Volume 78 Issue 4 (March 2010)

Research Articles

Molecular dynamics of leucine and dopamine transporter proteins in a model cell membrane lipid bilayer (p 797-811)
Patrick C. Gedeon, Martín Indarte, Christopher K. Surratt, Jeffry D. Madura
Published Online: Aug 31 2009 3:15PM
DOI: 10.1002/prot.22601

Slow formation of aggregation-resistant $\beta$-sheet folding intermediates (p 812-824)
Mirco Junker, Patricia L. Clark
Published Online: Sep 11 2009 2:56PM
DOI: 10.1002/prot.22609

A novel and efficient tool for locating and characterizing protein cavities and binding sites (p 825-842)
Ashutosh Tripathi, Glen E. Kellogg
Published Online: Sep 11 2009 2:56PM
DOI: 10.1002/prot.22608

Titration_DB: Storage and analysis of NMR-monitored protein pH titration curves (p 843-857)
Damien Farrell, Emanuel Sá Miranda, Helen Webb, Nikolaj Georgi, Peter B. Crowley, Lawrence P. McIntosh, Jens Erik Nielsen
Published Online: Sep 11 2009 2:56PM
DOI: 10.1002/prot.22611

Solid-state NMR and simulation studies of equinatoxin II N-terminus interaction with lipid bilayers (p 858-872)
Yuen Han Lam, Andrew Hung, Raymond S. Norton, Frances Separovic, Anthony Watts
Published Online: Sep 17 2009 3:13PM
DOI: 10.1002/prot.22612

Molecular mechanism of allosteric communication in the human PPAR$\alpha$-RXR$\alpha$ heterodimer (p 873-887)
Tuomas Venäläinen, Ferdinánd Molnár, Chris Oostenbrink, Carsten Carlberg, Mikael Peräkylä
Published Online: Sep 17 2009 3:13PM
DOI: 10.1002/prot.22613

Binding of nitrogen-containing bisphosphonates (N-BPs) to the Trypanosoma cruzi farnesyl diphosphate synthase homodimer (p 888-899)
Chuan-Hsiang Huang, Sandra B. Gabelli, Eric Oldfield, L. Mario Amzel
Published Online: Sep 17 2009 3:13PM
DOI: 10.1002/prot.22614

A novel approach to segregate and identify functional loop regions in protein structures using their Ramachandran maps (p 900-916)
Mattaparthi Venkata Satish Kumar, Rajaram Swaminathan
Published Online: Sep 17 2009 3:13PM
DOI: 10.1002/prot.22615

The structure and NO binding properties of the nitrophorin-like heme-binding protein from Arabidopsis thaliana gene locus At1f79260.1 (p 917-931)
Christopher M. Bianchetti, George C. Blouin, Eduard Bitto, John S. Olson, George N. Phillips Jr.
Published Online: Sep 28 2009 2:45PM
DOI: 10.1002/prot.22617
Symmetry-restrained molecular dynamics simulations improve homology models of potassium channels (p 932-949)
Andriy Anishkin, Adina L. Milac, H. Robert Guy
Published Online: Sep 28 2009 2:45PM
DOI: 10.1002/prot.22618

Thermodynamics of protein-cation interaction: Ca$^{2+}$ and Mg$^{2+}$ binding to the fifth binding module of the LDL receptor (p 950-961)
Xabier Arias-Moreno, Santiago Cuesta-Lopez, Oscar Millet, Javier Sancho, Adrian Velazquez-Campoy
Published Online: Oct 8 2009 3:31PM
DOI: 10.1002/prot.22619

Unraveling the molecular basis for ligand binding in truncated hemoglobins: The trHbO Bacillus subtilis case (p 962-970)
Leonardo Boechi, Pau Arroyo Mañez, F. Javier Luque, Marcelo A. Marti, Dario A. Estrin
Published Online: Sep 28 2009 2:45PM
DOI: 10.1002/prot.22620

Improving the analysis of NMR spectra tracking pH-induced conformational changes: Removing artefacts of the electric field on the NMR chemical shift (p 971-984)
Predrag Kukić, Damien Farrell, Chresten R. Søndergaard, Una Bjarnadottir, John Bradley, Gianluca Pollastri, Jens Erik Nielsen
Published Online: Sep 28 2009 2:45PM
DOI: 10.1002/prot.22621

Computational exploration of the network of sequence flow between protein structures (p 985-1003)
Baoqiang Cao, Ron Elber
Published Online: Sep 28 2009 2:45PM
DOI: 10.1002/prot.22622

Multi-scale characterization of the energy landscape of proteins with application to the C3D/Efb-C complex (p 1004-1014)
Nurit Haspel, Brian V. Geisbrecht, John Lambris, Lydia Kavraki
Published Online: Sep 28 2009 2:45PM
DOI: 10.1002/prot.22624

Highly conserved glycine 86 and arginine 87 residues contribute differently to the structure and activity of the mature HIV-1 protease (p 1015-1025)
Rieko Ishima, Qingguo Gong, Yunfeng Tie, Irene T. Weber, John M. Louis
Published Online: Sep 28 2009 2:45PM
DOI: 10.1002/prot.22625

Predicting protein complex geometries with a neural network (p 1026-1039)
Myong-Ho Chae, Florian Krull, Stephan Lorenzen, Ernst-Walter Knapp
Published Online: Oct 8 2009 3:31PM
DOI: 10.1002/prot.22626

Relation between pH, structure, and absorption spectrum of Cerulean: A study by molecular dynamics and TD DFT calculations (p 1040-1054)
Germain Vallverdu, Isabelle Demachy, Fabienne Mérola, Hélène Pasquier, Jacqueline Ridard, Bernard Lévy
Published Online: Oct 16 2009 3:53PM
DOI: 10.1002/prot.22628

Computational design of second-site suppressor mutations at protein-protein interfaces (p 1055-1065)
Deanne W. Sammond, Ziad M. Eletr, Carrie Purbeck, Brian Kuhlman
Published Online: Oct 16 2009 3:53PM
DOI: 10.1002/prot.22631

Structure Notes