

## REFERENCES

- ❖ Badenhuizen IP (1969) *The Biogenesis of Starch Granules in Higher Plants*. Appleton-Century Crofts, New York.
- ❖ Ball K, Preiss J (1994) Allosteric sites of the large subunit of the spinach leaf ADPglucose pyrophosphorylase. *The Journal of Biological Chemistry*. 269(40): 24706-24711.
- ❖ Ball S, Marianne T, Dirick L, Fresnoy M, Delrue B, Decq A (1991) A *Chlamydomonas reinhardtii* low starch mutant is defective for 3-phosphoglycerate activation and orthophosphate inhibition of ADPglucose pyrophosphorylase. *Planta*. 185(1): 17-26.
- ❖ Ballicora MA, Dubay JR, Devillers CH, Preiss J (2005) Resurrecting the ancestral enzymatic role of a modulatory subunit. *The Journal of Biological Chemistry*. 280(11): 10189-10195.
- ❖ Ballicora MA, Frueauf JB, Fu Y, Schurmann P, Preiss J (2000) Activation of the potato tuber ADP-glucose pyrophosphorylase by thioredoxin. *The Journal of Biological Chemistry*. 275(2): 1315-1320.
- ❖ Ballicora MA, Fu Y, Nesbitt NM, Preiss J (1998) ADPglucose pyrophosphorylase from potato tubers Site-directed mutagenesis studies of the regulatory sites. *Plant Physiology*. 118(1): 265-274.
- ❖ Ballicora MA, Iglesias AA, Preiss J (2003) ADP-glucose pyrophosphorylase, a regulatory enzyme for bacterial glycogen synthesis. *Microbiology and Molecular Biology Reviews*. 67(2): 213-225.

- ❖ Ballicora MA, Iglesias AA, Preiss J (2004) ADP-glucose pyrophosphorylase: a regulatory enzyme for plant starch synthesis. *Photosynthesis Research*. 79(1): 1-24.
- ❖ Ballicora MA, Laughlin MJ, Fu Y, Okita TW, Barry GF, Preiss J (1995) Adenosine 5'-diphosphate-glucose pyrophosphorylase from potato tuber. Significance of the N-terminus of the small subunit for catalytic properties and heat stability. *Plant Physiology*. 109(1): 245-251.
- ❖ Bates PA, Kelley LA, MacCallum RM, Sternberg MJ (2001) Enhancement of protein modeling by human intervention in applying the automatic programs 3D-JIGSAW and 3DPSSM. *Proteins. Suppl* 5: 39-46.
- ❖ Benedix A, Becker CM, de Groot BL, Caflisch A, Böckmann RA (2009) Predicting free energy changes using structural ensembles. *Nature Methods*. 6(1): 3-4.
- ❖ Benkert P, Tosatto SC, Schomburg D (2008) QMEAN: A comprehensive scoring function for model quality assessment. *Proteins*. 71(1): 261-277.
- ❖ Bhattacharya D, Cheng J (2013a) 3Drefine: consistent protein structure refinement by optimizing hydrogen bonding network and atomic-level energy minimization. *Proteins*. 81(1): 119-131.
- ❖ Bhattacharya D, Cheng J (2013b) i3Drefine software for protein 3D structure refinement and its assessment in CASP10. *PLoS One*. 8:e69648.
- ❖ Bissantz C, Kuhn B, Stahl M (2010) A medicinal chemist's guide to molecular interactions. *Journal of Medicinal Chemistry*. 53(14): 5061-5084.

- ❖ Blundell TL, Sibanda BL, Sternberg MJ, Thornton JM (1987) Knowledge-based prediction of protein structures and the design of novel molecules. *Nature*. 326(611): 347-352.
- ❖ Bodade RG, Beedkar SD, Manwar AV, Khobragade CN (2010) Homology modeling and docking study of xanthine oxidase of *Arthrobacter* sp XL26. *International Journal of Biological Macromolecules*. 47(2): 298-303.
- ❖ Boehlein SK, Shaw JR, Stewart JD, Hannah LC (2007) Heat stability and allosteric properties of the maize endosperm ADP-glucose pyrophosphorylase are intimately intertwined. *Plant Physiology*. 146(1):289-299.
- ❖ Bogan AA, Thorn KS (1998) Anatomy of hot spots in protein interfaces. *Journal of Molecular Biology*. 280(1): 1-9.
- ❖ Boyd SE, Pike RN, Rudy GB, Whisstock JC, Garcia de la Banda M (2005) PoPS: a computational tool for modeling and predicting protease specificity. *Journal of Bioinformatics and Computational Biology*. 3(3): 551-585.
- ❖ Brooks BR, Brooks CL 3rd, Mackerell AD Jr, Nilsson L, Petrella RJ, Roux B, Won Y, Archontis G, Bartels C, Boresch S, Caflisch A, Caves L, Cui Q, Dinner AR, Feig M, Fischer S, Gao J, Hodoscek M, Im W, Kuczera K, Lazaridis T, Ma J, Ovchinnikov V, Paci E, Pastor RW, Post CB, Pu JZ, Schaefer M, Tidor B, Venable RM, Woodcock HL, Wu X, Yang W, York DM, Karplus M (2009) CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*. 30(10): 1545-1614.
- ❖ Burrell MM (2003) Starch: the need for improved quality and quantity- an overview. *Journal of Experimental Botany*. 54(382): 451-456.

- ❖ Caspar T, Huber SC, Somerville C (1985) Alterations in growth, photosynthesis and respiration in a starchless mutant of *Arabidopsis thaliana* (L.) deficient in chloroplast phosphoglucomutase activity. *Plant Physiology*. 79(1): 11-17.
- ❖ Chaturvedi N, Singh VK, Pandey PN (2013) Computational identification and analysis of arsenate reductase protein in *Cronobacter sakazakii* ATCC BAA-894 suggests potential microorganism for reducing arsenate. *Journal of Structural and Functional Genomics*. 14(2): 37-45.
- ❖ Chen BY, Wang Y, Janes HW (1998) ADP-glucose pyrophosphorylase is localized to both the cytoplasm and plastids in developing pericarp of tomato fruit. *Plant Physiology*. 116(1):101-106.
- ❖ Chen SW, Pellequer JL (2004) Identification of functionally important residues in proteins using comparative models. *Current Medicinal Chemistry*. 11(5): 595-605.
- ❖ Chen VB, Arendall WB 3rd, Headd JJ, Keedy DA, Immormino RM, Kapral GJ, Murray LW, Richardson JS, Richardson DC (2010) MolProbity: All-atom structure validation for macromolecular crystallography. *Acta Crystallographica. Section D, Biological crystallography*. 66(Pt 1): 12-21.
- ❖ Chivian D, Kim DE, Malmström L, Bradley P, Robertson T, Murphy P, Strauss CE, BonneauR, Rohl CA, Baker D (2003) Automated prediction of CASP-5 structures using the Robetta server. *Proteins*. 53(Suppl 6): 524-533.
- ❖ Chivian D, Kim DE, Malmström L, Bradley P, Robertson T, Murphy P, Strauss CE, BonneauR, Rohl CA, Baker D (2003) Automated prediction of CASP-5 structures using the Robettaserver. *Proteins*. 53(Suppl 6): 524-533.

- ❖ Chong LT, Duan Y, Wang L, Massova I, Kollman PA (1999) Molecular dynamics and free energy calculations applied to affinity maturation in antibody 48G7. *Proceeding of the National Academy of Sciences of the United States of America*. 96(25): 14330-14335.
- ❖ Chothia C, Lesk AM (1986) The relation between the divergence of sequence and structure in proteins. *EMBO Journal*. 5(4): 823-826.
- ❖ Clackson T, Wells JA (1995) A hot spot of binding energy in a hormone-receptor interface. *Science* 267(5196): 383-386.
- ❖ Colovos C, Yeates TO (1993) Verification of protein structures: patterns of nonbonded atomic interactions. *Protein Science*. 2(9): 1511-1519.
- ❖ Combet C, Jambon M, Deléage G, Geourjon C (2002) Geno3D: automatic comparative molecular modeling of protein. *Bioinformatics*. 18(1): 213-214.
- ❖ Cornell DW, Cieplak P, Bayly IC, Gould RI, Merz MK, Ferguson MD, Spellmeyer DC, Fox T, Caldwell WJ, Kollman A P (1995) 2nd generation force-field for the simulation of proteins, nucleic-acids, and organic molecules. *Journal of the American Chemical Society*. 117(19): 5179-5197.
- ❖ Cross JM, Clancy M, Shaw JR (2005) A polymorphic motif in the small subunit of ADP-glucose pyrophosphorylase modulates interactions between the small and large subunits. *The Plant Journal*. 41(4): 501-511.
- ❖ Cross JM, Clancy M, Shaw JR, Greene TW, Schmidt RR, Okita TW, Hannah LC (2004) Both subunits of ADP-glucose pyrophosphorylase are regulatory. *Plant Physiology*. 135(1): 137-144

- ❖ Cui M, Mezei M, Osman R (2008) Prediction of protein loop structures using a local move Monte Carlo approach and a grid-based force field. *Protein Engineering Design and Selection*. 21(12): 729-735.
- ❖ Dantas G, Corrent C, Reichow SL, Havranek JJ, Eletr ZM, Isern NG, Kuhlman B, Varani G, Merritt EA, Baker D (2007) High-resolution structural and thermodynamic analysis of extreme stabilization of human procarboxypeptidase by computational protein design. *Journal of Molecular Biology*. 366(4): 1209-1221.
- ❖ Darnell SJ, LeGault L, Mitchell JC (2008) KFC Server: interactive forecasting of protein interaction hot spots. *Nucleic Acids Research*. 36(Web Server issue): W265-W269.
- ❖ Darnell SJ, Page D, Mitchell JC (2007) An automated decision-tree approach to predicting protein interaction hot spots. *Proteins*. 68(4): 813-823.
- ❖ Davies JN, Cocking EC (1965) Changes in carbohydrates, proteins and nucleic acids during cellular development in tomato fruit locule tissue. *Planta*. 67: 242-253.
- ❖ De Genst E, Areskoug D, Decanniere K, Muyldermans S, Andersson K (2002) Kinetic and affinity predictions of a protein-protein interaction using multivariate experimental design. *The Journal of Biological Chemistry*. 277(33): 29897-29907.
- ❖ de Vries SJ, van Dijk M, Bonvin AM (2010) The HADDOCK web server for data-driven biomolecular docking. *Nature Protocols*. 5(5): 883-897.

- ❖ Dehury B, Sahu M, Sahu J, Sarma K, Sen P, Modi MK, Barooah M, Choudhury MD (2013) Structural analysis and molecular dynamics simulations of novel  $\delta$ -endotoxin Cry1Id from *Bacillus thuringiensis* to pave the way for development of novel fusion proteins against insect pests of crops. *Journal of Molecular Modelling*. 19(12): 5301-5316.
- ❖ deVries SJ, van Dijk M, Bonvin AM (2010) The HADDOCK web server for data-driven biomolecular docking. *Nature Protocols*. 5(5): 883-897.
- ❖ Dinar M, Stevens MA (1981) The relationship between starch accumulation and soluble solids content of tomato fruits. *Journal of the American Society for Horticultural Science*. 106: 415-418.
- ❖ Dominguez C, Boelens R, Bonvin AM (2003) HADDOCK: a protein-protein docking approach based on biochemical or biophysical information. *Journal of American Chemical Society*. 125(7): 1731-1737.
- ❖ Edwards GE and Walker DA (1983) C3, C4: Mechanisms of Cellular and Environmental Regulation of Photosynthesis. University of California Press, Berkeley.
- ❖ Eramian D, Shen MY, Devos D, Melo F, Sali A, Marti-Renom MA (2006) A composite score for predicting errors in protein structure models. *Protein Sciences*. 15(7): 1653-1666.
- ❖ Espada J (1962) Enzymic synthesis of adenosine diphosphate glucose from glucose-1-phosphate and adenosine triphosphate. *The Journal of Biological Chemistry*. 237: 3577-3581.

- ❖ Espadaler J, Fernandez-Fuentes N, Hermoso A, Querol E, Aviles FX, Sternberg MJ, Oliva B (2004) ArchDB: automated protein loop classification as a tool for structural genomics. *Nucleic Acids Research*. 32(Database issue): D185-D188.
- ❖ Ewing RM, Chu P, Elisma F, Li H, Taylor P, Climie S, McBroom-Cerajewski L, RobinsonMD, O'Connor L, Li M, Taylor R, Dharsee M, Ho Y, Heilbut A, Moore L, Zhang S, OrnatskyO, Bukhman YV, Ethier M, Sheng Y, Vasilescu J, Abu-Farha M, Lambert JP, Duewel HS, Stewart II, Kuehl B, Hogue K, Colwill K, Gladwish K, Muskat B, Kinach R, Adams SL, Moran MF, Morin GB, Topaloglou T, Figeys D (2007) Large-scale mapping of human protein-protein interactions by mass spectrometry. *Molecular Systems Biology*. 3: 89.
- ❖ Felsenstein J (1981) Evolutionary Trees from DNA Sequences: A Maximum Likelihood Approach. *Journal of Molecular Evolution*. 17: 368-376.
- ❖ Felts AK, Gallicchio E, Chekmarev D, Paris KA, Friesner RA, Levy RM (2008) Prediction of Protein Loop Conformations using the AGBNP Implicit Solvent Model and Torsion Angle Sampling. *Journal of Chemical Theory and Computation*. 4(5): 855-868.
- ❖ Fernandez-Fuentes N, Madrid-Aliste CJ, Rai BK, Fajardo JE, Fiser A (2007) M4T: a comparative protein structure modeling server. *Nucleic Acids Research*. 35(Web Server issue): W363-W368.
- ❖ Finn RD, Bateman A, Clements J, Coggill P, Eberhardt RY, Eddy SR, Heger A, Hetherington K, Holm L, Mistry J, Sonnhammer EL, Tate J, Punta M (2014) Pfam: the protein families database. *Nucleic Acids Research*. 42 (Database issue): D222-D230.



- ❖ Fitch WM, Margoliash E (1967) Construction of Phylogenetic Trees. *Science*. 155: 279-284.
- ❖ Friesner RA, Banks JL, Murphy RB, Halgren TA, Klicic JJ, Mainz DT, Repasky MP, Knoll EH, Shelley M, Perry JK, Shaw DE, Francis P, Shenkin PS (2004) Glide: a new approach for rapid, accurate docking and scoring. 1. Method and assessment of docking accuracy. *Journal of Medicinal Chemistry*. 47(7): 1739-1749.
- ❖ Frishman D, Argos P (1995) Knowledge-based protein secondary structure assignment. *Proteins*. 23(4): 566-579.
- ❖ Frueauf JB, Ballicora MA, Preiss J (2003) ADP-glucose pyrophosphorylase from potato tuber: site-directed mutagenesis of homologous aspartic acid residues in the small and large subunits. *The Plant Journal: for cell and molecular biology*. 33(3): 503-511.
- ❖ Fu Y, Ballicora MA, Leykam JF, Preiss J (1998b) Mechanism of reductive activation of potato tuber ADP-glucose pyrophosphorylase. *The Journal of Biological Chemistry*. 273(39): 25045-25052.
- ❖ Fujitani H, Tanida Y, Ito M, Jayachandran G, Snow CD, Shirts MR, Sorin EJ, Pande VS (2005) Direct calculation of the binding free energies of FKBP ligands. *The Journal of Chemical Physics*. 123(8): 084108.
- ❖ Ganguly B, Prasad S (2012) Homology modeling and functional annotation of bubaline pregnancy associated glycoprotein 2. *Journal of Animal Science and Biotechnology*. 3: 13.

- ❖ Gasteiger E, Hoogland C, Gattiker A, Duvaud S, Wilkins MR, Appel RD, Bairoch A (2005). Protein identification and analysis tools on the ExPASy Server. In: John M. Walker (ed): *The Proteomics Protocols Handbook*, Humana Press, pp 571-607.
- ❖ Geer LY, Domrachev M, Lipman DJ, Bryant SH (2002) CDART: protein homology by domain architecture. *Genome Research*. 12(10): 1619-1623.
- ❖ Gilson MK, Zhou HX (2007) Calculation of protein-ligand binding affinities. *Annual Review of Biophysics and Biomolecular Structure*. 36: 21-42.
- ❖ Ginalski K (2006) Comparative modeling for protein structure prediction. *Current Opinion in Structural Biology*. 16(2): 172-177.
- ❖ Giroux MJ, Hannah LC (1994) ADP-glucose pyrophosphorylase in shrunken-2 and brittle-2 mutants of maize. *Molecular & General Genetics*. 243(4): 400-408.
- ❖ Giroux MJ, Shaw J, Barry G, Cobb BG, Greene T, Okita T, Hannah LC (1996) A single mutation that increases maize seed weight. *Proceedings of the National Academy of Sciences of the United States of America*. 93(12): 5824-5829.
- ❖ Gohlke H, Kiel C, Case DA (2003) Insights into protein-protein binding by binding freeenergy calculation and free energy decomposition for the Ras-Raf and Ras-Ral GDS complexes. *Journal of Molecular Biology*. 330(4): 891-913.
- ❖ Gohlke H, Klebe G (2002) Approaches to the description and prediction of the bindingaffinity of small-molecule ligands to macromolecular receptors. *Angewandte Chemie (International Ed in English)*. 41(15): 2644-2676.
- ❖ Goldemberg J (2007) Ethanol for a sustainable energy future. *Science*. 315(5813): 808-810.

- ❖ Gomez-Casati DF, Iglesias AA (2002) ADP-glucose pyrophosphorylase from wheat endosperm. Purification and characterization of an enzyme with novel regulatory properties. *Planta*. 214(3): 428-434.
- ❖ Greene TW, Chantler SE, Kahn ML, Barry GF, Preiss J, Okita TW (1996) Mutagenesis of the potato ADPglucose pyrophosphorylase and characterization of an allosteric mutant defective in 3-phosphoglycerate activation. *Proceedings of the National Academy of Sciences of the United States of America*. 93(4): 1509-1513.
- ❖ Guerois R, Nielsen JE, Serrano L (2002) Predicting changes in the stability of proteins and protein complexes: a study of more than 1000 mutations. *Journal of Molecular Biology*. 320(2): 369-387.
- ❖ Guimarães CR, Boger DL, Jorgensen WL (2005) Elucidation of fatty acid amide hydrolase inhibition by potent alpha-ketoheterocycle derivatives from Monte Carlo simulations. *Journal of the American Chemical Society*. 127(49): 17377-17384.
- ❖ Halperin I, Wolfson H, Nussinov R (2004) Protein-protein interactions; coupling of structurally conserved residues and of hot spots across interfaces. Implications for docking. *Structure*. 12(6): 1027-1038.
- ❖ Hannah L, Tuschall D, Mans R (1980) Multiple forms of maize endosperm ADP-glucose pyrophosphorylase and their control by Shrunken-2 and Brittle-2. *Genetics*. 95(4): 961-970.

- ❖ Hannah LC, Nelson OE Jr. (1976) Characterization of ADP glucose pyrophosphorylase from shrunken 2 and brittle 2 mutants of maize. *Biochemical Genetics*. 14(7-8): 547- 560.
- ❖ Hartmann C, Antes I, Lengauer T (2007) IRECS: a new algorithm for the selection of most probable ensembles of side-chain conformations in protein models. *Protein Science*. 16(7): 1294-1307.
- ❖ Haugen TH, Ishaque A, Preiss J (1976) Biosynthesis of bacterial glycogen Characterization of the subunit structure of *Escherichia coli* B glucose 1 phosphate adenylyltransferase (EC 27727). *The Journal of Biological Chemistry*. 251(24): 7880-7885.
- ❖ Hizukuri S (1995) Starch: analytical aspects. In: Eliansson AC (ed) *Carbohydrates in Food*, pp 347-429. Marcel Dekker, New York.
- ❖ Holder M, Lewis PO (2003) Phylogeny estimation: traditional and Bayesian approaches. *Nature Reviews Genetics*. 4: 275-284.
- ❖ Hu Z, Ma B, Wolfson H, Nussinov R (2000) Conservation of polar residues as hot spots at protein interfaces. *Proteins*. 39(4): 331-342.
- ❖ Huey R, Morris GM, Olson AJ, Goodsell DS (2007) A semiempirical free energy force field with charge-based desolvation. *Journal of Computational Chemistry*. 28(6): 1145-1152.
- ❖ Huo S, Massova I, Kollman PA (2002) Computational alanine scanning of the human growth hormone-receptor complex. *Journal of Computational Chemistry*. 23(1): 15-27.

- ❖ Hwang SK, Hamada S, Okita TW (2006) ATP binding site in the plant ADP-glucose pyrophosphorylase large subunit. *FEBS Letters*. 580(28-29): 6741-6748.
- ❖ Hwang SK, Nagai Y, Kim D, Okita TW (2008) Direct appraisal of the potato tuber ADP-glucose pyrophosphorylase large subunit in enzyme function by study of a novel mutant form. *The Journal of Biological Chemistry*. 283(11): 6640-6647.
- ❖ Hwang SK, Salamone PR, Okita TW (2005) Allosteric regulation of the higher plant ADP-glucose pyrophosphorylase is a product of synergy between the two subunits. *FEBS Letter*. 579(5): 983-990
- ❖ Iglesias AA, Barry GF, Meyer C, Bloksberg L, Nakata PA, Greene T, Laughlin MJ, Okita TW, Kishore GM, Preiss J. (1993) Expression of the potato tuber ADP-glucose pyrophosphorylase in *Escherichia coli*. *The Journal of Biological Chemistry*. 268(2): 1081-1086.
- ❖ Iglesias AA, Barry GF, Meyer C, Bloksberg L, Nakata PA, Greene T, Laughlin MJ, Okita TW, Kishore GM, Preiss J (1993) Expression of the potato tuber ADP-glucose pyrophosphorylase in *Escherichia coli*. *The Journal of Biological Chemistry*. 268(2): 1081-1086.
- ❖ Iglesias AA, Preiss J (1992) Bacterial glycogen and plant starch biosynthesis. *Biochemical Education*. 20(4): 196-203.
- ❖ Ito T, Chiba T, Yoshida M (2001) Exploring the protein interactome using comprehensive two-hybrid projects. *Trends in Biotechnology*. 19(Suppl 10): S23-S27.

- ❖ Jacobson MP, Pincus DL, Rapp CS, Day TJ, Honig B, Shaw DE, Friesner RA (2004) Ahierarchical approach to all-atom protein loop prediction. *Proteins*. 55(2): 351-367.
- ❖ Jin XS, Ballicora MA, Preies J, Geiger JH (2005) Crystal structure of potato tuberADP-glucose pyrophosphorylase. *The EMBO Journal*. 24(4): 694-704.
- ❖ Jones DA, Jones JDG (1997) The role of leucine-rich repeat protein in plant defense. *Advances in Botanical Research*. 24: 89-167.
- ❖ Jones P, Binns D, Chang HY, Fraser M, Li W, McAnulla C, McWilliam H, Maslen J, Mitchell A, Nuka G, Pesseat S, Quinn AF, Sangrador-Vegas A, Scheremetjew M, Yong SY, Lopez R, Hunter S (2014) InterProScan 5: genome-scale protein function classification. *Bioinformatics*. 30(9): 1236-1240.
- ❖ Jorgensen WL (1991) Rusting of the lock and key model for protein-ligand binding. *Science*. 254(5034): 954-955.
- ❖ Kamaraj B, Purohit R (2013) In-silico analysis of Betaine AldehydeDehydrogenase2 of *Oryza sativa* and significant mutations responsible for fragrance. *Journal of Plant Interactions*. 8: 321-333.
- ❖ Kashyap S (2013) *In Silico* modeling and functional interpretations of Cry1Ab15 toxin from *Bacillus thuringiensis* BtB-Hm-16. *BioMed Research International*. 2013: 471636.
- ❖ Kavakli IH, Greene TW, Salamone PR, Choi S, Okita T W (2001) Investigation of subunit function in ADP-glucose pyrophosphorylase. *Biochemical and Biophysical Research Communications*. 281(3): 783-787.

- ❖ Kavakli IH, Kato C, Choi SB, Kim KH, Salamone PR, Ito H, Okita TW (2002) Generation, characterization, and heterologous expression of wild-type and up-regulated forms of *Arabidopsis thaliana* leaf ADP-glucose pyrophosphorylase. *Planta*. 215(3): 430-439.
- ❖ Kavakli IH, Park JS, Slattery CJ, Salamone PR, Frohlick J, Okita TW (2001) Analysis of allosteric effector binding sites of potato ADP-glucose pyrophosphorylase through reverse genetics. *The Journal of Biological Chemistry*. 276(44): 40834-40840.
- ❖ Kelley LA, Sternberg MJE (2009) Protein structure prediction on the web: a case study using the Phyre server. *Nature Protocols*. 4(3): 363-371
- ❖ Kitchen DB, Decornez H, Furr JR, Bajorath J (2004) Docking and scoring in virtual screening for drug discovery: methods and applications. *Nature Reviews. Drug Discovery* 3(11): 935-949.
- ❖ Kleczkowski LA (2000) Is leaf ADP-glucose pyrophosphorylase an allosteric enzyme? *Biochimica et Biophysica Acta*. 1476(1): 103-108.
- ❖ Kleczkowski LA, Villand P, Lüthi E, Olsen OA, Preiss J (1993c) Insensitivity of barley endosperm ADP-Glc pyrophosphorylase to 3-phosphoglycerate and orthophosphate regulation. *Plant Physiology*. 101(1): 179-186.
- ❖ Koehler P, Weiser H (2013) Chapter 2: Chemistry of cereal grains. In: M. Gobbetti and M. Ganzle (eds.), *Handbook on Sourdough Biotechnology*, Springer Science + Business Media, New York, pp 11-45.
- ❖ Kokh DB, Wenzel W (2008) Flexible side chain models improve enrichment rates in in silico screening. *Journal of Medicinal Chemistry*. 51(19): 5919-5931.

- ❖ Kolodny R, Kosloff M (2013) From protein structure to function via computational tools and approaches. *Israel Journal of Chemistry*. 53(3-4): 147-156.
- ❖ Kong L, Ranganathan S (2004) Delineation of modular proteins: domain boundary prediction from sequence information. *Briefings in bioinformatics*. 5(2): 179-192.
- ❖ Kortemme T, Baker D (2002) A simple physical model for binding energy hot spots in protein-protein complexes. *Proceedings of the National Academy of Sciences of the United States of America*. 99(22): 14116-21.
- ❖ Kozakov D, Beglov D, Bohnuud T, Mottarella SE, Xia B, Hall DR, Vajda S (2013) How good is automated protein docking? *Proteins*. 81(2): 2159-2166.
- ❖ Kryshchuk A, Fidelis K, Mouton R (2007) Progress from CASP6 to CASP7. *Proteins*. 69(Suppl 8): 194-207.
- ❖ Kurowski MA, and Bujnicki JM. (2003). GeneSilico protein structure prediction meta-server. *Nucleic Acids Research*. 31(13): 3305-3307.
- ❖ La Cognata U, Willmitzer L, Muller-Rober B (1995) Molecular cloning and characterization of novel isoforms of potato ADP-glucose pyrophosphorylase. *Molecular & General Genetics*. 246(5): 538-548.
- ❖ Lakshmanan M, Mohanty B, Lee D Y (2013) Identifying essential genes/reactions of the rice photorespiration by in silico model-based analysis. *Rice*. 6: 1-5.
- ❖ Larsson P, Wallner B, Lindahl E, Elofsson A (2008) Using multiple templates to improve quality of homology models in automated homology modeling. *Protein Science*. 17(6): 990-1002.



- ❖ Laskowski RA, MacArthur MW, Moss DS, Thornton JM (1993) PROCHECK-a program to check the stereochemical quality of protein structures. *Journal of Applied Crystallography*. 26(2): 283-291.
- ❖ Laskowski RA, Watson JD, Thornton JM (2005) ProFunc: a server for predicting protein function from 3D structure. *Nucleic Acids Research*. 33(Web Server issue): W89-W93.
- ❖ Laughlin MJ, Payne JW, Okita TW (1998) Substrate binding mutants of the higher plant ADP-glucose pyrophosphorylase. *Phytochemistry*. 47(4): 621-629.
- ❖ Le Gac G, Ka C, Joubrel R, Gourlaouen I, Lehn P, Mornon JP, Férec C, Callebaut I (2013) Structure-function analysis of the human ferroportin iron exporter (SLC40A1): effect of hemochromatosis type 4 disease mutations and identification of critical residues. *Human Mutation*. 34(10): 1371-1380.
- ❖ Lengauer T, Rarey M (1996) Computational methods for biomolecular docking. *Current Opinion in Structural Biology*. 6(3): 402-406.
- ❖ Lensink MF, Méndez R, Wodak SJ (2007) Docking and scoring protein complexes: CAPRI3rd Edition. *Proteins*. 69(4): 704-718.
- ❖ Letunic I, Doerks T and Bork P (2012) SMART 7: recent updates to the protein domain annotation resource. *Nucleic Acids Research*. 40 (Database issue): D302-D305.
- ❖ Lin TP, Caspar T, Somerville C and Preiss J (1988a) A starch deficient mutant of *Arabidopsis thaliana* with low ADPglucose pyrophosphorylase activity lacks one of the two subunits of the enzyme. *Plant Physiol*. 88(4): 1175-1181.

- ❖ Lin TP, Caspar T, Somerville C, Preiss J (1988b) Isolation and characterization of a starchless mutant of *Arabidopsis thaliana* L. Henyh lacking ADPglucose pyrophosphorylase activity. *Plant Physiology*. 86(4): 1131-1135.
- ❖ Ma B, Elkayam T, Wolfson H, Nussinov R (2003) Protein-protein interactions: structurally conserved residues distinguish between binding sites and exposed protein surfaces. *Proceeding of the National Academy of Sciences of the United States of America*. 100(10): 5772-5777.
- ❖ Mandell JG, Roberts VA, Pique ME, Kotlovyi V, Mitchell JC, Nelson E, Tsigelny I, TenEyck LF (2001) Protein docking using continuum electrostatics and geometric fit. *Protein Engineering*. 14(2): 105-113.
- ❖ Manners DJ, Matheson NK (1981) The fine structure of amylopectin. *Carbohydrate Research*. 90: 99-110.
- ❖ Manning JR, Bailey MA, Soares DC, Dunbar DR, Mullins JJ (2010) In silico structure-function analysis of pathological variation in the HSD11B2 gene sequence. *Physiological Genomics*. 42(3): 319-330.
- ❖ Marchler-Bauer A, Lu S, Anderson JB, Chitsaz F, Derbyshire MK, DeWeese-Scott C, Fong JH, Geer LY, Geer RC, Gonzales NR, Gwadz M, Hurwitz DI, Jackson JD, Ke Z, Lanczycki CJ, Lu F, Marchler GH, Mullokandov M, Omelchenko MV, Robertson CL, Song JS, Thanki N, Yamashita RA, Zhang D, Zhang N, Zheng C, Bryant SH (2011) CDD: a Conserved Domain Database for the functional annotation of proteins. *Nucleic Acids Research*. 39(Database Issue): D225-D229.

- ❖ Marrero-Ponce Y, Medina-Marrero R, Torrens F, Martinez Y, Romero-Zaldivar V, Castro EA (2005) Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: a promising approach for modeling of antibacterial activity. *Bioorganic and Medicinal Chemistry*. 13(8): 2881-2899.
- ❖ Martin C, Smith AM (1995) Starch biosynthesis. *Plant Cell*. 7(7): 971-985.
- ❖ Marti-Renom MA, Madhusudhan MS, Sali A (2004) Alignment of protein sequences by their profiles. *Protein Science*. 13(4): 1071-1087.
- ❖ Matheson NK (1996) The chemical structure of amylose and amylopectin fractions of starch from tobacco leaves during development and diurnally-nocturnally. *Carbohydrate Research*. 282(2): 247-262.
- ❖ McGuffin LJ (2007) Benchmarking consensus model quality assessment for protein fold recognition. *BMC Bioinformatics*. 8: 345.
- ❖ McGuffin LJ (2008) Intrinsic disorder prediction from the analysis of multiple protein fold recognition models. *Bioinformatics*. 24(16): 1798-1804.
- ❖ Melo F, Feytmans E (1998) Assessing protein structures with a non-local atomic interaction energy. *Journal of Molecular Biology*. 277(5): 1141-1152.
- ❖ Mereghetti P, Ganadu ML, Papaleo E, Fantucci P, De Gioia L (2008) Validation of protein models by a neural network approach. *BMC Bioinformatics*. 9: 66.
- ❖ Michel J, Verdonk ML, Essex JW (2006) Protein-ligand binding affinity predictions by implicit solvent simulations: a tool for lead optimization? *Journal of Medicinal Chemistry*. 49(25): 7427-7439.
- ❖ Mobley DL, Dill KA (2009) Binding of small-molecule ligands to proteins: "what you see" is not always "what you get". *Structure*. 17(4): 489-498.

- ❖ Montgomerie S, Cruz JA, Shrivastava S, Arndt D, Berjanskii M, Wishart DS (2008) PROTEUS2: a web server for comprehensive protein structure prediction and structure-based annotation. *Nucleic Acids Research*. 36(Web Server issue): W202-W209.
- ❖ Mooney BP (2009) The second green revolution? Production of plant-based biodegradable plastics. *The Biochemical Journal*. 418(2): 219-232.
- ❖ Morrison WR, Karkalas J (1990) Starch. In: Dey PM (ed) *Methods in Plant Biochemistry*, pp 323-352. Academic Press, London.
- ❖ Morrison WR, Karkalas J (1990) Starch. In: Dey PM (ed) *Methods in Plant Biochemistry*, pp 323-352. Academic Press, London.
- ❖ Muller-Rober B, Sonnewald U, Willmitzer L(1992) Inhibition of the ADP-glucose pyrophosphorylase in transgenic potatoes leads to sugar-storing tubers and influences tuber formation and expression of tuber storage protein genes. *The EMBO Journal*. 11(4): 1229-1238.
- ❖ Murtagh F (1984) Complexities of Hierarchic Clustering Algorithms: The State of the Art. *Computational Statistics Quarterly*. 1: 101-113.
- ❖ Neuhaus HE, Stitt M (1990) Control analysis of photosynthate partitioning: Impact of reduced activity of ADPglucose pyrophosphorylase or plastid phosphoglucomutase on the fluxes to starch and sucrose in *Arabidopsis*. *Planta*. 182: 445-454.
- ❖ Obiol-Pardo C, Rubio-Martinez J (2007) Comparative evaluation of MMPBSA and XSCOREto compute binding free energy in XIAP-peptide complexes. *Journal of Chemical Information and Modelling*. 47(1): 134-142.

- ❖ Ofraan Y, Rost B (2007) Protein-protein interaction hotspots carved into sequences. *PLoS Computational Biology*. 3(7): e119.
- ❖ Ohlson T, Wallner B, Elofsson A (2004) Profile-profile methods provide improved fold recognition: a study of different profile-profile alignment methods. *Proteins*. 57(1): 188-197.
- ❖ Okita T, Nakata P, Anderson J, Sowokinos J, Morell M, Preiss J (1990) The subunit structure of potato tuber ADP glucose pyrophosphorylase. *Plant Physiology*. 93(2): 785-790.
- ❖ Olson MA, Feig M, Brooks CL 3rd (2008) Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. *Journal of Computational Chemistry*. 29(5): 820-831.
- ❖ Outlaw Jr WH, Manchester J (1979) Guard cells starch concentration quantitatively related to stomatal aperture. *Plant Physiology*. 64(1): 79-82.
- ❖ Peng HP, Yang AS (2007) Modeling protein loops with knowledge-based prediction of sequence-structure alignment. *Bioinformatics*. 23(21): 2836-2842.
- ❖ Peng J, Xu J (2010) Low-homology protein threading. *Bioinformatics*. 26(12): i294-300.
- ❖ Petersen TN, Brunak S, von Heijne G, Nielsen H (2011) SignalP 4.0: discriminating signal peptides from transmembrane regions. *Nature Methods*. 8(10): 785-786.
- ❖ Peterson JA, Graham SE (1998) A close family resemblance: the importance of structure in understanding cytochromes P450. *Structure*. 6(9): 1079-1085.

- ❖ Petrey D, Xiang Z, Tang CL, Xie L, Gimpelev M, Mitros T, Soto CS, Goldsmith-Fischman S, Kernytsky A, Schlessinger A, Koh IY, Alexov E, Honig B (2003) Using multiple structure alignments, fast model building, and energetic analysis in fold recognition and homology modeling. *Proteins*. 53(Suppl 6): 430-435.
- ❖ Pettitt CS, McGuffin LJ, Jones DT (2005) Improving sequence-based fold recognition by using 3D model quality assessment. *Bioinformatics*. 21(17): 3509-3515.
- ❖ Plaxton WC, Preiss J (1987) Purification and properties of non proteolytically degraded ADPglucose pyrophosphorylase from maize endosperm. *Plant Physiology*. 83(1): 105-112.
- ❖ Preiss J (1984) Bacterial glycogen synthesis and its regulation. *Annual Review of Microbiology*. 38: 419-458.
- ❖ Preiss J (1991) Biology and molecular biology of starch synthesis and its regulation *Plant Molecular and Cellular Biology*. 7: 59-114.
- ❖ Preiss J (1999) Biosynthesis of bacterial and mammalian glycogen and plant starch synthesis and their regulation. In: Hecht SM (ed) *Biorganic Chemistry: carbohydrates*, pp 489-554. Oxford University Press, Oxford.
- ❖ Preiss J, Sivak MN (1998a) Starch and glycogen biosynthesis. In: Pinto BM (ed) *Comprehensive Natural Products Chemistry*, pp 441-495. Pergamon Press, Oxford.
- ❖ Preiss J, Sivak MN (1998b) Biochemistry, molecular biology and regulation of starch synthesis. *Genetic Engineering*. 20: 177-223.

- ❖ Prioul JL, Jeannette E, Reyss A, Grégory N, Giroux M, Hannah LC, Causse M (1994) Expression of ADP-glucose pyrophosphorylase in maize (*Zea mays* L.) grain and source leaf during grain filling. *Plant Physiology*. 104(1): 179-187.
- ❖ Qiu J, Sheffler W, Baker D, Noble WS (2008) Ranking predicted protein structures with support vector regression. *Proteins*. 71(3): 1175-1182.
- ❖ R. Luthy, J. U. Bowie, and D. Eisenberg (1992) Assessment of protein models with three-dimensional profiles. *Nature*. 356(6364): 83-85.
- ❖ Rai DK, Rieder E (2012) Homology modeling and analysis of structure predictions of the bovine rhinitis B virus RNA dependent RNA polymerase (RdRp). *International Journal of Molecular Sciences*. 13(7): 8998-9013.
- ❖ Rajamani D, Thiel S, Vajda S, Camacho CJ (2004) Anchor residues in protein-protein interactions. *Proceeding of the National Academy of Sciences of the United States of America*. 101(31): 11287-11292.
- ❖ Raman S, Vernon R, Thompson J, Tyka M, Sadreyev R, Pei J, Kim D, Kellogg E, DiMaio F, Lange O, Kinch L, Sheffler W, Kim BH, Das R, Grishin NV, Baker D (2009) Structure prediction for CASP8 with all-atom refinement using Rosetta. *Proteins*. 77(Suppl 9): 89-99.
- ❖ Randall A, Baldi P (2008) SELECTpro: effective protein model selection using a structure based energy function resistant to BLUNDERs. *BMC Structural Biology*. 8: 52.
- ❖ Rarey M, Kramer B, Lengauer T, Klebe G (1996) A fast flexible docking method using an incremental construction algorithm. *Journal of Molecular Biology*. 261(3): 470-489.

- ❖ Ritte G, Raschke K (2003) Metabolite export of isolated guard cell chloroplasts of *Vicia faba*. *New Phytologist*. 159: 195-202.
- ❖ Roy A, Kucukural A, and Zhang Y. (2010). I-TASSER: A unified platform for automated protein structure and function prediction. *Nature Protocols*. 5(4): 725-738.
- ❖ Roy SS, Dasgupta R, Bagchi A (2014) A review on Phylogenetics analysis: A Journey through Modern Era. *Computational Molecular Bioscience*. 4(3): 521816.
- ❖ Rzhetsky A, Nei M (1993) Theoretical Foundation of the Minimum-Evolution Method of Phylogenetic Inference. *Molecular Biology and Evolution*. 10: 1073-1095.
- ❖ Sachs J (1887) In: Ward HM (ed) *Lectures of the Physiology of Plants*, pp 304-325. Clarendon Press, Oxford.
- ❖ Saitou N, Nei M (1987) The neighbor-joining method: a new method for reconstructing phylogenetic tree. *Molecular Biology and Evolution*. 4(4): 406-425.
- ❖ Salamone PR, Greene TW, Kavakli IH, Okita TW (2000) Isolation and characterization of a higher plant ADP-glucose pyrophosphorylase small subunit homotetramer *FEBS Letters* 482(1-2): 113-118.
- ❖ Salamone PR, Kavakli IH, Slattery CJ, Okita TW (2002) Directed molecular evolution of ADP-glucose pyrophosphorylase. *Proceedings of the National Academy of Sciences of the United States of America*. 99(2): 1070-1075.
- ❖ Sali A, Blundell TL (1993) Comparative protein modelling by satisfaction of spatial restraints. *Journal of Molecular Biology*. 234(3): 779-815.



- ❖ Sali A, Potterton L, Yuan F, van Vlijmen H, Karplus M (1995) Evaluation of comparative protein modeling by MODELLER. *Proteins*. 23(3): 318-326.
- ❖ Sándor M, Kiss R, Keseru GM (2010) Virtual fragment docking by Glide: a validation study on 190 protein-fragment complexes. *Journal of Chemical Information and Modelling*. 50(6): 1165-1172.
- ❖ Sarma K, Dehury B, Sahu J (2012) A comparative proteomic approach to analyse structure, function and evolution of rice chitinases: a step towards increasing plant fungal resistance. *Journal of Molecular Modeling*. 18(11): 4761-4780.
- ❖ Schaffer AA, Petreikov M (1997) Sucrose-to-starch metabolism in tomato fruit undergoing transient starch accumulation. *Plant Physiology*. 113:739-746.
- ❖ Schwede T, Kopp J, Guex N, Peitsch MC (2003) SWISS-MODEL: An automated protein homology-modeling server. *Nucleic Acids Research*. 31(13): 3381-3385.
- ❖ Schymkowitz J, Borg J, Stricher F, Nys R, Rousseau F, Serrano L (2005) The FoldX webserver: an online force field. *Nucleic Acids Research*. 33(Web Server issue): W382-W388.
- ❖ Sievers F, Wilm A, Dineen D, Gibson TJ, Karplus K, Li W, Lopez R, McWilliam H, Remmert M, Soding J, Thompson JD, Higgins DG (2011) Fast, Scalable generation of high-quality protein multiple sequence alignments using Clustal Omega. *Molecular System Biology* 7:539.
- ❖ Simons KT, Kooperberg C, Huang E, Baker D (1997) Assembly of protein tertiary structures from fragments with similar local sequences using simulated annealing and Bayesian scoring functions. *Journal of Molecular Biology*. 268(1): 209-225.

- ❖ Simonson T, Archontis G, Karplus M (2002) Free energy simulations come of age: protein ligand recognition. *Accounts of Chemical Research*. 35(6): 430-437.
- ❖ Singh BK, Greenberg E, Preiss J (1984) ADPglucose pyrophosphorylase from the CAM plants *Hoya carnosa* and *Xerosicyos danguyi*. *Plant Physiology*. 74(3): 711-716.
- ❖ Singletary GW, Banisadr R, Keeling PL (1994) Heat stress during grain filling in maize: effects of carbohydrate storage and metabolism. *Australian Journal of Plant Physiology*. 21(6): 829-841.
- ❖ Sivak MN, Preiss J (1998) Starch: basic science to biotechnology. In: Taylor SL (ed) *Advances in Food and Nutrition Research*, pp 1-199. Academic Press, San Diego, California.
- ❖ Slattery CJ, Kavakli IH, Okita TW (2000) Engineering starch for increased quantity and quality. *Trends in Plant Science*. 5(7): 291-298.
- ❖ Smidansky ED, Clancy M, Meyer FD, Lanning SP, Blake NK, Talbert LE, Giroux MJ (2002) Enhanced ADPglucose pyrophosphorylase activity in wheat endosperm increases seed yield. *Proceedings of the National Academy of Sciences of the United States of America*. 99(3): 1724-1729.
- ❖ Smidansky ED, Martin JM, Hannah LC, Fischer AM, Giroux MJ (2003) Seed yield and plant biomass increases in rice are conferred by deregulation of endosperm ADP-glucose pyrophosphorylase. *Planta*. 216(4): 656-664.
- ❖ Smith GR, Sternberg MJ (2002) Prediction of protein-protein interactions by docking methods. *Current Opinion in Structural Biology*. 12(1): 28-35.

- ❖ Smith-White BJ, Preiss J (1992) Comparison of proteins of ADP-glucose pyrophosphorylase from diverse sources. *Journal of Molecular Evolution*. 34(5): 449-464.
- ❖ Sober E (1983) Parsimony in Systematics: Philosophical Issues. *Annual Review of Ecology and Systematics*. 14: 335-357.
- ❖ Soding J (2005) Protein homology detection by HMM-HMM comparison. *Bioinformatics*. 21(7): 951-960.
- ❖ Soto CS, Fasnacht M, Zhu J, Forrest L, Honig B (2008) Loop modeling: Sampling, filtering, and scoring. *Proteins*. 70(3): 834-843.
- ❖ Sowokinos J, Preiss J (1982) Pyrophosphorylases in *Solanum tuberosum* III Purification, physical, and catalytic properties of ADP glucose pyrophosphorylase in potatoes. *Plant Physiology*. 69(6): 1459-1466.
- ❖ Spassov VZ, Flook PK, Yan L (2008) LOOPER: a molecular mechanics-based algorithm for protein loop prediction. *Protein Engineering Design and Selection*. 21(2): 91-100.
- ❖ Spassov VZ, Yan L, Flook PK. (2007) The dominant role of side-chain backbone interactions in structural realization of amino acid code. ChiRotor: a side-chain prediction algorithm based on side-chain backbone interactions. *Protein Science*. 16(3): 494-506.
- ❖ Stark DM, Timmerman KP, Barry GI, Preiss J, Kishore GM (1992) Regulation of the amount of starch in plant tissues by ADP glucose pyrophosphorylase. *Science*. 258(5080): 287-292.

- ❖ Sternberg MJ, Aloy P, Gabb HA, Jackson RM, Moont G, Querol E, Aviles FX (1998) Acomputational system for modelling flexible protein-protein and protein-DNA docking. *Proceedings/ International Conference on Intelligent Systems for Molecular Biology*. 6: 183-192.
- ❖ Stoddard BL, Koshland DE Jr (1992) Prediction of the structure of a receptor-proteincomplex using a binary docking method. *Nature*. 358(6389): 774-776.
- ❖ Tamura K, Stecher G, Peterson D, Filipski A, Kumar S (2013) MEGA6: Molecular Evolutionary Genetics Analysis version 6.0. *Molecular Biology and Evolution*. 30(12): 2725-2729.
- ❖ Tang CL, Xie L, Koh IY, Posy S, Alexov E, Honig B (2003) On the role of structuralinformation in remote homology detection and sequence alignment: new methods usinghybrid sequence profiles. *Journal of Molecular Biology*. 334(5): 1043-1062.
- ❖ Taylor RD, Jewsbury PJ, Essex JW (2002) A review of protein-small molecule dockingmethods. *Journal of Computer Aided Molecular Design*. 16(3): 151-166.
- ❖ Thorsell AG, Lee WH, Persson C (2011) Comparative structural analysis of lipid binding START domains. *PLoS ONE*. 6(6): e19521.
- ❖ Tiessen A, Hendriks JH, Stitt M, Branscheid A, Gibon Y, Farre EM, Geigenberger P (2002) Starch synthesis in potato tubers is regulated by post-translational redox modification of ADP-glucose pyrophosphorylase: a novel regulatory mechanism linking starch synthesis to the sucrose supply. *Plant Cell*. 14(9): 2191-2213.

- ❖ Tsai CY, Nelson OE (1966) Starch-deficient maize mutant lacking adenosine diphosphate glucose pyrophosphorylase activity. *Science*. 151(3708): 341-343.
- ❖ Tuncel A, Kavakli IH, Keskin O (2008) Insights into Subunit Interactions in the Heterotetrameric Structure of Potato ADP-Glucose Pyrophosphorylase. *Biophysical Journal*. 95: 3628-3639.
- ❖ Uetz P, Giot L, Cagney G, Mansfield TA, Judson RS, Knight JR, Lockshon D, Narayan V, Srinivasan M, Pochart P, Qureshi-Emili A, Li Y, Godwin B, Conover D, Kalbfleisch T, Vijayadamodar G, Yang M, Johnston M, Fields S, Rothberg JM (2000) A comprehensive analysis of protein-protein interactions in *Saccharomyces cerevisiae*. *Nature*. 403(6770): 623-627.
- ❖ Vakser IA (1997) Evaluation of GRAMM low-resolution docking methodology on the hemagglutinin-antibody complex. *Proteins. Suppl* 1: 226-230.
- ❖ Van den Koornhuysen N, Libessart N, Delrue B, Zabawinski C, Decq A, Iglesias A, Carton A, Preiss J, Ball S (1996) Control of starch composition and structure supply in the monocellular alga *Chlamydomonas reinhardtii*. *The Journal of Biological Chemistry*. 271(27): 16281-16287.
- ❖ Ventriglia T, Kuhn ML, Ruiz MT, Ribeiro-Pedro M, Valverde F, Ballicora MA, Preiss J, Romero JM (2008) Two *Arabidopsis* ADP-Glucose Pyrophosphorylase Large Subunits (APL1 and APL2) Are Catalytic<sup>1</sup>. *Plant Physiology*. 148: 65-76.
- ❖ Villand P, Aalen R, Olsen OA, Lüthi E, Lönneborg A, Kleczkowski LA (1992a) PCR amplification and sequences of cDNA clones for the small and large subunits of ADP-glucose pyrophosphorylase from barley tissues. *Plant Molecular Biology*. 19(3): 381-389.

- ❖ Villand P, Olsen OA, Kleczkowski LA (1993) Molecular characterization of multiple cDNA clones of ADP-glucose pyrophosphorylase from *Arabidopsis thaliana*. *Plant Molecular Biology*. 23(6), 1279- 1284.
- ❖ Wallner B, Fang H, Elofsson A (2003) Automatic consensus-based fold recognition using Pcons, ProQ, and Pmodeller. *Proteins*. 53(Suppl 6): 534-541.
- ❖ Wallner B, Larsson P, Elofsson A (2007) Pcons.net: protein structure prediction meta server. *Nucleic Acids Research*. 35(Web Server issue): W369-W374.
- ❖ Wallrapp FH, Pan JJ, Ramamoorthy G (2013) Prediction of function for the polyprenyl transferase subgroup in the isoprenoid synthase superfamily. *Proceedings of the National Academy of Sciences of the United States of America*. 110(13): E1196-E1202.
- ❖ Wang R, Lu Y, Wang S (2003) Comparative evaluation of 11 scoring functions for molecular docking. *Journal of Medicinal Chemistry*. 46(12): 2287-2303.
- ❖ Warren GL, Andrews CW, Capelli AM, Clarke B, LaLonde J, Lambert MH, Lindvall M, Nevins N, Semus SF, Senger S, Tedesco G, Wall ID, Woolven JM, Peishoff CE, Head MS (2006) Critical assessment of docking programs and scoring functions. *Journal of Medicinal Chemistry*. 49(20): 5912-5931.
- ❖ Watson JD, Laskowski RA, Thornton JM (2005) Predicting protein function from structure and structural data. *Current Opinion in Structural Biology* 15(3): 275-284.
- ❖ Weber H, Heim U, Borisjuk L, Wobus U (1995) Cell-type specific, coordinate expression of two ADP-glucose pyrophosphorylase genes in relation to starch biosynthesis during seed development of *Vicia faba* L. *Planta*. 195(3): 352-61.

- ❖ Wei BQ, Weaver LH, Ferrari AM, Matthews BW, Shoichet BK (2004) Testing a flexible receptor docking algorithm in a model binding site. *Journal of Molecular Biology*. 337(5): 1161-1182.
- ❖ Wei Y, Thompson J, Floudas CA (2012) CONCORD: a consensus method for protein secondary structure prediction via mixed integer linear optimization. *Proceeding of the Royal Society A*. 468: 831-850.
- ❖ Wenzel W, Hamacher K (1999) Stochastic tunneling approach for global minimization of complex potential energy landscapes. *Physical Review Letters*. 82: 3003-3007.
- ❖ Wheeler WC, Lucarini N, Hong L, Crowley LM, Varon A (2014) POY version 5: phylogenetic analysis using dynamic homologies under multiple optimality criteria. *Cladistics*. 31(2): 189-196.
- ❖ Wiederstein S (2007) ProSA-web: interactive web service for the recognition of errors in three-dimensional structures of proteins. *Nucleic Acids Research* 35(Web Server issue): W407-W410.
- ❖ Wiehe K, Peterson MW, Pierce B, Mintseris J, Weng Z (2008) Protein-protein docking: overview and performance analysis. *Methods in Molecular Biology*. 413: 283-314.
- ❖ Witz S, Panwar P, Schober M (2014) Structure-function relationship of a plant NCS1 member-homolog modeling and mutagenesis identified residues critical for substrate specificity of PLUTO, a nucleobase transporter from arabidopsis. *PLoS ONE*. 9: e91343.

- ❖ Wootton JC (1994) Non-globular domains in protein sequences: automated segmentation using complexity measures. *Computers and Chemistry*. 18(3): 269-285.
- ❖ Wu G, Robertson DH, Brooks CL, Vieth M (2003) Detailed analysis of grid-based molecular docking: a case study of CDOCKER-a CHARMM-based MD docking algorithm. *Journal of Computational Chemistry*. 24(13): 1549- 562.
- ❖ Wu GS, Robertson DH, Brooks CL, Michal V (2003) Detailed analysis of grid based molecular docking: a case study of CDOCKER-A CHARMM-based MD docking algorithm, *Journal of Computational Chemistry*. 24(13):1549-1562.
- ❖ Wu S, Zhang Y (2007) LOMETS: a local meta-threading-server for protein structure prediction. *Nucleic Acids Research*. 35(10): 3375-3382.
- ❖ Xiang Y, Cao Y, Xu C, Li X, Wang S. Xa3 (2006) Conferring resistance for rice bacterial blight and encoding a receptor kinase-like protein, is the same as Xa26. *Theoretical and Applied Genetics*. 113(7): 1347-1355.
- ❖ Xiang Z, Soto CS, Honig B (2002) Evaluating conformational free energies: the colony energy and its application to the problem of loop prediction. *Proceeding of the National Academy of Sciences of the United States of America*. 99(11): 7432-7437.
- ❖ Xu R, Zhang S, Huang J, Zheng C (2013) Genome-wide comparative in silico analysis of the RNA helicase gene family in *Zea mays* and *Glycine max*: a comparison with *Arabidopsis* and *Oryza sativa*. *PLoS ONE*. 8: e78982.



- ❖ Yan A, Kloczkowski A, Hofmann H, Jernigan RL (2007) Prediction of side chain orientations in proteins by statistical machine learning methods. *Journal of Biomolecular Structure and Dynamics*. 25(3): 275-288.
- ❖ Yogurtcu ON, Erdemli SB, Nussinov R, Turkay M, Keskin O (2008) Restricted mobility of conserved residues in protein-protein interfaces in molecular simulations. *Biophysics Journal*. 94(9): 3475-3485.
- ❖ Zaki MJ, Bystroff C (2008) Protein structure prediction. Preface. *Methods in Molecular Biology*. 413: v-vii.
- ❖ Zeiger E, Talbott LD, Frechilla S, Srivastava A, Zhu J (2002) The guard cell chloroplast: a perspective for the twenty-first century. *New Phytologist*. 153: 415-424.
- ❖ Zhang W, Duan Y (2006) Grow to Fit Molecular Dynamics (G2FMD): an ab initio method for protein side-chain assignment and refinement. *Protein Engineering Design and Selection*. 19(2): 55-65.
- ❖ Zhang Y (2007) Template-based modeling and free modeling by I-TASSER in CASP7. *Proteins*. 69(Suppl 8): 108-117.
- ❖ Zhang Y (2008) I-TASSER server for protein 3D structure prediction. *BMC Bioinformatics*. 9: 40.
- ❖ Zhang Z, Li Y, Lin B, Schroeder M, Huang B (2011) Identification of cavities on protein surface using multiple computational approaches for drug binding site prediction. *Bioinformatics*. 27(15): 2083-2088.

- ❖ Zhou R, Cheng L (2005) Binding of 3-phosphoglycerate leads to both activation and stabilization of ADP-glucose pyrophosphorylase from apple leaves. *Functional Plant Biology*. 32: 839-848.
- ❖ Zhu K, Pincus DL, Zhao S, Friesner RA (2006) Long loop prediction using the protein localoptimization program. *Proteins*. 65(2): 438-452.