MMCC Results

MOLECULAR MODELING & COMPUTATIONAL CHEMISTRY

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About 108 papers from 14 journals are cited.

Editorial and News

Two very significant advances are reported in the **Molecular Dynamics** and **Free Energy Methods** sections of the **Methodology** section this issue. In the first, Christen and van Gunsteren analyse the structural and energetic consequences of flexibly constraining bond lengths. Energy fluctuations are much greater than with Shake, which gives an inflexible bond length constraint, and are similar to those seen with unconstrained simulations, but at no greater compute time cost than Shake. Simulations of neopentane are stable (for 20 ps) with time steps of up to 19 fs, whereas with Shake, system energy diverges with time steps of >14 fs. Using a thermostat, the kinetic energy can be held constant, but partitioning and transfer between modes is not accurate and pressure can be affected. However, energy fluctuations are similar to the level seen with unconstrained simulations (rather than much lower as with Shake).

Shirts and Pande analyze the variance and bias for free energy perturbation methods. The two standard free energy methods, TI and exponential averaging (which takes advantage of the Jarzynski result to accommodate the non-equilibrium nature of perturbations), are compared to the theoretically preferable but overlooked Bennet acceptance ratio method. It turns out that using WHAM in FEP (i.e. with a mutated molecule *in situ*) reduces to the Bennett acceptance ratio method. This latter method turns out to give less variance and bias for FEP than TI or the exponential averaging methods in a complete atomistic simulation (although each of the other two might be preferable for some "toy" examples).

David D. Busath, Editor

1. APPLICATIONS

1.1. *Small Molecules*

General and Model Systems

Molecular dynamics studies of melting and some liquid-state properties of 1-ethyl-3-methylimidazolium hexafluorophosphate [emim][PF_6].

S. Alavi* [U Missouri] and D.L. Thompson

J. Chem. Phys. **122,** 15470401-15470412 (2005)

MD simulations of 1-ethyl-3-methylimidazolium hexafluorosphosphate in the crystal state. The melting point is 375 K, which compares to the experimental value of 333 K.

Water and Solvation

Structure-breaking effects of solvated Rb(I) in dilute aqueous solution - An *ab initio* QM/MM MD approach.

I. Horenko* [Freie U Berlin], S. Lorenz, C. Schütte, and W. Huisinga

J. Comput. Chem. **26,** 949-956 (2005)

Inner shell water occupancy time is 2.0 ps according to this thorough analysis of water structure using QM/MM.

A linear-scaling self-consistent generalization of the multistate empirical valence bond method for multiple excess protons in aqueous systems.

F. Wang and G.A. Voth* [U Utah]

J. Chem. Phys. **122**, 14410501-14410509 (2005)

With the introduction of a generalization of EVB to allow simulations of multiple protons in MD, it is now possible to study HCl solution. 0.44 M HCl showed considerable hydronium^{+} – Cl^{-} pairing with a concomitant reduction in the Eigen complex ($H_9O_4^{+}$) density in favor of smaller complexes.

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Water and Solvation (cont'd)

Temperature dependence of quantum effects in liquid water.

L. Hernandez de la Pena, and P. G. Kusalik

J. Amer. Chem. Soc. **127**, 5246-5251 (2005)

Classical and quantum rigid-body centroid dynamics of liquid water at tempereatures ranging from 100 to -35° C "explore the interplay between structure and dynamics in the context of effective tunneling". To get the correct dynamical behavior, quantum effects are essential.

Molecular origin of anticooperativity in hydrophobic association.

C. Czaplewski, A. Liwo, D. R. Ripoll, and H. A. Scheraga* [Cornell U]

J. Phys. Chem. B **109**, 8108-8119 (2005)

The PMFs of methane dimer and trimer formation are calculated to give insight into the hydrophobic effect. The simulations suggest cooperativity and suggest problems with the information theory model of hydrophobic association with respect to trimers.

Structure and vibrational spectroscopy of salt water/air interfaces: Predictions from classical molecular dynamics simulations.

E. C. Brown, M. Mucha, P. Jungwirth, and D. J. Tobias* [UCI]

J. Phys. Chem. B **109**, 7934-7940 (2005)

Sum frequency generation spectra for NaI interfaces are estimated from MD simulation and shown to qualitatively agree with experiment. Changes in spectra intensity are related to ordering of subsurface water molecules.

Molecular dynamics study of hydration in ethanol-water mixtures using a polarizable force field.

S. Y. Noskov, G. Lamoureux, and B. Roux* [Weill Med Col]

J. Phys. Chem. B **109**, 6705-6713 (2005)

A drude oscillator model is applied to water/ethanol mixtures.

Medicinal Chemistry and Drug Design

A pharmacophore hypothesis for P-glycoprotein substrate recognition using GRIND-based 3D-QSAR.

G. Cianchetta, R.W. Singleton, M. Zhang, M. Wildgoose, D. Giesing, A. Fravolini, G. Cruciani, and R.J. Vaz* [Sanofi-Aventis]

J. Med. Chem. **48**, 2927-2935 (2005)

New experimental data on PGP transport inhibition by both public and proprietary small molecules is used to build a 3D-QSAR model using Volsurf and Almond descriptors and GRID fields. The strong predictability (q^2=0.75) of pharmacophore features suggests that PGP binding, and not diffusion across the membrane, is the key step in PGP inhibition.

T

Computational identification of proteins for selectivity assays.

S. Yoon, A. Smellie, D. Hartsough, and A. Filikov* [ArQule]

Proteins **59***,* 434-443 (2005)

A representative panel of proteins for selectivity assays is selected based on comparison of a set of high-ranked docked substrates. The method is tuned on CDK2-homologous kinases, and applied to estradiol-, tamoxifen- and riboflavin-binding proteins, and shown to be able to recover known, as well as homologous and non-homologous proteins.

Medicinal Chemistry and Drug Design (cont'd)

T

LEA3D: A computer-aided ligand design for structure-based drug design.

D. Douguet* [CNRS], H. Munier-Lehmann, G. Labesse, and S. Pochet

J. Med. Chem. **48**, 2457-2468 (2005)

LEA3D is a new structure-based program for generating denovo ligands by combining docked fragments of ligands from the Comprehensive Medicinal Chemistry and KEGG LIGAND databases. The approach is used to find >12uM inhibitors of thymidine monophosphate kinase.

T

Drugability indices for protein targets derived from NMR-based screening data.

P.J. Hajduk* [Abbott], J.R. Huth, and S.W. Fesik

J. Med. Chem. **48**, 2518-2525 (2005)

A regression-based model based on computationally-calculated protein surface parameters predicts NMR screening hit rates with a r^2 of 0.72 and a q^2 of 0.56.

A theoretical study on the activation of Ser70 in the acylation mechanism of cephalosporin antibiotics.

Y.-Y. Ke and T.-H. Lin* [Natl Tsing Hua U]

J. Biophys. Chem. **114**, 103-113 (2005)

Insight II and Grid20 is used to determine the most favored activation process for Ser70 in the acylation mechanism for the cephalosporin antibiotics. The B3LYP/6−31+G level and the Polarized Continuum Model is used and water is treated as a solvent for each activation process. The most favorable activation process for Ser70 in the acylation mechanism involves a proton transfer mediated by the catalytic water and the catalytic residues Glu166 and Ser70.

Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: A promising approach for modeling of antibacterial activity.

Y.M. -Ponce* [Cent U Las Villas], R.M. Marrero, F. Torrens, Y. Martinez, V.R. Zaldivar and E.A. Castro

Bioorg. Med. Chem. **13**, 2881-2899 (2005)

The TOpological MOlecular COMputer Design approach is used and a complete data set containing 1006 antimicrobial agents is collected. Two structure-based antibacterial activity classification models are generated. This approach is more satisfactorily compares with respect to nine of the most useful models for antimicrobial selection reported earlier.

Investigations of linker structure on the potency of a series of bidentate protein tyrosine phosphatase inhibitors.

J. Xie and C.T. Seto* [Brown U.]

Bioorg. Med. Chem. **13**, 2981-2991 (2005)

Protein tyrosine phosphatases such as PTP1B and the *Yersinia* PTPase play an important role in diseases including type II diabetes and bubonic plague. The correlation between linker structure and inhibitor activity showed that aromatic groups in the linker played an important role in determining binding affinity in this class of inhibitors.

In silico ADME modelling: prediction models for blood–brain barrier permeation using a systematic variable selection method.

R. Narayanan* [TCS] and B.G. Sitarama

Bioorg. Med. Chem. **13**, 3017-3028 (2005)

The Variable Selection and Modeling method based on the prediction (VSMP) is proposed to develop QSPR models based on in vivo blood-brain permeation data (logBB) of 88 diverse compounds, 324 descriptors. The three-descriptor model is the best one based on Atomic type E-state index, AlogP98 and Van der Waal's surface area. The success rate of these models is 82% in the case of BBB+ compounds and a similar success rate is observed with BBB− compounds.

Synthesis and biological evaluation of novel 6-nitro-5-substituted aminoquinolines as local anesthetic and anti-arrhythmic agents: molecular modeling study.

F.E. Goda* [U Mansoura], A.A.M. Abdel-Aziz and H.A. Ghoneim

Bioorg. Med. Chem. **13**, 3175-3183 (2005)

The AM1 method is used to study the local anesthetic and anti-arrhythmic activity of lidocaine and the active compounds. HyperChem program is used to study the superposition of the stable conformations of these compounds.

Molecular basis of the low activity of antitumor anthracenediones, mitoxantrone and ametantrone, in oxygen radical generation catalyzed by NADH dehydrogenase: Enzymatic and molecular modelling studies.

J. Tarasiuk* [Gdansk U. of Tech.], J. Mazerski, K.T. -Gobis and E. Borowski

Eur. J. Med. Chem. 40, 321-328 (2004)

The distribution of the molecular electrostatic potential, around the quinone system is important for the ability of anthracenediones to stimulate reactive oxygen species formation in NADH dehydrogenase system. The clouds of positive molecular electrostatic potential (MEP) cover the quinone carbon atoms for non-stimulating anthracenediones, while for agents effective in stimulating reactive oxygen species formation the clouds of negative (MEP) cover continuously the aromatic core together with the quinone system.

Quantitative Structure-Activity Relations

3D-QSAR CoMFA studies on trypsin-like serine protease inhibitors: A comparative selectivity analysis.

B.A. Bhongade, V.V. Gouripur and A.K. Gadad* [J. N. Med.Coll.]

Bioorg. Med. Chem. **13**, 2773-2782 (2005)

CoMFA models are generated using steric and electrostatic fields for tPA, fXa, thrombin, plasmin, and trypsin inhibition. These models exhibited better statistical significance than the CoMFA models generated using ClogP as an additional descriptor. These models were used to generate 3D contour maps, provided possible modification of molecules for better selectivity/activity of serine protease inhibitors of therapeutic interest.

QSAR by LFER model of cytotoxicity data of anti-HIV 5-phenyl-1-phenylamino-1*H*-imidazole derivatives using principal component factor analysis and genetic function approximation.

Kunal Roy* [Jadavpur U.] and J.T. Leonard

Bioorg. Med. Chem. **13**, 2967-2973 (2005)

Linear free energy related model of Hansch using electronic, hydrophobicity and steric parameters of phenyl ring substituents of the compounds are used in QSAR study. The coefficients of molar refractivity and steric parameters for meta substituents of the phenyl ring of 1-phenylamino fragment indicated that the length, width and overall size of meta substituents are conducive factors for the cytotoxicity.

Topological models for prediction of anti-HIV activity of acylthiocarbamates.

S. Bajaj, S.S. Sambi and A.K. Madan* [MD Univ.]

Bioorg. Med. Chem. **13**, 3263-3268 (2005)

Relationship of anti-HIV activity of acylthiocarbamates with distance based *Wiener's index*, adjacency based *first-order molecular connectivity index* and distance-cum-adjacency based *augmented eccentric connectivity index* was investigated. The values of all the three indices for each of the 61 compounds involved in the dataset were calculated using an in-house computer program. The results showed high accuracy of prediction was observed with these topological models.

Quantitative Structure-Activity Relations (cont'd)

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Quantitative structure-activity relationship to predict differential inhibition of aldose reductase by flavonoid compounds.

M. Fernández, J. Caballero, A.M. Helguera, E.A. Castro and M.P. González* [Cent. U. of Las Villas]

Bioorg. Med. Chem. **13**, 3269-3277 (2005)

Galvez indices showed the relationship between the inhibitor structures and its activity by describing the molecular topology and charge transfer through the molecule. Artificial neural networks were trained using charge indices from the linear models but the obtaining networks overfitted the data having low predictive power.

A structure-activity relationship study of quinone compounds with trypanocidal activity.

F.A. Molfetta, A.T. Bruni, K.M. Honório and A.B.F. da Silva* [Univ. de Sao Paulo]

Eur. J. Med. Chem. **40**, 329-338 (2004)

A DFT method is used to study the anti-trypanocidal activity to calculate atomic and molecular properties correlated with the biological activity. Torsion angle (T_5), sum of absolute values of the atomic charges (QTS1), volume of the substituent at region B (VOLS2) and energy of the molecular orbital below HOMO (HOMO-1) descriptors were responsible for the separation between the active and inactive compounds.

Connecting traditional QSAR and molecular simulations of papain hydrolysis-importance of charge transfer.

Z. Lepp and H. Chuman* [U Tokushima Shomachi]

Bioorg. Med. Chem. **13**, 3093-3105 (2005)

MD and semi-empirical QM calculations are used to investigate the structure-activity relationship for the papain hydrolysis of a series of *N*-benzoylglycine esters. The results are useful to understand how QSAR descriptors, like F or σ, interacts with other electronic effects during complex formation.

Carbon Nanoparticles

Molecular modeling of freezing of simple fluids confined within carbon nanotubes.

F.R. Hung* [N Carolina State U], B. Coasne, E.E. Santiso, K.E. Gubbins, F.R. Siperstein,and M. Sliwinska-Bartkowiak

J. Chem. Phys. **122,** 14470601- 14470614 (2005)

Carbon tetrachloride exhibits numerous ice phases in confinement, consistent with dielectric relaxation spectroscopy measurements.

1.2. *Biopolymers*

Bioinformatics

Identification and distribution of protein families in 120 completed genomes using Gene3D.

D. Lee* [U Coll London], A. Grant, R.L. Marsden, and C. Orengo

Proteins **59***,* 603-615 (2005)

A large scale, semi-automated protein family and domain clustering from all available complete genomes is presented, and comparisons with CATH and Pfam classifications are made. All classifications obey a power-law, but with different exponents, and steeper for domains than proteins, indicative of evolutionary domain-shuffling mechanisms.

Bioinformatics (cont'd)

Linking tumor cell cytotoxicity to mechanism of drug action: An integrated analysis of gene expression, small-molecule screening and structural databases.

D.G. Covell* [NCI], A. Wallqvist, R. Huang, N. Thanki, A.A. Rabow, and X.J. Lu

Proteins **59***,* 403-433 (2005)

A large-scale, thorough statistical analysis of genomic, chemical and cytotoxicity information from three respective databases, and combination with available structural data, is presented. Insights in mechanism of action, described in thirteen conserved compound classes are gained.

Assembly factors of F_1F_O-ATP synthase across genomes.

A. Pícková, M. Potocký, and J. Houštěk* [Acad Sci Czech]

Proteins **59***,* 393-402 (2005)

A detailed phylogenetic analysis ATP synthase subunits in 39 eukaryotic genomes shows the F_1 part to be relatively highly conserved, while the F_o part shows more variability in composition as well as apparent assembly.

Protein Structure Prediction

Addressing the intrinsic disorder bottleneck in structural proteomics.

C.J. Oldfield, E.L. Ulrich, Y. Cheng, A.K. Dunker, and J.L. Markley* [U Wisconsin]

Proteins **59***,* 444-453 (2005)

The effectiveness several screening methods in use to avoid spending time on structure determination of disordered proteins, is evaluated and compared to disorder determination by NMR for 13 proteins. Implications for the protein structure initiative are discussed at length.

A new method to determine the structure of the metal environment in metalloproteins: Investigation of the prion protein octapeptide repeat Cu^{2+} complex.

M. Mentler, A. Weiss, K. Grantner, P. del Pino, D. Deluca, S. Fiori, C. Renner, W.M. Klaucke, L. Moroder, U. Bertsch, H.A. Kretzschmar, P. Tavan and F.G. Parak* [Tech U München]

Europ. Biophys. J. **34,** 97-112 (2005)

A new method is proposed, which combines computations with spectroscopic data. Computations are used to select sterically possible structures with correct H and N positions from ENDOR and ESEEM measurements. The structure of this octarepeat complex is similar to a pentapeptide complex determined by X-ray structure. The tryptophan residue has a different orientation: the axial water is on the other side of the Cu.

Solvent accessibility in native and isolated domain environments: General features and implications to interface predictability.

M.F. Raih, S. Ahmad* [Kyushu Inst Tech], R. Zheng and R. Mohamed

J. Biophys. Chem. **114**, 63-69 (2005)

Non-redundant databases of 4536 structural domains are used for the calculation of their solvent accessibility in the native protein environment. The interfacings of these amino acid residues are calculated and their variation for different secondary structure types is analyzed. The results have significant implications towards determining interacting residues in proteins and for the prediction of protein-protein, protein-ligand, protein-DNA and similar interactions.

Protein Structure Prediction (cont'd)

Understanding the structural characteristics of compstatin by conformational space annealing.

M.K. Song, S.–Y. Kim and J. Lee*
[Korea Inst for Adv Study]

J. Biophys. Chem. **115**, 201-207 (2005)

The conformational space annealing (CSA) method with CHARMM force field and the GBSA continuum solvent model is used to investigate the structural characteristics of the 13-residue compstatin molecule. It was found that most of the conformations (94.4%) are in the coil state and other conformers containing a 3_{10}-helix, a π-helix, a β-hairpin, and an α-helix.

Protein structure prediction based on fragment assembly and parameter optimization.

J. Lee, S.–Y. Kim and J. Lee* [Korea Inst for Adv Study]

J. Biophys. Chem. **115**, 209-214 (2005)

A novel method is proposed for ab-initio prediction of protein tertiary structures based on fragment assembly and global optimization. The secondary structure prediction method, PREDICT, is used to construct fifteen residue long fragment libraries and fragments in these libraries are assembled to generate full-length chains of a query protein. The linear parameters of the energy function are optimized and the native-like conformations become energetically more favorable than the non-native ones for proteins with known structures.

Protein linear indices of the 'macromolecular pseudograph α-carbon atom adjacency matrix' in bioinformatics. Part 1: Prediction of protein stability effects of a complete set of alanine substitutions in Arc repressor.

Y.M. -Ponce* [Cent. U. of Las Villas], R.M. -Marrero*, J.A.C. Garit, V.R. Zaldivar, F. Torrens and E.A. Castro

Bioorg. Med. Chem. **13**, 3003-3015 (2005)

The TOMOCOMD-CAMPS method produced a linear regression between protein backbone descriptors and melting temperature values for alanine mutants of the Arc repressor. The linear discriminant analysis is used to predict the stability of the mutant Arc homodimers. These models permitted the interpretation of the driving forces of such folding process, indicating that topologic/ topographic protein backbone interactions control the stability profile of wild-type Arc and its alanine mutants.

Comparative or Homology Modeling

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.

J.Mol.Graph.Mod. **23**, 409-418 (2005)

A homology model of the active site region of tripeptidyl peptidase II was constructed. The structure-activity relationships observed for the prepared TPP II inhibitors are correlated with the structural details of the TPP II active site model. This model is validated and useful for structure-based drug design and pharmacophore searching experiments.

Peptide Conformational Analysis

Molecular dynamics simulation of the aggregation of the core-recognition motif of the islet amyloid polypeptide in explicit water.

G. Colombo* [CNR], I. Daidone, E. Gazit, A. Amadei, and A. Di Nola

Proteins **59***,* 519-527 (2005)

Conformational clustering and detailed structural analysis reveal the initial stages of self-assembly of an amyloid-forming peptide, going from random, isolated peptides to a proto-fibril.

Peptide Conformational Analysis (cont'd)

Thermodynamic and kinetic characterization of a beta-hairpin peptide in solution: An extended phase space sampling by molecular dynamics simulations in explicit water.

I. Daidone, A. Amadei* [U Roma], and A. Di Nola

Proteins **59***,* 510-518 (2005)

Thorough statistical-mechanical analysis of over 1μsec of simulations with several folding-unfolding events, show a ~200ns β-hairpin folding time, and a distinct funnel-type free energy landscape in essential space.

Monte Carlo studies of folding, dynamics, and stability in α–helices.

D.Shental-Bechor, S. Kirca, N. Ben-Tal, and T. Haliloglu* [Bogazici U]

Biophys. J. **88,** 2391-2402 (2005)

Polyalanine, (but not polyglycine), folds into a helix when represented as a chain of interaction site pairs, one for Cα and one for Cβ. Fewer intermediate states are observed in the path to helix at lower temperatures.

Molecular dynamics simulations indicate a possible role of parallel β-helices in seeded aggregation of poly-Gln.

M. Stork, A. Giese, H.A. Kretzschmar, and P. Tavan* [LMU]

Biophys. J. **88,** 2442-2451 (2005)

Simulations in explicit water show that triangular (but not circular) β-helices with 18 residues per turn of at least 3 turns are stable, and may be a plausible nucleus for aggregation.

Exploring the helix-coil transition via all-atom equilibrium ensemble simulations.

E.J. Sorin and V.S. Pande* [Standford U]

Biophys. J. **88,** 2472-2493 (2005)

Based on distributed processing, the folding of two 21-residue helix-forming peptides from time domains orders of magnitude greater than the folding process shows that the landscapes is for denatured and folded states are flat and that folding involves conformational diffusion more than an exponential process. AMBER-99 was tuned to match experimental data.

Protein Structure Analysis

The pairwise energy content estimated from amino acid composition discriminates between folded and intrinsically unstructured proteins.

Z. Dosztányi, V. Csizmók, P. Tompa, and I. Simon* [Hungarian Academy Sci]

J. Mol. Biol. **347**, 827-839 (2005)

The "pair-wise energy content" of disordered proteins is less favorable than structured proteins, and thus can be used to predict disordered proteins based solely on sequence. The pair-wise energy content is calculated using residue-pair statistical potential matrices derived from PDB structures.

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 Med Sci]

J. Mol. Graph. Mod. **23**, 389-394 (2005)

3D-structures of hPer1-PTD and its mutant analogs were simulated by the Rosetta method to investigate physico-chemical properties. The electrostatic potentials and energies of these structures were calculated using the Delphi algorithm. Arg836 is the key residue for peptide internalization and if this Arg is mutated into Ala, the peptide cannot cross the membrane.

A

Protein Folding

Multiple folding mechanisms of protein ubiquitin.

J. Zhang, M. Qin, and W. Wang* [Nanjing U]

Proteins **59***,* 565-579 (2005)

Go-type (C_α) MD simulations of the folding of ubiquitin, show glass-state kinetic traps at low temperatures, distinct from 'real' intermediate states found at higher temperatures. Folding events and differences at different temperatures are analysed in detail.

Native geometry and the dynamics of protein folding.

P.F.N. Faisca* [CFTC] and M.M. Telo da Gama

J. Biophys. Chem. **115**, 169-175 (2005)

The role of native geometry on the kinetics of protein folding is investigated based on simple lattice models and MC simulations. The Miyazawa-Jernigan approach indicates the existence of two dynamical folding regimes depending on the protein chain length. The folding performance is sensitive, for chains larger than 80 amino acids, to the native state's conformation.

Heat capacity effects in protein folding and ligand binding: A re-evaluation of the role of water in biomolecular thermodynamics.

A. Cooper* [Glasgow U]

J. Biophys. Chem. **115**, 89-97 (2005)

The contribution of the heat capacity changes is evaluated for cooperative biomolecular folding and binding processes. Based on the hydrogen-bonding propensity of water as a function of temperature, quantitative estimates of ΔC_p compare well with experimental observations for both protein folding and ligand binding. Significant ΔC_p effects are expected for any macromolecular process involving a multiplicity of cooperative weak interactions.

Protein Dynamics

Analysis of correlated domain motions in IgG light chain reveals possible mechanisms of immunological signal transduction.

M. Król* [Cancer Research UK], I. Roterman, B. Piekarska, L. Konieczny, J. Rybarska, B. Stopa, and P. Spólnik

Proteins **59***,* 545-554 (2005)

Large structural changes in the V domain, decreased stability and loss of domain motional correlation are seen in 1-ns MD simulations at three temperatures of free and congo-red bound IgG. Implications for IgG function are discussed.

Ligand Binding

Hierarchical database screenings for HIV-1 reverse transcriptase using a pharmacophore model, rigid docking, solvation docking, and MM-PB/SA.

J. Wang* [Encysive Inc] , X. Kang, I.D. Kuntz, and P.A. Kollman

J. Med. Chem. **48**, 2432-2444 (2005)

A retrospective analysis using the hierarchical ligand screening approach described in the title finds that 16 of the 37 known non-nucleoside reverse transcriptase inhibitors used survive all the filters.

Ligand Binding (cont'd)

Quantum study of mutational effect in binding of efavirenz to HIV-1 RT.

Y. Mei, X. He, Y. Xiang, D.W. Zhang, and J.Z. Zhang* [NY U]

Proteins **59***,* 489-495 (2005)

Ab-initio calculations using the 'molecular fractionation with conjugate caps' (MFCC) approximation of the HIV-1 RT-inhibitor complex and mutants, reveals key interacting residues and furthers understangding of viral resitance traits.

A

***LigScore:* a novel scoring function for predicting binding affinities**.

A. Krammer* [Accelrys Inc], P.D. Kirchhoff, X. Jiang, C.M. Venkatachalam and M. Waldman

J. Mol. Graph. Mod. **23**, 395-407 (2005)

Two new empirical *LigScore* functions, *LigScore1* and *LigScore2* are introduced, which describe the van der Waals interaction, the polar attraction between the ligand and protein, and the desolvation penalty attributed to the binding of the polar ligand atoms to the protein and vice versa. LigScore2 has good predictability with r^2 of 0.75 and 1.04 of S.D over the training data set, consists of a diverse set of proteins that span more than seven protein families.

Modeling kinase-substrate specificity: implication of the distance between substrate nucleophilic oxygen and attacked phosphorus of ATP analog on binding affinity.

M. Sun* [Tsinghua U], X.-H. Liu, S.-H. Ji and Y.-F. Zhao

J. Mol. Graph. Mod. **23**, 433-438 (2005)

MD simulations are used to establish a relationshipbetween structural features and binding ability of the kinase-substrate complexes. It was found that the distance between substrate nucleophilic oxygen (OG) and attacked phosphorus (PG) of ATP analog correlated closely with the binding affinity.

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, C.A. Willoughby, K. Chapman, B. McKeever and R. Mosley

J. Mol. Graph. Mod. **23**, 457-464 (2005)

Molecular modeling techniques are used to develop a novel series of potent glycogen phosphorylase inhibitors based on a phenyl diacid lead compound. Characterization of the binding pocket by a grid-based surface calculation of the docking model revealed a large unfilled hydrophobic region near the central phenyl ring, suggested that compounds with larger hydrophobic groups in this region would improve binding.

Enzyme Catalysis

Quantum chemical modeling of CO oxidation by the active site of molybdenum CO dehydrogenase.

P.E.M. Siegbahn* [Stockholm U] and A. F. Shestakov

J. Comput. Chem. **26,** 888-898 (2005)

The enzyme crystal structure revealed that Mb is connected to Cu in the active site. DFT studies with large fragments of the crystal structure were used to evaluate the catalytic process in coversion of CO to CO_2 and the reason that sulfinated CO_2 is produced rapidly even though single molecules don't leave the site readily.

Using a library of structural templates to recognise catalytic sites and explore their evolution in homologous families.

J.W. Torrance* [EMBL], G.J. Bartlett, C.T. Porter, and J.M. Thornton

J. Mol. Biol. **347**, 565-581 (2005)

A database of enzyme active site templates, which are curated three-dimensional arrangements of catalytic residues, can be queried and downloaded at http://www.ebi.ac.uk/thornton-srv/databases/CSS.

Enzyme Catalysis (cont'd)

Sequence-structure-function relationships of a tRNA (m(7)G46) methyltransferase studied by homology modeling and site-directed mutagenesis.

E. Purta, F. van Vliet, C. Tricot, L.G. De Bie, M. Feder, K. Skowronek, L. Droogmans* [U Libre Bruxelles], and J.M. Bujnicki* [Genesilico]

Proteins **59***,* 482-488 (2005)

A strong combination of experimental data and modeling is used to elucidate key residues in the activity of the enzyme.

Predicting enzyme function from protein sequence.

J. Minshull* [DNA2.0], J.E. Ness, C. Gustafsson, and S. Govindarajan

Curr. Opi. Chem. Biol. **9**, 202-209 (2005)

This review focuses on the applicability of what is learned from natural enzymes to improve methods for catalyst design.

High-throughput screens and selections of enzyme-encoding genes.

A. Aharoni, A.D. Griffiths, and D.S. Tawfik* [Weizmann Inst Sci]

Curr. Opi. Chem. Biol. **9**, 210-216 (2005)

Recent developments in the selection of enzyme-coding genes for directed evolution and functional genomics were described. This study focused on HTS approaches that enable selection from large libraries (>10^6 gene variants) with relatively humble means (*i.e.* non-robotic systems), and particularly on *in vitro* compartmentalization.

Toward identification of the compound I reactive intermediate in cytochrome P450 chemistry: A QM/MM study of its EPR and Mossbauer parameters.

J. C. Schoneboom, F. Neese* [Max Planck Inst], and W. Thiel* [Max Plank Inst]

J. Amer. Chem. Soc. **127**, 5840-5853 (2005)

.DFT and correlated ab initio methods are applied to understand EPR and Maossbauer properties of coupound I in cytochrome $P40_{cam}$.

Theoretical study on the inhibition of ribonucleotide reductase by 2'-mercapto-2'-deoxyribonucleoside-5'-diphosphates.

S. Pereira, P. A. Fernandes, and M. J. Ramos* [Fac Ciencias Porto]

J. Amer. Chem. Soc. **127**, 5174-5179 (2005)

ONIOM calculations investigate the mechanism of inhibition of ribonucleotide reductase by mercapto-deoxyribonucleoside diphosphates. The results support previous hypotheses on the mechanisms in the presence and absence of oxygen.

The final catalytic step of cytochrome P450 aromatase: A density functional theory study.

J. C. Hackett* [Ohio State U], R. W. Brueggemeier, and C. M. Hadad

J. Amer. Chem. Soc. **127**, 5224-5237 (2005)

DFT and ab initio MD calculations probe possible mechanisms for the "mysterious third step" of aromatase catalysis (which convert androgens to estrogens aromatizing a ring). The calculations support a dehydrogenase like mechanism.

Protein-Protein Interactions

3D-Epitope-Explorer (3DEX): Localization of conformational epitopes within three-dimensional structures of proteins.

A. Schreiber, M. Humbert, A. Benz, and U. Dietrich* [Inst Biomed Res]

J. Comput. Chem. **26,** 879-887 (2005)

3DEX is designed to identify possible peptide antigens that would mimic the epitopes for antibodies. The method was tested with antibodies to HIV gp120.

The relationship between the flexibility of proteins and their conformational states on forming protein–protein complexes with an application to protein–protein docking.

G.R. Smith, M.J.E. Sternberg, and P.A. Bates* [Cancer Research UK]

J. Mol. Biol. **347**, 1077-1101 (2005)

For a set of 22 protein-protein complexes, MD of the unbound forms suggests that although regions of the unbound protein-protein interface samples the bound form, the interface never completely samples the bound state. Interestingly, in 40 of the 41 proteins, the core protein-protein interface residues appear to be less mobile than the rest of the surface.

The effect of resolution-dependent global shape modifications on rigid-body protein-protein docking.

D. Segal and M. Eisenstein* [Weizmann]

Proteins **59***,* 580-591 (2005)

Fourier-series shape and electrostatic descriptors are used to explore docking approaches using low local resolution to compensate for shape misfits. An optimal intermediate resolution was found to significantly improve ranking for 23 test cases.

Probing metal-protein interactions using a *de novo* design approach.

D. Ghosh and V.L. Pecoraro* [Univ. of Michigan]

Curr. Opi. Chem. Biol. **9**, 97-103 (2005)

De novo design of metalloproteins provides a valuable tool for understanding the structural constraints and functional attributes of natural biological systems. This study focused at probing interactions between metals and proteins in designed systems. The results indicated that the field of metalloprotein design is contributing significantly to the understanding of metals in biology.

The role of Phe in the formation of well-ordered oligomers of amyloidogenic hexapeptide (NFGAIL) observed in molecular dynamics simulations with explicit solvent.

C. Wu, H. Lei, and Y. Duan* [U Calif Davis]

Biophys. J. **88:** 2897-2906 (2005)

Both β-sheet extension and β-sheet stacking were observed as possible amyloid formation mechanisms in these peptide octamer simulations of ~1 μs aggregate duration. The Phe in NFGAIL directed stacking, but the peptide still retained substantial disorder (92%).

Membrane Proteins and Lipid-Peptide Interactions

Empirical lipid propensities of amino acid residues in multispan alpha helical membrane proteins.

L. Adamian, V. Nanda, W.F. Degrado* [U Pennsylvania], and J. Liang* [U Illinois]

Proteins **59***,* 496-509 (2005)

A statistical analysis of 'lipid-accessibility' for headgroup or tail regions of residue types in transmembrane helices from 29 crystal structures, is presented. Comparison with various general hydrophobicity scales is made, and application in structure prediction is explored.

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

Prediction of the mutation-induced change in thermodynamic stabilities of membrane proteins from free energy simulations.

Hwangseo Park* [Seoul National U] and Sangyoub Lee

J. Biophys. Chem. **114**, 191-197 (2005)

Comparative protein structure modeling and FEP simulation are applied to investigate the mutation-induced stabilization of membrane proteins (MPs) in aqueous solution. The calculated difference in protein solvation free energy between the wild type and a mutant compares well with their relative thermodynamic stabilities in solution. This tool is useful for assessing the relative stability of a mutant MP with respect to its wild type in solution.

Ligand-induced conformational change in the α7 nicotinic receptor ligand binding domain.

R.H. Henchman* [U Calif San Diego], H.-L. Wang, S.M. Sine, P.Taylor, and J.A. McCammon

Biophys. J. **88,** 2564-2576 (2005)

Five 15-ns simulations with a pentamer of α7 extracellular domains (based on the ACh binding protein structure) in the unit cell. Periodic boundary conditions and explicit saline were used to provide NPT ensemble conditions. The simulations without a ligand or with antagonist d-tubocurarine yielded asymmetric structures that might be imagined to lead to closed transmembrane pores, whereas those with agonist ACh or ACh plus enhancer Ca^{2+} led to expanded, more open-prone states.

Assembly of lipoprotein particles containing apolipoprotein-B: Structural model for the nascent lipoprotein particle.

P.E. Richardson, M. Manchekar, N. Dashti, M. K. Jones, A. Beigneux, S.G. Young, S.C. Harvey, and J.P. Segrest* [U Alabama Birmingham Med Center]

Biophys. J. **88,** 2789-2800 (2005)

A homology model of 1000 residues of ApoB suggests a lipid bilayer binding pocket motif that may nucleate lipoprotein assembly.

Protein-Nucleic Acid Interactions

Molecular dynamics simulation of clustered DNA damage sites containing 8-oxoguanine and abasic site.

H. Fujimoto* [Natl Inst Inf Dis], M. Pinak, T. Nemoto, P. O'Neill, E. Kume, K. Saito, and H. Maekawa

J. Comput. Chem. **26,** 788-798 (2005)

MD simulations show that when repair of an abasic site is going within a few bases of an 8-oxoguanine oxidized site, the intermediate base pairs lose contact force with each other and the repair would be inhibited.

Nucleic Acids

Does water play a structural role in the folding of small nucleic acids?

E.J. Sorin, Y.M. Rhee, and V.S. Pande* [Stanford U]

Biophys. J. **88,** 2516-2524 (2005)

5'-GGGC[GCAA]GCCU-3, a RNA hairpin-loop motif, folds in 8.8±2 μs according to explicit saline simulations of aggregate length 500 μs (using distributed processing). Water is excluded in a final step. Hydrophobic collapse is more rapid than and independent of ion motions.

Nucleic Acids (cont'd)

Recognition of RNA by amide modified backbone nucleic acids: Molecular dynamics simulations of DNA-RNA hybrids in aqueous solution.

M. Nina* [Syngenta Corp], R. Fonne-Pfister, R. Beaudegnies, H. Chekatt, P. M. J. Jung, F. Murphy-Kessabi, A. De Mesmaeker, and S. Wenderborn

J. Amer. Chem. Soc. **127**, 6027-6038 (2005)

MD simulation with and Ewald treatment and MM-PBSA continuum analysis help understand the nature of amide backbone modifications to nucleic acids, aiding interpretation of experiment. Most interesting about this work is that it is performed by an industrial group suggesting that these methods have moved into practice.

Carbohydrates

Free energy surfaces for the α(1→4)-glycosidic linkage: Implications for polysaccharide solution structure and dynamics.

M. M. Kuttel, and K. J. Naidoo* [U Cape Town]

J. Phys. Chem. B **109**, 7468-7474 (2005)

The PMF for rotation around the f and y dihedral angles of the α(1→4) linkage in maltose disaccharide is calculation in solution and in vacuo. An adaptive umbrella sampling method in CHARMM with the CSFF parameter set is applied.

1.3. Surfaces, Catalysts, and Material Subjects

Unified molecular picture of the surfaces of aqueous acid, base, and salt solutions.

M. Mucha, T. Frigato, L. M. Levering, H. C. Allen, D. J. Tobias, L. X. Dang, and P. Jungwirth* [Acad Sci Czech Rep]

J. Phys. Chem. B **109**, 7617-7623 (2005)

This feature article discusses current knowledge and theory applied to overcome the controversies regarding the molecular structure of the interfacial regions of aqueous electrolytes.

Application of accelerated molecular dynamics schemes to the production of amorphous silicon.

D. Choudhary* [Cornell U] and P. Clancy

J. Chem Phys. **122,** 15450901- 15450908 (2005)

Hyperdynamics and self-guided dynamics schemes yield a boost in the dynamics by a factor of 20 without increased overhead compared to conventional MD. A boost of 4-12 for small systems did not affect the evolution, but for larger systems, anomalies develop.

2. METHODOLOGY

Conformational Search and Analysis

Modified replica exchange simulation methods for local structure refinement.

X. Cheng, G. Cui, V. Hornak, and C. Simmering* [Stony Brook U]

J. Phys. Chem. B **109**, 8220-8230 (2005)

A variant of replica-exchange that applies only to local regions of the structure is proposed and applied to an RNA hairpin. The results suggest more efficient sampling of the structure than is observed in standard MD or REMD simulations.

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Potentials and Parameters

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Electrostatic energies and forces computed without explicit interparticle interactions: A linear time complexity formulation.

R.J. Petrella* [Harvard U] and M. Karplus

J. Comput. Chem. **26,** 755-787 (2005)

A method of computing pairwise interactions by partitioning of the double sum based on a polynomial fit to the inverse distances can increase accuracy and speed. It is applicable to periodic systems, but also usable as an approcximation in condensed phase liquid systems. Compute time only grows linearly with number of particles.

New AMBER force field parameters of heme iron for cytochrome P450s determined by quantum chemical calculations of simplified models.

A. Oda* [Toyama Chem], N. Yamaotsu, and S. Hirono

J. Comput. Chem. **26,** 818-826 (2005)

A hybrid DFT with the MIDI basis set for iron yields good force field parameters for the porphyrin in cytochrome P450.

T

A knowledge-based energy function for protein-ligand, protein-protein, and protein-DNA complexes.

C. Zhang, S. Liu, Q. Zhu, and Y. Zhou* [SUNY Buffalo]

J. Med. Chem. **48**, 2325-2335 (2005)

A previously described novel knowledge-based potential based on a distance-scaled, finite, ideal-gas reference (DFIRE) state is parameterized using only 19 atom types and applied to prediction of intermolecular binding affinities. Correlation coefficients of predicted versus known affinities are in the 0.6-0.8 range.

Molecular Dynamics

Efficient charge assignment and back interpolation in multigrid methods for molecular dynamics.

S. Banerjee* [Duke U] and J. A. Board Jr.

J. Comput. Chem. **26,** 957-967 (2005)

A convolution method is found to speed both grid charge assignment and back interpolation to atomic charges with improved accuracy and scalability for multigrid analysis based on the truncated Gaussian grid charge assignment method.

!

An approximate but fast method to impose flexible distance constraints in molecular dynamics simulations.

M. Christen and W.F. van Gunsteren

J. Chem. Phys. **122,** 14410601- 14410612 (2005)

Flexible distance constraints are something between bond energies, which don't specifically constrain the distance between atoms, and Shake, which completely constrains the distance. They do not lead to constant energy MD, but are as fast as Shake and, when used with a thermostat produce stable simulations at time steps up to 19 fs in a neopentane test case.

Free Energy Methods

Automated computation of low-energy pathways for complex rearrangements in proteins: Application to the conformational switch of Ras p21.

F. Noe, F. Ille, J.C. Smith, and S. Fischer* [U Heidelberg]

Proteins **59***,* 534-544 (2005)

A novel method for finding multiple free energy paths for conformational transitions is presented, combining initial sidechain shrinking and subsequent conjugate peak refinement steps. For the Ras p21 'switch' transition a limiting barrier is found that corresponds to experimental rates.

Free Energy Methods (cont'd)

Comparison of efficiency and bias of free energies computed by exponential averaging, the Bennett acceptance ratio, and thermodynamic integration.

M.R. Shirts* [Stanford U] and V.S. Pande

J. Chem. Phys. **122,** 14410701-14410716 (2005)

The Bennett acceptance ratio method, which is what WHAM reduces to when used for alchemical FEP, can be used directly to efficiently determine free energy differences in atomistic simulations, and yields lower variance and bias than TI or exponential averaging methods, in that it is better able to handle many small simulations far from equilibrium.

Secondary Structure Prediction

Protein secondary structure prediction with dihedral angles.

M.J. Wood and J.D. Hirst* [U Nottingham]

Proteins **59***,* 476-481 (2005)

A novel method for secondary structure and [psi]-angle prediction outperforms several others on the CB513 dataset, and performs equally well on the 2245 member set for training PSIPRED, as well as on the CASP4 and 5 targets.

Combining prediction of secondary structure and solvent accessibility in proteins.

R. Adamczak, A. Porollo, and J. Meller* [CHRF]

Proteins **59***,* 467-475 (2005)

Incorporation of predicted solvent accessibility (SA) in a neural net-based secondary structure prediction method gives a slight (2.5%) enhancement of prediction accuracy. Maximal improvement is estimated at 4% (for perfect SA prediction), and inclusion of two-state SA decreases accuracy.

Protein Structure Prediction

Automated use of mutagenesis data in structure prediction.

V. Nanda and W.F. Degrado* [U Pennsylvania]

Proteins **59***,* 454-466 (2005)

A method is presented to use information on deleterious and neutral mutations from various sources in combination with coarse-grained forcefields, and tested on 2D lattice models with chains of up to 12 binary 'Large-Small' units. Implications for all-atom models, protein-protein and protein-small molecule interactions are discussed.

Ligand Docking

Importance of accurate charges in molecular d ocking: Quantum mec hanical/molecular mechanical (QM/MM) approach.

A.E. Cho, V. Guallar, B.J. Berne, and R. Friesner* [Columbia U]

J. Comput. Chem. **26,** 915-931 (2005)

With the ligand specified as QM, ligand redocking (for a sample of 40 PDB complexes) was often times much more structurally accurate than when fixed charges were used on the ligand.

Ligand Docking (cont'd)

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Binding mode prediction of cytochrome P450 and thymidine kinase protein-ligand complexes by consideration of water and rescoring in automated docking.

C. de Graaf, P. Pospisil, W. Pos, G. Folkers, and N.P.E. Vermeulen [Vrije U]

J. Med. Chem. **48**, 2308-2318 (2005)

Results from docking against Cyp P450 and TK binding sites with no water, crystallographic waters, and computationally predicted waters, suggests that the computationally predicted water scheme sometimes increases docking accuracy. A consensus scoring function combining results from three docking programs also helps.

Validation of the binding site structure of the cellular retinol-binding protein (CRBP) by ligand NMR chemical shift perturbations.

B. Wang, and K. M. Merz, Jr. *[Penn State U]

J. Amer. Chem. Soc. **127**, 5310-5311 (2005)

Divide and conquer semi-empirical methods (at the MNDO level) are applied and compared to NMR results in the estimation of chemical shift perturbations upon ligand binding by protein.

Structure Determination

!

Fluctuations and correlations in crystalline protein dynamics: A simulation analysis of staphylococcal nuclease.

L. Meinhold and J.C. Smith* [U Heidelberg]

Biophys. J. **88,** 2554-2563 (2005)

Short range interatomic distance correlation times are < 1 ns, but long range correlation times would be up to ~1 μs based on extrapolations from 10 ns simulations with four copies of the protein per unit cell. Simulation-derived *B*-factors are similar but slightly larger than experimental and computed *R*-factors drop to 8% by 10 ns.

3. JOURNAL REVIEWS

Journal of Computational Chemistry 26(8), June 2005

755-787 **Electrostatic energies and forces computed without explicit interparticle interactions: A linear time complexity formulation.** R.J. Petrella* [Harvard U] and M. Karplus. See **Methodology, Potentials and Parameters.**

788-798 **Molecular dynamics simulation of clustered DNA damage sites containing 8-oxoguanine and abasic site.** H. Fujimoto* [Natl Inst Inf Dis], M. Pinak, T. Nemoto, P. O'Neill, E. Kume, K. Saito, and H. Maekawa. See **Applications, Protein-Nucleic Acid Interactions.**

799-802 **Carbon boronyls: Species with higher viable possibility than boron carbonyls at the density functional theory.** S.-D. Li* [Shanxi U], C.-Q. Miao, J.-C. Guo, and G.-M. Ren.

Carbon boronyls should be more stable than their boron carbonyl isomers, according to DFT.

803-806 **Stability of $(C_{60})_2$ and epoxide dimers, $(C_{60})_2O_N$, and their anions.** F.J. Owens* [US Army, Hunter Coll]

$C_{60}O$ molecules are more stable with negative charge than without according to semiempirical calculations, and should be ferromagnet due to unpaired electron spin.

807-817 **Theoretical study on the reaction mechanism of the methyl radical with nitrogen oxides.** J.-X. Zhang, J.-Y. Liu, Z.-S. Li* [Jilin U], and C.-C. Sun

The CH_3 radical should react readily with NO_2, forming CH_3O + NO or CH_2O + HNO , but not with NO according to DFT computations.

818-826 **New AMBER force field parameters of heme iron for cytochrome P450s determined by quantum chemical calculations of simplified models.** A. Oda* [Toyama Chem], N. Yamaotsu, and S. Hirono. See **Methodology, Potentials and Parameters.**

827-835 **Optimal virtual orbitals to relax wave functions built up with transferred extremely localized molecular orbitals.** A. Genoni, A. Fornili, and M. Sironi* [U Studi Milano]

Virtual orbitals can be used to approximate electron delocalization when using transferable extrememly localized molecular orbitals for molecular fragments to build a macromolecule.

836-845 **Computations on the Ã-X transition of isoprene-OH-O2 peroxy radicals.** T.S. Dibble* [SUNY]

Configuration interaction with single excitations (CIS) method and time-dependent density functional theory (TD-DFT) were compared for computations of fragment components of isoprene and its excitation energies.

846-855 **Translation of STO charge distributions.** J. Fernández Rico * [U Autónoma Madrid], R. López, I. Ema, and G. Ramírez

The Barnett and Carlson algorithm for computing multicenter orbitals with Slater functions is expanded here for use with two-center charge distributions.

856-862 **Zori 1.0: A parallel quantum Monte Carlo electronic structure package.** A. Aspuru-Guzik* [U Calif Berkeley], R. Salomón-Ferrer, B. Austin, R. Perusquía-Flores, M.A. Griffin, R.A. Oliva, D. Skinner, D. Domin, and W.A. Lester Jr.

Zori computes electronic structures using a quantum MC method.

863 **Erratum to "Solvation forces on biomolecular structures: A comparison of explicit solvent and Poisson-Boltzmann models," by Jason Wagoner and Nathan A. Baker.** J. Wagoner* [Washington U] and N.A. Baker

Simulation energies should have been reported as kcal/mol rather than kJ/mol, which in turn means that the Poisson equation underestimates rather than overestimating the solvation energy by a factor of 2.

Journal of Computational Chemistry 26(9), July 15, 2005

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865-870 **Quantum chemical modeling of the reduction of cis-diammineplatin um(IV) tetrachloride [Pt(NH3)2Cl4] by methyl thiolate anion.** I.I. Dobrogorskaia-Méreau* [U Bordeaux 1] and A.V. Nemukhin.

QM/MM MD simulations with and without water give an excellent match to the experimental reduction energy for this system intended to mimic glutathione reduction.

871-878 **The relationship between adsorption energies of methyl on metals and the metallic electronic properties: A first-principles DFT study.** G.-C. Wang 1* [Nankai U], J. Li, X.-F. Xu, R.-F. Li, and J. Nakamura

> Methyl prefers to bind to the hollow site rather than the "top one for Fe, Ni, Rh, and Cu, but it is the other way for Pt, Pd, Au, and Ag."

879-887 **3D-Epitope-Explorer (3DEX): Localization of c onformational epito pes within three-dimensional structures of proteins.** A. Schreiber, M. Humbert, A. Benz, and U. Dietrich* [Inst Biomed Res]. See **Applications, Protein-Protein Interactions.**

888-898 **Quantum chemical modeling of CO oxidation by the active site of molybdenum CO dehydrogenase.** P.E.M. Siegbahn* [Stockholm U] and A. F. Shestakov. See **Applications, Enzyme Catalysis.**

899-906 **An unbiased population-based search for the g eometry optimizatio n of Lennard-Jones clusters: 2 ≤ N ≤ 372.** W. Pullan* [Griffith U]

> A global optimization technique, Population Based Search, was shown to produce all of the global minima for LJ clusters (2 - 372 atoms) previously determined and stored in the Cambridge Cluster Database.

907-914 **Hydration process as an activation of trans- and cisplatin compl exes in anticancer treatment. DFT and ab initio computational study of thermodynamic and kinetic parameters.** J.V. Burda* [Charles U], M. Zeizinger, and J. Leszczynski

> Cisplatin dechlorination is computed with DFT/polarizable continuum to have a rate constant of $1.4x10^4$/s, consistent with experiment and 3-4 orders of magnitude faster than deammination.

915-931 **Importance of accurate charges in molecular d ocking: Quantum mec hanical/molecular mechanical (QM/MM) approach.** A.E. Cho, V. Guallar, B.J. Berne, and R. Friesner* [Columbia U]. See **Methodology, Ligand Docking.**

932-940 **An accurate relativistic universal Gaussian b asis set for hydrog en through Nobelium without variational prolapse and to be used with both uniform sphere and Gaussian nucleus models.** R.L.A. Haiduke, L.G.M. de Macedo, and A.B.F. da Silva* [U São Paulo]

> "The largest error between our Dirac-Fock-Coulomb total energy values and those calculated numerically is 8.8 mHartree for the No atom."

941-948 **Adaptive approach for nonlinear sensitivity a nalysis of reaction kinetics.** T.S. Hofer, B.R. Randolf, and B.M. Rode* [U Innsbruck]

> The "Trail" algorithm (from MD simulations) is used for the Fokker-Planck PDE derived from recasting the ODE's of kinetic theory into a density transport problem.

949-956 **Structure-breaking effects of solvated Rb(I) in dilute aqueous solution - An *ab initio* QM/MM MD approach.** I. Horenko* [Freie U Berlin], S. Lorenz, C. Schütte, and W. Huisinga. **See Applications, Water and Solvation.**

957-967 **Efficient charge assignment and back interpolation in multigrid methods for molecular dynamics.** S. Banerjee* [Duke U] and J. A. Board Jr. See **Methodology, Molecular Dynamics.**

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