Title:
Protein Function Annotation: The next frontier in molecular biology

140 word brief abstract:
Protein folding has been called the “major unsolved challenge” in understanding proteins. But, one could argue that the real challenge involves understanding, in molecular detail, what those proteins actually do—their detailed molecular function. In 2006, Protein Science published the results from the first Automated Function Prediction meeting, held in Detroit, MI, in 2005. Since then, protein function prediction has become a field in its own right, with researchers trying to make sense of the masses of proteins of unknown function, whose sequences and structures are determined by today’s high-throughput techniques. This virtual issue of Protein Science highlights some of the important articles published at that first AFP meeting, as well as more recently published articles in this relatively young, but exciting, area of protein science.

Key featured articles:


Figure:
All featured articles:

Recent articles-general protein function prediction


Toward prediction of functional protein pockets using blind docking and pocket search algorithms PROTEIN SCIENCE Volume 20, Issue 5, May 2011, Pages: 880–893, Csaba Hetényi and David van der Spoel

Prediction of ligand-binding sites of proteins by molecular docking calculation for a random ligand library PROTEIN SCIENCE Volume 20, Issue 1, January 2011, Pages: 95–106, Yoshifumi Fukunishi and Haruki Nakamura

Recent articles- function prediction in a specific protein or protein family


Analysis and prediction of calcium-binding pockets from apo-protein structures exhibiting calcium-induced localized conformational changes PROTEIN SCIENCE Volume 19, Issue 6, June 2010, Pages: 1180–1190, Xue Wang, Kun Zhao, Michael Kirberger, Hing Wong, Guantao Chen and Jenny J. Yang

Recent articles-examples of why protein function prediction is so hard

Predicting memapsin 2 (β-secretase) hydrolytic activity PROTEIN SCIENCE Volume 19, Issue 11, November 2010, Pages: 2175–2185, Xiaoman Li, Huang Bo, Xuejun C. Zhang, Jean A. Hartsuck and Jordan Tang


Analysis of the plasticity of location of the Arg244 positive charge within the active site of the TEM-1 β-lactamase PROTEIN SCIENCE Volume 18, Issue 10, October 2009, Pages: 2080–2089, David C. Marciano, Nicholas G. Brown and Timothy Palzkill

Comparative surface geometry of the protein kinase family† PROTEIN SCIENCE Volume 18, Issue 10, October 2009, Pages: 2016–2026, Elaine E. Thompson, Alexandr P. Kornev, Natarajan Kannan, Choel Kim, Lynn F. Ten Eyck and Susan S. Taylor
Future of function prediction is functional site design

Motif-directed flexible backbone design of functional interactions†PROTEIN SCIENCE Volume 18, Issue 6, June 2009, Pages: 1293–1305, James J. Havranek and David Baker

From the first Automated Protein Function Prediction (AFP) meeting in 2005:

New avenues in protein function prediction (pages 1527–1529) Iddo Friedberg, Martin Jambon and Adam Godzik Article first published online: 1 JAN 2009 | DOI: 10.1110/ps.062158406

Recurrent use of evolutionary importance for functional annotation of proteins based on local structural similarity (pages 1530–1536) David M. Kristensen, Brian Y. Chen, Viacheslav Y. Fofanov, R. Matthew Ward, Andreas Martin Lisewski, Marek Kimmel, Lydia E. Kavraki and Olivier Lichtarge Article first published online: 1 JAN 2009 | DOI: 10.1110/ps.062152706

Structure-based function inference using protein family-specific fingerprints (pages 1537–1543) Deepak Bandyopadhyay, Jun Huan, Jinze Liu, Jan Prins, Jack Snoeyink, Wei Wang and Alexander Tropsha Article first published online: 1 JAN 2009 | DOI: 10.1110/ps.062189906

A categorization approach to automated ontological function annotation (pages 1544–1549) Karin Verspoor, Judith Cohn, Susan Mniszewski and Cliff Joslyn Article first published online: 1 JAN 2009 | DOI: 10.1110/ps.062184006

Enhanced automated function prediction using distantly related sequences and contextual association by PFP (pages 1550–1556) Troy Hawkins, Stanislav Luban and Daisuke Kihara Article first published online: 1 JAN 2009 | DOI: 10.1110/ps.062153506

Functional annotation prediction: All for one and one for all (pages 1557–1562) Ori Sasson, Noam Kaplan and Michal Linial Article first published online: 1 JAN 2009 | DOI: 10.1110/ps.062185706