Short Communications

Structural insights into a low-spin myoglobin variant with bis-histidine coordination from molecular modeling (pages 679–684)
Ying-Wu Lin

Research Articles

Remeasuring HEWL pK, values by NMR spectroscopy: Methods, analysis, accuracy, and implications for theoretical pK, calculations (pages 685–702)
Helen Webb, Barbara Mary Tynan-Connolly, Gregory M. Lee, Damien Farrell, Fergal O’Meara, Chresten R. Søndergaard, Kaare Teilum, Chandralal Hewage, Lawrence P. McIntosh and Jens Erik Nielsen

Kinetics, in silico docking, molecular dynamics, and MM-GBSA binding studies on prototype indirubins, KT5720, and staurosporine as phosphorylase kinase ATP-binding site inhibitors: The role of water molecules examined (pages 703–719)

Predicting kinetic constants of protein–protein interactions based on structural properties (pages 720–734)
Hongjun Bai, Kun Yang, Daqi Yu, Changsheng Zhang, Fangjin Chen and Luhua Lai

FINDSITE-metal: Integrating evolutionary information and machine learning for structure-based metal-binding site prediction at the proteome level (pages 735–751)
Michal Brylinski and Jeffrey Skolnick

Solution structures of chicken parvalbumin 3 in the Ca²⁺-free and Ca²⁺-bound states (pages 752–764)
Michael T. Henzl, John J. Tanner and Anmin Tan

Recognition of β–calcineurin by the domains of calmodulin: Thermodynamic and structural evidence for distinct roles (pages 765–786)
Susan E. O'Donnell, Liping Yu, C. Andrew Fowler and Madeline A. Shea
Simplified modeling approach suggests structural mechanisms for constitutive activation of the C5a receptor (pages 787–802)
Gregory V. Nikiforovich, Garland R. Marshall and Thomas J. Baranski

Structures of parasitic CDPK domains point to a common mechanism of activation (pages 803–820)
Amy K. Wernimont, Merhnaz Amani, Wei Qiu, Juan C. Pizarro, Jennifer D. Artz, Yu-Hui Lin, Jocelyn Lew, Ashley Hutchinson and Raymond Hui

Effects of somatic mutations on CDR loop flexibility during affinity maturation (pages 821–829)
Sergio E. Wong, Ben D. Sellers and Matthew P. Jacobson

Role of conformational sampling in computing mutation-induced changes in protein structure and stability (pages 830–838)
Elizabeth H. Kellogg, Andrew Leaver-Fay and David Baker

Predicting protein flexibility through the prediction of local structures (pages 839–852)
Aurélie Bornot, Catherine Etchebest and Alexandre G. de Brevern

Protein domain assignment from the recurrence of locally similar structures (pages 853–866)
Chin-Hsien Tai, Vichetra Sam, Jean-Francois Gibrat, Jean Garnier, Peter J. Munson and Byungkook Lee

The effects of the L29F mutation on the ligand migration kinetics in crystallized myoglobin as revealed by molecular dynamics simulations (pages 867–879)
Massimiliano Anselmi, Alfredo Di Nola and Andrea Amadei

Application of long-range order to predict unfolding rates of two-state proteins (pages 880–887)
B. Harihar and S. Selvaraj

Prediction of protein binding regions (pages 888–897)
Naresh Chennamsetty, Vladimir Voynov, Veysel Kayser, Bernhard Helk and Bernhardt L. Trout

Salt bridges: Geometrically specific, designable interactions (pages 898–915)
Jason E. Donald, Daniel W. Kulp and William F. DeGrado

Exploring the role of structure and dynamics in the function of chymotrypsin inhibitor 2 (pages 916–924)
Matthew J. Whitley and Andrew L. Lee

In silico modeling of pH-optimum of protein–protein binding (pages 925–936)
Rooplekha C. Mitra, Zhe Zhang and Emil Alexov
The $\alpha$-sheet: A missing-in-action secondary structure? (pages 937–946)
Volodymyr Babin, Christopher Roland and Celeste Sagui

Analysis of the peroxiredoxin family: Using active-site structure and sequence information for global classification and residue analysis (pages 947–964)
Kimberly J. Nelson, Stacy T. Knutson, Laura Soito, Chananat Klomsiri, Leslie B. Poole and Jacquelyn S. Fetrow

Crystal structures of a family 8 polysaccharide lyase reveal open and highly occluded substrate-binding cleft conformations (pages 965–974)

The mechanism of papain inhibition by peptidyl aldehydes (pages 975–985)
Michael Shokhen, Netaly Khazanov and Amnon Albeck

Molecular dynamics simulation of $\beta$-microglobulin in denaturing and stabilizing conditions (pages 986–1001)
Federico Fogolari, Alessandra Corazza, Nicola Varini, Matteo Rotter, Devrim Gumral, Luca Codutti, Enrico Rennella, Paolo Viglino, Vittorio Bellotti and Gennaro Esposito

Fingerprint-based structure retrieval using electron density (pages 1002–1009)
Shuangye Yin and Nikolay V. Dokholyan

The structure of the ends of $\alpha$-helices in globular proteins: Effect of additional hydrogen bonds and implications for helix formation (pages 1010–1019)
David P. Leader and E. James Milner-White

Structure Notes

Crystal structure of toll-like receptor 2-activating lipoprotein IlpA from Vibrio vulnificus (pages 1020–1025)
Sangheon Yu, Na Yeon Lee, Soon-Jung Park and Sangkee Rhee