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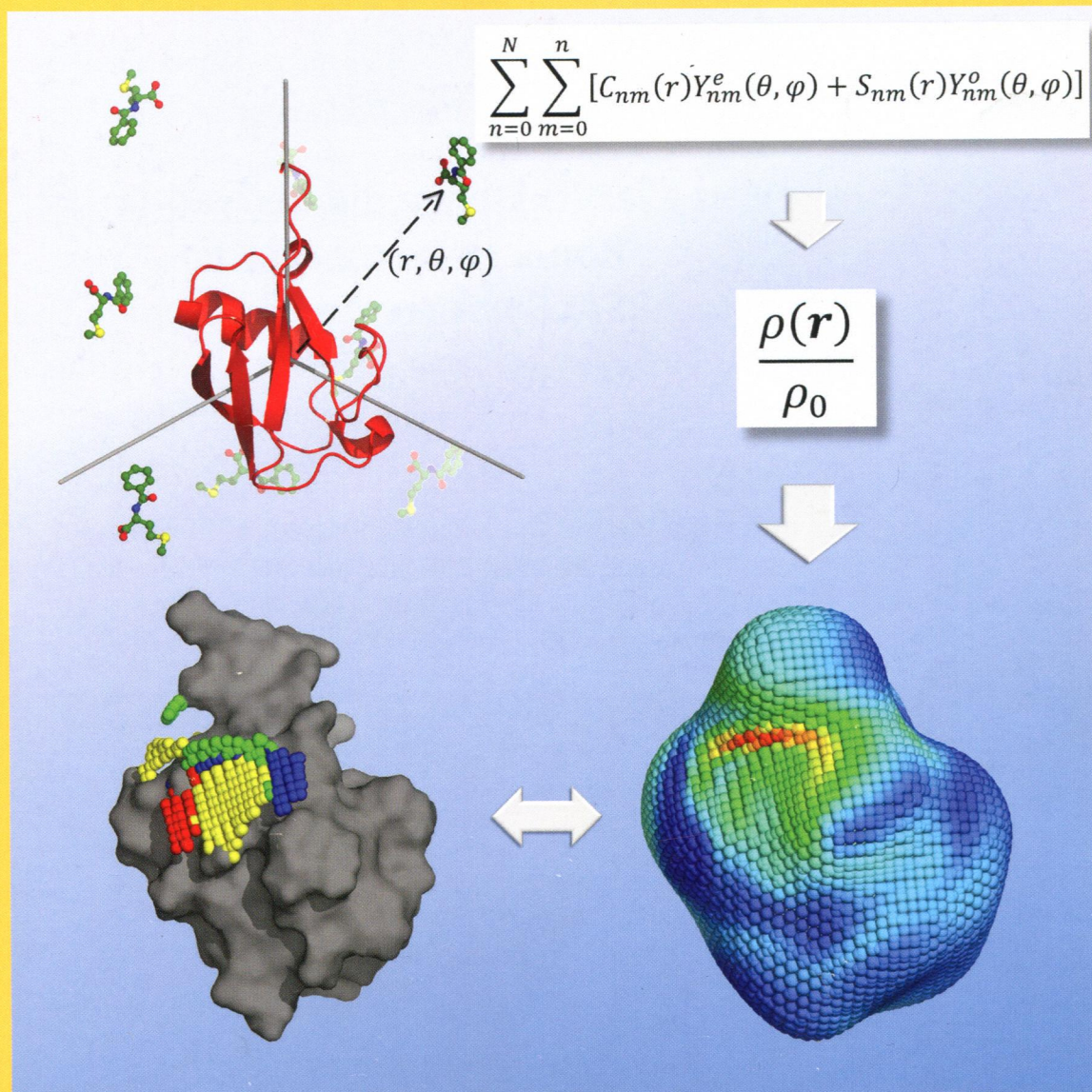
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B



Understanding the
Ligand Distribution
and Binding around
Proteins Using a
Spherical Harmonic
Expansion Approach
(see page 13066)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: Parimal et al. employ a spherical harmonic expansion approach to obtain spatially resolved three-dimensional distributions of multimodal ligands around proteins from molecular dynamics simulations. Representing ligand densities using color maps on surface envelopes surrounding proteins provides an understanding of ligand binding, orientation, and synergistic interactions that may drive protein–ligand interactions. This understanding is central to modern bioseparations processes (e.g., through the design of new classes of multimodal chromatographic ligands) and in drug discovery and design. See page 13066.

Articles

Biophysical Chemistry and Biomolecules

- 13025  DOI: 10.1021/jp501515g
pH-Dependent Differential Interacting Mechanisms of Sodium Dodecyl Sulfate with Bovine Serum Fetuin: A Biophysical Insight
Nida Zaidi, Saima Nusrat, Fatima Kamal Zaidi, and Rizwan H. Khan*
- 13037 DOI: 10.1021/jp503749a
Coarse-Grained Model of Glycosaminoglycans in Aqueous Salt Solutions. A Field-Theoretical Approach
Andrei L. Kolesnikov, Yuriy A. Budkov, and Evgenij A. Nogovitsyn*
- 13050  DOI: 10.1021/jp508423s
Novel Approach for Identifying Key Residues in Enzymatic Reactions: Proton Abstraction in Ketosteroid Isomerase
Mika Ito and Tore Brinck*
- 13059  DOI: 10.1021/jp505885j
DNA Recognition Process of the Lactose Repressor Protein Studied via Metadynamics and Umbrella Sampling Simulations
Simone Furini* and Carmen Domene
- 13066  DOI: 10.1021/jp506849k
Application of a Spherical Harmonics Expansion Approach for Calculating Ligand Density Distributions around Proteins
Siddharth Parimal, Steven M. Cramer, and Shekhar Garde*
- 13077  DOI: 10.1021/jp5068704
Binding of the Iminium and Alkanolamine Forms of Sanguinarine to Lysozyme: Spectroscopic Analysis, Thermodynamics, and Molecular Modeling Studies
Chandrima Jash, Pavan V. Payghan, Nanda Ghoshal, and Gopinatha Suresh Kumar*

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DOI: 10.1021/jp507618f

One Protein, Two Chromophores: Comparative Spectroscopic Characterization of 6,7-Dimethyl-8-ribityllumazine and Riboflavin Bound to Lumazine Protein

Bernd Paulus, Boris Illarionov, Daniel Nohr, Guillaume Roellinger, Sylwia Kacprzak, Markus Fischer, Stefan Weber, Adelbert Bacher, and Erik Schleicher*

13106 

DOI: 10.1021/jp5078906

Effect of Including Torsional Parameters for Histidine–Metal Interactions in Classical Force Fields for Metalloproteins

Raúl Mera-Adasme,* Keyarash Sadeghian, Dage Sundholm, and Christian Ochsenfeld

13112 

DOI: 10.1021/jp507936a

R102Q Mutation Shifts the Salt-Bridge Network and Reduces the Structural Flexibility of Human Neuronal Calcium Sensor-1 Protein

Yuzhen Zhu, Ying Wu, Yin Luo, Yu Zou, Buyong Ma, and Qingwen Zhang*

13123

DOI: 10.1021/jp508170c

Loss of Cellular Transformation Efficiency Induced by DNA Irradiation with Low-Energy (10 eV) Electrons

Saloua Kouass Sahbani,* Leon Sanche, Pierre Cloutier, Andrew D. Bass, and Darel J. Hunting

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DOI: 10.1021/jp508729z

Molecular Simulations of the Pairwise Interaction of Monoclonal Antibodies

Mauro Lapelosa, Thomas W. Patapoff, and Isidro E. Zarraga*

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DOI: 10.1021/jp5089417

“Building Block Picture” of the Electronic Structure of Aqueous Cysteine Derived from Resonant Inelastic Soft X-ray Scattering

F. Meyer, M. Blum, A. Benkert, D. Hauschild, S. Nagarajan, R. G. Wilks, J. Andersson, W. Yang, M. Zharnikov, M. Bär, C. Heske, F. Reinert, and L. Weinhardt*

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DOI: 10.1021/jp509326r

Thermodynamic Study of Rhodamine 123–Calf Thymus DNA Interaction: Determination of Calorimetric Enthalpy by Optical Melting Study

Abdulla Al Masum, Maharudra Chakraborty, Prateek Pandya, Umesh Chandra Halder, Md. Maidul Islam,* and Subrata Mukhopadhyay

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DOI: 10.1021/jp5094146

Peptide Backbone Effect on Hydration Free Energies of Amino Acid Side Chains

Timir Hajari and Nico F. A. van der Vegt*

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DOI: 10.1021/jp5106423

Disorder in Cholesterol-Binding Functionality of CRAC Peptides: A Molecular Dynamics Study

Cayla M. Miller, Angela C. Brown, and Jeetain Mittal*

13175 DOI: 10.1021/jp5074945
Semihydrophobic Nanoparticle-Induced Disruption of Supported Lipid Bilayers: Specific Ion Effect
Benxin Jing, Rosary C. T. Abot, and Yingxi Zhu*

13183 DOI: 10.1021/jp507999g
Nonviral Gene Delivery: Gemini Bispyridinium Surfactant-Based DNA Nanoparticles
Emilia Fiscaro,* Carlotta Compari, Franco Bacciottini, Laura Contardi, Nadia Barbero, Guido Viscardi, Pierluigi Quagliotto, Gaetano Donofrio, Bożenna Różycka-Roszak, Paweł Misiak, Edyta Woźniak, and Francesco Sansone

13192 DOI: 10.1021/jp508488c
Atomistic Description of the Solubilisation of Testosterone Propionate in a Sodium Dodecyl Sulfate Micelle
Daniel T. Allen, Yussif Saaka, M. Jayne Lawrence, and Christian D. Lorenz*

13202 DOI: 10.1021/jp508549m
Structures, Dynamics, and Water Permeation Free Energy across Bilayers of Lipid A and Its Analog Studied with Molecular Dynamics Simulation
Tao Wei,* Tiefan Huang, Baofu Qiao, Mo Zhang, Heng Ma, and Lin Zhang

13210 DOI: 10.1021/jp509099h
Gelation: The Role of Sugars and Polyols on Gelatin and Agarose
Seishi Shimizu* and Nobuyuki Matubayasi

Liquids; Chemical and Dynamical Processes in Solution

13217 DOI: 10.1021/jp506410w
Quantum Mechanics/Molecular Mechanics Modeling of Photoelectron Spectra: The Carbon 1s Core–Electron Binding Energies of Ethanol–Water Solutions
T. Löytynoja, J. Niskanen,* K. Jänkälä, O. Vahtras, Z. Rinkevicius, and H. Ågren

13226 DOI: 10.1021/jp507752e
The Role of Quantum Effects on Structural and Electronic Fluctuations in Neat and Charged Water
Federico Giberti, Ali A. Hassanali,* Michele Ceriotti,* and Michele Parrinello

13236 DOI: 10.1021/jp507959q
Reaction Coordinate of Incipient Methane Clathrate Hydrate Nucleation
Brian C. Barnes, Brandon C. Knott, Gregg T. Beckham,* David T. Wu,* and Amadeu K. Sum

13244 

DOI: 10.1021/jp5079778

Rotational Dynamics of Imidazolium-Based Ionic Liquids: Do the Nature of the Anion and the Length of the Alkyl Chain Influence the Dynamics?

Sugosh R. Prabhu and G. B. Dutt*

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DOI: 10.1021/jp5105054

Accurate Quadrupolar NMR Relaxation Rates of Aqueous Cations from Classical Molecular Dynamics

Antoine Carof, Mathieu Salanne, Thibault Charpentier, and Benjamin Rotenberg*

Glasses, Colloids, Polymers, and Soft Matter

13258 

DOI: 10.1021/jp505348t

Solvent Structuring and Its Effect on the Polymer Structure and Processability: The Case of Water–Acetone Poly- ϵ -caprolactone Mixtures

Nicodemo Di Pasquale,* Daniele Luca Marchisio, Antonello Alessandro Barresi, and Paola Carbone

13268 

DOI: 10.1021/jp507772t

Synergistic and Competitive Aspects of the Adsorption of Poly(ethylene glycol) and Poly(vinyl alcohol) onto Na-Bentonite

Francis Clegg,* Chris Breen, and Khairuddin

13279 

DOI: 10.1021/jp5079339

Preferential Molecular Encapsulation of an ICT Fluorescence Probe in the Supramolecular Cage of Cucurbit[7]uril and β -Cyclodextrin: An Experimental and Theoretical Approach

Anuva Samanta, Nikhil Guchhait,* and Subhash Chandra Bhattacharya*

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DOI: 10.1021/jp508284n

The Minimum Amount of "Matrix" Needed for Matrix-Assisted Pulsed Laser Deposition of Biomolecules

Marshall Tabetah, Andreea Matei, Catalin Constantinescu, Ninell P. Mortensen, Maria Dinescu, Jorgen Schou, and Leonid V. Zhigilei*

13300 

DOI: 10.1021/jp508329s

Chain Dynamics of Ethylene Oxide Oligomer Melts. An Ultrasonic Spectroscopy Study

Elke Wald and Udo Kaatzé*

13312 

DOI: 10.1021/jp510025j

Cooperativity of the Assembly Process in a Low Concentration Chromonic Liquid Crystal

Benjamin R. Mercado, Kenneth J. Nieser, and Peter J. Collings*

Correction to "Polarizable Water Models from Mixed Computational and Empirical Optimization"

Philip Tröster, Konstantin Lorenzen, Magnus Schwörer, and Paul Tavan*

[The main body of the page contains extremely faint, illegible text, likely bleed-through from the reverse side of the paper.]