/Medicinal Chemistry and Drug Design.**

447-456   **Structure and property correlation for Ag deposition on α-Al$_2$O$_3$ - a first principle study,**
  Abhijit Chatterjee* [Accelrys K.K.], Syuichi Niwa and Fujio Mizukami, See **Applications/ Surfaces**,
  Catalysts and Material subjects.

457- 464   **Modeling aided design of potent glycogen phosphorylase inhibitors**. Q. Deng* [Merck Res. Labs.],
  Z. Lu, J. Bohn, K.P. Ellsworth, R.W. Myers, W.M. Geissler, G. Harris, K. Chapman, C.A. Willoughby,
  B. McKeever and R. Mosley, See **Applications / Ligand Binding.**

Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta), 113(3), April 2005

133-151   **Accurate partial atomic charges for high-energy molecules using class IV charge models with the
  MIDI! basis set**. C.P. Kelly, C.J. Cramer* [Univ. of Minnesota] and D.G. Truhlar.

  A new charge model (CM3) was developed for calculations on molecules containing H, Li, C, N, O,F,
  Si, S, P, Cl, and Br. Hartree-Fock and hybrid density functional (HDFT) theories and MIDI! basis set
  are used to calculate partial atomic charges.

152-160   **Towards a complete basis set limit of Hartree-Fock method: correlation-consistent versus
  polarized-consistent basis sets**, S. Shahbazian and M. Zahedi* [Shahid Beheshti Univ.]

  The potential energy surfaces derived from basis-set-dependent solution of the Hartree-Fock equations
  achieves the exact numerical derived potential energy surfaces in an ordered manner.

161-166   **Hydrogen bonding motif in 2-hydroxy-1,4-naphthoquinone**, N.R. Dhumal, A.V. Todkary, S.Y. Rane and
  S.P. Gejji* [Univ. of Pune]

  The (HNQ)$_n$ (n=1–4) series modeled systems are used to investigate the self-assemblies of
  2-hydroxy-1,4-naphthoquinone (HNQ) using *ab initio* Hartree-Fock calculations. The energetics and
  charge distribution in these molecular systems are presented.

167-177 **Molecular electrostatic potentials and electron densities in azatriprismanes and nitroazatriprismanes**, S.P. Gejji* [Univ. of Pune] and K.A. Joshi

Ab initio Hartree-Fock (HF)-derived molecular electrostatic potentials and molecular electron densities are used to analyze the energy and charge distributions in a series of aza ($C_6N_\alpha H_{6-\alpha}$) and nitroaza ($CNO_2)_{6-\alpha} N_\alpha$, (with $\alpha=1...6$) derivatives of triprismane.

178-182 **Monte Carlo simulation of polarizable systems: Early rejection scheme for improving the performance of adiabatic nuclear and electronic sampling Monte Carlo simulations,** M. Medeiros* [Univ. Nat. Aut. de México]

The new method was employed in Gibbs ensemble Monte Carlo simulations of the polarizable simple point charge-fluctuating charge (SPC-FQ) model of water. The proposed method allows this number to increase, enhancing the chemical potential equalization.

183-186 **Average electron momenta in many-electron atoms**, T. Koga* [Muroran Inst. of Tech.]

The sum and the difference of the two momenta constitute upper and lower bounds to the electron-pair relative momentum and to the electron-pair center-of-mass momentum.

187-190 **On the accuracy of numerical Hartree-Fock energies**, Frank Jensen* [Univ. of Southern Denmark]

The convergence with respect to the computational parameters are systematically investigated. HF energies accurate to at least 1 microHartree are generated for 42 diatomic systems containing first and second row elements, encompassing both cationic, neutral and anionic systems.

191-196 **Self-interaction correction and isotropic hyperfine parameter of light atoms,** D. Guenzburger* [Cent. Brasil. de Pesquisas Físicas], D.E. Ellis and Joice Terra
Numerical SCF calculations in DFT and the local spin-density approximation were performed for the light atoms H, Li, B, C, N, O and F to investigate the effect of the self-interaction correction on the isotropic hyperfine parameter AISO.

Theoretical Chemistry Accounts: Theory, Computation, & Modeling, 113(4), May, 2005

197-204 **New designs for inhibitors of the NF-B: DNA binding**, P.A. Fernandes, E.S. Henriques, V. Pande, M.J. Ramos* [U do Porto], A.R.R. Maia, A.A.S. Almeida, B.F.B. Silva, C.M. S. Ribeiro, C.F.B. Ribeiro, D.S.M. Ribeiro, D.A.P. Fonseca, E.M.S. Cunha, F.R.N.C. Maia, J.A.A. Pereira, J.P.G. Pacheco, J.A.A.D. Ferreira, L.R.C. Matos, M.A.B. P. Pinto, M.C.S. Borges, P.J.C.R. Magalhães, P.F.R.D. Teixeira, P.N.B.C. Veloso, R.J.F. Ferreira, S.S. Gomes, T.F. Barros, T.S.J.T. Selão, and V.M.C. Fernandes.

GOLD was used to calculate the binding mode of PGJ2 and other related inhibitors to NF-B. MM and DFT calculations identified some novel compounds with increased affinity.

205-211 **Geometric and electronic similarities between transition structures for electrocyclizations and sigmatropic hydrogen shifts**, R. Ponec, P. Bultinck* [Ghent U], S. Van Damme, R. Carbó-Dorca and D.J. Tantillo.

Theoretical evidence is provided for the similarity between transition structures for electrocyclizations and sigmatropic hydrogen shifts.

212-214 **Valence basis sets for lanthanide 4f-in-core pseudopotentials adapted for crystal orbital ab initio calculations**, J. Yang* [U Cologne] and M. Dolg.

> Crystal orbital adapted Gaussian (4s4p3d), (5s5p4d) and (6s6p5d) valence primitive basis sets are used to calculate atomic energies of free lanthanide atoms for the evaluation of cohesive energies for A-Ln_2O_3 within both conventional Kohn-Sham DFT and the *a posteriori*-HF correlation DFT schemes.

225-232 **Interpolated potential energy surface for abstraction and exchange reactions of $NH_3 + H$ and deuterated analogues**, G.E. Moyano and M.A. Collins* [Australian Natl U]

> An ab initio interpolated potential energy surface for the hydrogen abstraction and exchange reactions between ammonia and a hydrogen atom is reported.

233-237 **Basis set effects on relative energies and HOMO–LUMO energy gaps of fullerene C_{36},** K. Hoon Kim* [LG Chem. Ltd.], Young-Kyu Han and Jaehoon Jung

> Fifteen C_{36} isomers were examined to determine the influence that the quality of basis sets has on the geometry parameters, the relative stability and HOMO–LUMO energy gaps of fullerene isomers calculated with DFT.

Journal of Chemical Theory & Computation, Volume 1(3) May, 2005

BIOMOLECULAR SYSTEMS
Model Systems
472-478 **Histidine-Aromatic interactions in proteins and protein-ligand complexes: Quantum chemical study of X-ray and model structures,** Emilie Cauët, Marianne Rooman, René Wintjens, Jacques Liévin, and Christophe Biot*[Univ. Libre de Bruxelles]

> The protonated complexes are much more stable than the neutral ones in gas phase. This higher stability is due to the electrostatic contributions, the electron correlation contributions are equally important in the two forms.

Methodology, Solvation Energy
484-493 **Optimized radii for Poisson-Boltzmann calculations with the AMBER force field,** Jessica M. J. Swanson* [Univ. of Cal. at San Diego], Stewart A. Adcock and J. Andrew McCammon.

> The results showed that an increase in accuracy of the molecular solvation energies and atomic forces relative to commonly used continuum parameter sets. These radii are suitable for Poisson-Boltzmann calculations with the AMBER force field and offer energetic congruence to any model that combines molecular mechanics and Poisson-Boltzmann solvation energies.

Enzyme Catalysis
494-505 **Enzymatic hydroxylation in *p*-Hydroxybenzoate hydroxylase: A case study for QM/MM molecular dynamics,** H. Martin Senn, S. Thiel, and W. Thiel* [Max-Planck-Inst. for Kohlenforschung].

> The QM region is treated at the AM1 level, while the MM part is described by the GROMOS force field. The MD simulations provide insight into the dynamics of the hydrogen bonding network in the active site along the course of the reaction.

4.   A D D R E S S E S   O F   P R I N C I P A L   A U T H O R S

The production sites for the corresponding or principal authors are given in brackets in the citations. When not designated by the publisher, the first author is assumed to be the principal. Current addresses are listed here.

Nilesh Banavali
nilesh.banavali@cornell.edu
Dept. of Physiol, Biophys.,
 and Systems Biol.
Weill Medical College
Cornell University
1300 York Avenue
New York, NY 10021, USA

A. Baumgaertner
a.baumgaertner@fz-juelich.de
Inst. for Solid State Research
Forschungszentrum Jülich
Jülich, Germany

Ilan Benjamin
benjamin@chemistry.ucsc.edu
Department of Chemistry
University of California
Santa Cruz, CA 95064, USA

Avinoam Ben-Shaul
abs@fh.huji.ac.il
Dept. of Phys.Chem. &
 Fritz Haber Res.Cent.
The Hebrew Univ.
Jerusalem, 91904, Israel

David L. Beveridge
dbeveridge@wesleyan.edu
Wesleyan University
Hall-Atwater Labs
Middletown, CT 06457-0280, USA

T.N. Bhat
bhat@nist.gov
Biotechnology Div. (831), NIST
100 Bureau Drive, Gaithersburg
MD 20899-8314, USA

Thomas C. Bishop
bishop@tulane.edu
Dept. of Environ. Health Sci.
Tulane Univ. HSC
1430 Tulane Ave. SL-29
New Orleans, LA 70112, USA

Christophe Biot
Service de Chim. générale
Univ. Libre de Bruxelles
CP 206/04, Bld du Triomphe
B-1050 Bruxelles, Belgium

R. A. Böckmann
rainer.boeckmann@bioinf.uni-sb.de
Dept. of Biochemistry
University of Zürich
Winterthurerstrasse 190
CH-8057 Zürich, Switzerland

Alexandre M.J.J. Bonvin
a.m.j.j.bonvin@chem.uu.nl
Bijvoet C. for Biomol. Research
Utrecht University
Utrecht, The Netherlands

Stefano Borini
stef@chim251.unife.it
Dipartimento di Chimica
Università di Ferrara
Via Borsari 46
I-44100 Ferrara, Italy

Alexandre G. de Brevern
debrevern@ebgm.jussieu.fr
Eq. de Bioinf. Génom. et Moléc.
 (EBGM), INSERM U726
Univ. Denis DIDEROT—Paris 7
case 7113, 2, place Jussieu
75251 Paris, France

James M. Briggs
jbriggs@uh.edu
Dept. of Biology and Biochemistry
University of Houston
Houston, TX 77204-5001, USA

Patrick Bultinck
Patrick.Bultinck@UGent.be
Dept. of Inorg. & Phys. Chem.
Ghent Univ.
Krijgslaan 281 (S-3)
B-9000 Gent, Belgium

Amedeo Caflisch
caflisch@bioc.unizh.ch
Department of Biochemistry
University of Zurich
Winterthurerstrasse 190
CH-8057 Zurich, Switzerland

Shin-Ho Chung
shin-ho.chung@anu.edu.au
Department of Theoretical Physics
Res. School of Physical Sciences
Australian National University
Canberra, Australia

Michael A. Collins
collins@rsc.anu.edu.au
Res. Sch. of Chem.
Australian National Univ.
Canberra, ACT, 0200, Australia

Ben Corry
ben@theochem.uwa.edu.auSch. of
Biomed. & Chem. Sci.
The Univ. of W. Austr., Crawley
WA, 6009, Australia

Gordon M. Crippen
gcrippen@umich.edu
College of Pharmacy
University of Michigan
Ann Arbor, MI 48109-1065, USA

Q. Cui
Dept. Of Chemistry
Univ. of Wisconsin
1101 University Ave
Madison, WI 53706, USA

Antoine Danchin
adanchin@pasteur.fr
Genetics of Bacterial Genomes
CNRS/URA2171, Institut Pasteur
28 rue du Docteur Roux
75724 Paris Cedex 15, France

Yong Duan
duan@ucdavis.edu
UC Davis Genome Center
Dept. of Applied Sci.
Univ. of California
One Shields Ave.
Davis, CA 95616, USA

B. J. Edwards
bjedwards@chem.engr.utk.edu
Dept. of Chemical Engineering
University of Tennessee
Knoxville, TN 37996-2200, USA

Dario A. Estrin
dario@qi.fcen.uba.ar
Dept. Quimica Inorg.
Univ. Buenos Aires
Ciudad Univ. – Pab II
C1428EHA, Buenos Aires,
 Argentina

José D. Figueroa-Villar
Dept. de Química
Inst. Militar de Engenharia
Praça General Tibúrcio 80-Urca
22290-270 Rio de Janeiro, Brazil

Stefan Fischer
stefan.fischer
 @iwr.uni-heidelberg.de
IWR-Comp Bio.
Univ. Heidelberg
Im Neuenheimer Feld 368
69120 Heidelberg, Germany

Th. Frauenheim
Theoretische Physik
Univ. Paderborn
Warburger Strasse 100
33098 Paderborn, Germany

Richard A. Friesner
rich@chem.columbia.edu
Dept. of Chem.
Columbia Univ.
3000 Broadway, MC 3110
New York, NY 10025, USA

Patrick F.J. Fuchs
Patrick.Fuchs@ebgm.jussieu.fr
alain.alix@univreims.fr
Eq. de Bioinf. Génom. et Moléc.
 (EBGM), INSERM EMI 0346
Université Paris 7
Case Courrier 7113
2 place Jussieu
75251 Paris Cedex 05, France

Federico Gago
federico.gago@uah.es
Dept. of Pharmacology
Univ. of Alcala, E-28871
Alcala de Henares, Madrid, Spain

Oxana Galzitskaya
ogalzit@vega.protres.ru
Institute of Protein Research
Russian Academy of Sciences
142290, Pushchino,
 Moscow Region, Russia

Angel E. García
axg@lanl.gov
Theo. Biol. and Biophys. Group
T-10 MS K710
Los Alamos National Laboratory
Los Alamos, NM 87545, USA

Humberto González-Díaz
Dept. of Org. Chem.
Facu. of Pharm.
Univ. of Santiago de Compostela
15706, Spain

Philip S. Hammond
phil.hammond@targacept.com
Targacept, Inc.
200 East First Street, Suite 300
Winston-Salem, NC 27101-4165,
 USA

Corwin Hansch
Dept. of Chem.
Pomona Coll.
Claremont, CA 91711, USA

P. Shing Ho
hops@onid.orst.edu
Dept .of Biochem. & Biophys.
Oregon State Univ.
Agri. and Life Sci. Building 2011
Corvallis, OR 97331-7305, USA

Jorng-Tzong Horng
horng@db.csie.ncu.edu.tw
Department of Life Science
National Central University
Chung-Li 320
Taiwan, RO China

Hsien-Da Huang
bryan@mail.nctu.edu.tw
Dept. of Biol. Sc. and Tech.
Institute of Bioinformatics
National Chiao Tung University
Hsin-Chu 300
Taiwan, RO China

Jesús A. Izaguirre
izaguirr@nd.edu
Dept. of Comp. Sci. and Engg.
University of Notre Dame
Notre Dame, IN 46556 USA

Ask F. Jakobsen
MEMPHYS—Center for
  Biomembrane Physics
Physics Department
Univ. of Southern Denmark
Odense, Denmark

Dušanka Janežic
dusa@cmm.ki.si
National Institute of Chemistry
Hajdrihova 19
1000 Ljubljana, Slovenia

Joël Janin
janin@lebs.cnrs-gif.fr
Lab. d'Enzymologie et de
  Biochimie Structurales
CNRS UPR 9063
91198-Gif-sur-Yvette, France.

Harald Janovjak
harald.janovjak@biotec.tu-dresden.de
BioTechnological Center
University of Technology
01307 Dresden, Germany

Martin Karplus
marci@tammy.harvard.edu
Lab. Chimie Biophysique, ISIS
Univ. Louis Pasteur
4 rue Blaise Pascal
67000 Strasbourg, France
 and
Dept. of Chem. and Chem. Biol.
Harvard Univ.
Cambridge, MA 02138, USA

Tatsuyuki Kawakubo
Facu. of Engg.
Toin Univ. of Yokohama
Aoba-ku
Yokohama 225-8502, Japan

Kyoung Hoon Kim
ykhan@lgchem.com
Comp. Chem. Laboratory
Corporate R & D, LG Chem, Ltd.
Res. Park, Daejon, 305-380, Korea

Gerhard Klebe
klebe@ mailer.uni-marburg.de
Philipps Univ.
Marbacher Weg 6
35037 Marburg, Germany

Michael L. Klein
klein@lrsm.upenn.edu;
Center for Molecular Modeling
 and Department of Chemistry
University of Pennsylvania
Philadelphia, PA, USA

Ernst-Walter Knapp
knapp@chemie.fu-berlin.de
Dept. of Bio., Chem., and Pharm.
Inst. of Chemistry
Freie Univ. Berlin
Takustrasse 6
14195 Berlin, Germany

David A. Kofke
kofke@buffalo.edu
Dept. of Chemical and Biol. Engg.
University at Buffalo
The State University of New York
Buffalo, NY 14260-4200, USA

Laura Korhonen
Laura.Korhonen@uku.fi
University of Kuopio
POB 1627
70211 Kuopio, Finland

Daniel J. Lacks
daniel.lacks@case.edu
Dept. of Chemical Engineering
Case Western Reserve Univ.
Cleveland, OH, USA

Neocles B. Leontis
leontis@bgnet.bgsu.edu
Chemistry Dept. and
 Center for Biomol. Sci.
Bowling Green State Univ.
Bowling Green, OH 43403, USA

Jie Liang
jliang@uic.edu
Dept. of Bioeng., SEO, MC-063
University of Illinois at Chicago
851 S. Morgan Street, Room 218
Chicago, IL 60607-7052, USA

Klaus R. Liedl
Klaus.liedl@uibk.ac.at
Inst. of General, Inorganic, and
Theoretical Chemistry
Univ. Innsbruck
Innrain 52a
A-6020 Innsbruck, Austria

Thy-Hou Lin
thlin@life.nthu.edu.tw
Inst. Mol. Med.
Dept. of Life Science
Natl. Tsing Hua Univ.
Hsinchi 30013, Taiwan

Xiang Yang Liu
phyliuxy@nus.edu.sg
Department of Physics
Faculty of Science
National Univ. of Singapore
2 Science Drive 3
Singapore 117542, Singapore

Maria Grazia Mamolo
Dept. of Pharm. Sciences
Piazzale Europa 1
Univ. of Trieste
34127 Trieste, Italy

Neelan J. Marianayagam
neelanm@yahoo.com
Dept. of Chem.
Univ. of Cambridge
Cambridge CB2 1EW, U. K.

Claudio Margulis
Dept. of Chem.
319 CB
Univ. of Iowa
Iowa City, IA 52242, USA

Alan E. Mark
Dept. of Biophys. Chem.
Univ. of Groningen
Nijenborgh 4, 9747 AG
Groningen, The Netherlands

Kimmo Mattila
kimmo.mattila@csc.fi
CSC–Scientific Computing Ltd.
P.O. Box 405
FIN-02101 Espoo, Finland

Adrien Melquiond
Lab. de Biochimie Théorique
UPR 9080 CNRS
Inst. de Biol. Physico-Chimie
 et Université Paris 7
13 rue Pierre et Marie Curie
75005 Paris, France

Gaetano T. Montelione
guy@cabm.rutgers.edu
CABM–Rutgers University
679 Hoes Lane
Piscataway, NJ 08854, USA

Dr. Emanuele Paci
paci@bioc.unizh.ch
University of Zurich
Dept. of Biochemistry
Winterthurestrasse 190
Zurich, 8057, Switzerland

Géraldine Pascal
gpascal@genoscope.cns.fr
Genoscope/UMR 8030
Atelier de Genomique Comparative
2 rue Gaston Cremieux
91006 Evry Cedex, France

Nina Pastor
nina@servm.fc.uaem.mx
Facultad de Ciencias
Univ. Autó. del Estado de Morelos
Av. Universidad 1001
Col. Chamilpa
62210 Cuernavaca, Morelos,
 México

M. Germana Paterlini
germana@certusoft.com
Certusoft, Inc.
7900 W. 78th St., Suite 165
Minneapolis, MN 55439, USA

Stefano Piana
piana@power.curtin.edu.au
Department of Applied Chemistry
Curtin University of Technology
GPO Box U1987
Perth, WA 6845, Australia

Maria. J. Ramos
mjramos@fu.up.pt
REQUIMTE/Dept. de Química
Facu. de Ciências
Univ. do Porto
Rua do Campo Alegre, 687
4169-007 Porto, Portugal

Chaya S. Rapp
rappc@yu.edu
Stern College for Women
Yeshiva University
245 Lexington Avenue
New York, NY 10016, USA

Mauro C. C. Ribeiro
mccribei@quim.iq.usp.br
Lab. de Espectroscopia Molecular
Instituto de Química
Universidade de São Paulo
Caixa Postal 26077
CEP 05513-970
São Paulo, São Paulo, Brazil

Jeffrey Roach
roachjm@email.unc.edu
Dept. of Biochem. and Biophys.
University of North Carolina
Chapel Hill, NC 27599, USA

Adrian E. Roitberg
roitberg@qtp.ufl.edu
QTP and Dept. of Chem.
Univ. Florida
Gainesville, FL 32611, USA

Burkhard Rost
rost@columbia.edu
Dept. Molec. Biophysics
Columbia Univ.
650 W. 168th St. BB217
New York, NY 10032, USA

Benoît Roux
benoit.roux@med.cornell.edu.
Dept. of Physiol. and Biophys.
Weill Med. Coll. of Cornell Univ.
1300 York Avenue
New York, NY 10021, USA

Mark S. P. Sansom
mark.sansom@biop.ox.ac.uk
Department of Biochemistry
University of Oxford
Oxford OX1 3QU, UK

Alexander Schug
schug@int.fzk.de
Institute for Nanotechnology
Forschungszentrum Karlsruhe
P.O. Box 3640
76021 Karlsruhe, Germany

Hans Martin Senn
Max-Planck-Inst. für
Kohlenforschung
D-45470 Mülheim an der Ruhr,
 Germany

Brian Shoichet
shoichet@cgl.ucsf.edu
Graduate Group in Biophysics
Univ. of California San Francisco
1700 4th St.
San Francisco, CA 94143, USA

Jeremy C. Smith
IWR-Comp Mol. Biophys.
Univ. Heidelberg
Im Neuenheimer Feld 368
69120 Heidelberg, Germany

Jirí Ŝponer
sponer@ncbr.chemi.muni.cz
Institute of Biophysics
Acad. of Sci. of the Czech Rep.
Kralovopolska 135
61265 Brno, Czech Republic

Charlie E. M. Strauss
cems@lanl.gov
Los Alamos National Laboratory
Los Alamos, NM 87545, USA

Yuji Sugita
sugita@iam.u-tokyo.ac.jp
Inst. of Mol. and Cell. Biosci.
University of Tokyo
Yayoi, Bunkyo-ku
Tokyo 113-0032, Japan

Jessica M. J. Swanson
Howard Hughes Med. Inst.
Cent. for Theor. Biol. Phys.
Depts. of Chem. and Biochem.,
 and of Pharmacology
Univ. of Cali. at San Diego
La Jolla, CA 92093-0365, USA

Annabel Todd
annabel.todd@deshaw.com
Dept. Biochem. and Mol. Biol.
Univ. College London
Gower Street
London, WC1E 6BT, UK

Joseph W. Toporowski
Dept. of Chem. & Biochem.
Univ. of Calif.
Santa Barbara, CA 93106, USA

Mark E. Tuckerman
mark.tuckerman@nyu.edu
Dept. of Struct. Biol.
Stanford Univ.
Stanford, CA 93405, USA

W.F. van Gunsteren
wfvgn@igc.phys.chem.ethz.ch
Lab. of Phys. Chem.
Swiss Federal Inst. of Tech.
Eidgenössische Tech.
 Hochschule-Hönggerberg
CH-8093 Zurich, Switzerland

Ilpo Vattulainen
ilpo.vattulainen@csc.fi
Laboratory of Physics
 and Helsinki Institute of Physics
Helsinki University of Technology
Helsinki, Finland

Gregory A. Voth
voth@chem.utah.edu
Dept. of Chemistry
University of Utah
315 S. 1400 E., Rm. 2020
Salt Lake City, UT 84112-0850, USA

Michael E. Wall
mewall@lanl.gov
Comp. and Comput'l Sci. Div.
Los Alamos National Laboratory
Mail Stop B256
Los Alamos, NM, 87545, USA

Wei Wang
wangwei@nju.edu.cn
Natl. Solid State Microstruct. Lab.
Institute of Biophysics
 and Department of Physics
Nanjing University
Nanjing 210093, PR China

William J. Welsh
welshwj@umdnj.edu
Univ. of Medicine and Dentistry
 of New Jersey
675 Hoes Lane
Piscataway, NJ 08554, USA

Di Wu
Dept. of Chem. and Biol. Engg.
University at Buffalo
The State University of New York
Buffalo, NY 14260-4200, USA

Yi Xiao
yxiao@mail.hust.edu.cn
Biomol. Physics and Mdlng. Group
Department of Physics
Huazhong Univ. of Sci. and Tech.
Wuhan 430074, Hubei, China

J. Yang
jyang0@uni-koeln.de
Inst. of Theor.Chem.
Univ. of Cologne
Greinstr. 4
D-50939 Cologne, Germany

Darrin M. York
york@chem.umn.edu
Dept. of Chem.
Univ. of Minnesota
Minneapolis, MN 55455, USA

F. Marty Ytreberg
fmy1@pitt.edu
Dept. of Comp. Bio.
Grad. School of Public Health
Univ. Pittsburgh
200 Lothrop St.
Pittsburgh, PA 15261, USA

Wenjun Zheng
zhengwj@helix.nih.gov
Laboratory of Comp. Biology
Natl. Heart, Lung, and Blood Inst.
National Institutes of Health
Bethesda, MD 20892, USA

Gerhard Zifferer
gerhard.zifferer@univie.ac.at
Institut für Physikalische Chemie
 der Universität Wien
Währinger Straße 42
A-1090 Wien, Austria

Huan-Xiang Zhou
zhou@sb.fsu.edu
Dept. of Physics
Florida State Univ.
Tallahassee, FL 32306, USA

5. DISCLAIMER, COPYRIGHT, AND PUBLISHER INFORMATION