

BIBLIOGRAPHY

- [1] UNAIDS. 2012. "Global report: UNAIDS report on the global AIDS epidemic 2012." [online]. Available <http://www.unaids.org/en/resources/publications/2012/name,76121,en.asp> (9 June 2013).
- [2] Hirsch MS, Gunthard HF, Schapiro JM, Brun-Vezinet F, Clotet B, Hammer SM, et al. Antiretroviral drug resistance testing in adult HIV-1 infection: 2008 recommendations of an International AIDS Society-USA panel. *Top HIV Med.* 2008 Aug-Sep; 16(3) : 266-85.
- [3] Huang G, Chen M, Wang K. Effect of neutral mutation on HIV-1 drug resistance in highly active antiretroviral therapy. *Academic Journals.* 2011; 6(30) : 6364-71.
- [4] Lieberman J. Defying death--HIV mutation to evade cytotoxic T lymphocytes. *N Engl J Med.* 2002 Oct 10; 347(15) : 1203-4.
- [5] Troyer RM, McNevin J, Liu Y, Zhang SC, Krizan RW, Abraha A, et al. Variable fitness impact of HIV-1 escape mutations to cytotoxic T lymphocyte (CTL) response. *PLoS Pathog.* 2009 Apr; 5(4) : e1000365.
- [6] Hasenkrug KJ, Brooks DM, Dittmer U. Critical role for CD4(+) T cells in controlling retrovirus replication and spread in persistently infected mice. *J Virol.* 1998 Aug; 72(8) : 6559-64.
- [7] Truneh A, Buck D, Cassatt DR, Juszczak R, Kassis S, Ryu SE, et al. A region in domain 1 of CD4 distinct from the primary gp120 binding site is involved in HIV infection and virus-mediated fusion. *J Biol Chem.* 1991 Mar 25; 266(9) : 5942-8.
- [8] Pugach P, Ketas TJ, Michael E, Moore JP. Neutralizing antibody and anti-retroviral drug sensitivities of HIV-1 isolates resistant to small molecule CCR5 inhibitors. *Virology.* 2008 Aug 1; 377(2) : 401-7.
- [9] Bruno CJ, Jacobson JM. Ibalizumab: an anti-CD4 monoclonal antibody for the treatment of HIV-1 infection. *J Antimicrob Chemother.* Sep; 65(9) : 1839-41.

- [10] Bolmstedt A, Hemming A, Flodby P, Berntsson P, Travis B, Lin JP, et al. Effects of mutations in glycosylation sites and disulphide bonds on processing, CD4-binding and fusion activity of human immunodeficiency virus envelope glycoproteins. *J Gen Virol.* 1991 Jun; 72 (Pt 6) : 1269-77.
- [11] Binz HK, Stumpp MT, Forrer P, Amstutz P, Pluckthun A. Designing repeat proteins: well-expressed, soluble and stable proteins from combinatorial libraries of consensus ankyrin repeat proteins. *J Mol Biol.* 2003 Sep 12; 332(2) : 489-503.
- [12] Li J, Mahajan A, Tsai MD. Ankyrin repeat: a unique motif mediating protein-protein interactions. *Biochemistry.* 2006 Dec 26; 45(51) : 15168-78.
- [13] Mosavi LK, Cammett TJ, Desrosiers DC, Peng ZY. The ankyrin repeat as molecular architecture for protein recognition. *Protein Sci.* 2004 Jun; 13(6) : 1435-48.
- [14] Schweizer A, Rusert P, Berlinger L, Ruprecht CR, Mann A, Cortesy S, et al. CD4-specific designed ankyrin repeat proteins are novel potent HIV entry inhibitors with unique characteristics. *PLoS Pathog.* 2008 Jul; 4(7) : e1000109.
- [15] Pugach P, Krarup A, Gettie A, Kuroda M, Blanchard J, Piatak M, et al. In vivo binding and retention of CD4-specific DARPin 57.2 in macaques. *PLoS One.* 2010; 5(8) : e12455.
- [16] Severino ME, Sipsas NV, Nguyen PT, Kalams SA, Wallker BD, Johnson RP, et al. Inhibition of human immunodeficiency virus type 1 replication in primary CD4(+) T lymphocytes, monocytes, and dendritic cells by cytotoxic T lymphocytes. *J Virol.* 2000; 74(14) : 6695-9.
- [17] Khanolkar A, Fuller MJ, Zajac AJ. T cell responses to viral infections: lessons from lymphocytic choriomeningitis virus. *Immunol Res.* 2002; 26(1-3) : 309-21.
- [18] Borrow P, Lewicki H, Hahn BH, Shaw GM, Oldstone MB. Virus-specific CD8+ cytotoxic T-lymphocyte activity associated with control of viremia in primary human immunodeficiency virus type 1 infection. *J Virol.* 1994 Sep; 68(9) : 6103-10.
- [19] O'Connor D, Friedrich T, Hughes A, Allen TM, Watkins D. Understanding cytotoxic T-lymphocyte escape during simian immunodeficiency virus infection. *Immunol Rev.* 2001 Oct; 183 : 115-26.
- [20] Wahren B, Morfeldt-Mansson L, Biberfeld G, Moberg L, Sonnerborg A, Ljungman P, et al. Characteristics of the specific cell-mediated immune

- response in human immunodeficiency virus infection. *J Virol.* 1987 Jun; 61(6) : 2017-23.
- [21] Krowka JF, Stites DP, Jain S, Steimer KS, George-Nascimento C, Gyenes A, et al. Lymphocyte proliferative responses to human immunodeficiency virus antigens in vitro. *J Clin Invest.* 1989 Apr; 83(4) : 1198-203.
- [22] Altfeld M, Rosenberg ES. The role of CD4(+) T helper cells in the cytotoxic T lymphocyte response to HIV-1. *Curr Opin Immunol.* 2000 Aug; 12(4) : 375-80.
- [23] Matloubian M, Concepcion RJ, Ahmed R. CD4+ T cells are required to sustain CD8+ cytotoxic T-cell responses during chronic viral infection. *J Virol.* 1994 Dec; 68(12) : 8056-63.
- [24] *HIV InSite, February 2003. "Molecular Insights Into HIV Biology."* [Online]. Available <http://hivinsite.ucsf.edu/InSite?page=kb-00&doc=kb-02-01-01> (2011 June 09).
- [25] Wang JH, Yan YW, Garrett TP, Liu JH, Rodgers DW, Garlick RL, et al. Atomic structure of a fragment of human CD4 containing two immunoglobulin-like domains. *Nature.* 1990 Nov 29; 348(6300) : 411-8.
- [26] Garrett TP, Wang J, Yan Y, Liu J, Harrison SC. Refinement and analysis of the structure of the first two domains of human CD4. *J Mol Biol.* 1993; 234(3) : 763-78.
- [27] Moebius U, Clayton LK, Abraham S, Diener A, Yunis JJ, Harrison SC, et al. Human immunodeficiency virus gp120 binding C'C" ridge of CD4 domain 1 is also involved in interaction with class II major histocompatibility complex molecules. *Proc Natl Acad Sci U S A.* 1992 Dec 15; 89(24) : 12008-12.
- [28] Wang JH, Meijers R, Xiong Y, Liu JH, Sakihama T, Zhang R, et al. Crystal structure of the human CD4 N-terminal two-domain fragment complexed to a class II MHC molecule. *Proc Natl Acad Sci U S A.* 2001 Sep 11; 98(19) : 10799-804.
- [29] Houlgatte R, Scarmato P, Marhomy S, Matin M, Ostankovitch M, Lafosses S, et al. HLA class II antigens and the HIV envelope glycoprotein gp120 bind to the same face of CD4. *J Immunol.* 1994; 152(9) : 4475-88.
- [30] Bowman MR, MacFerrin KD, Schreiber SL, BURakoff SJ. Identification and structural analysis of residues in the V1 region of CD4 involved in interaction with human immunodeficiency virus envelope glycoprotein gp120 and class II major histocompatibility complex molecules. *Proc Natl Acad Sci U S A.* 1990; 87(22) : 9052-6.

- [31] Moebius U, Clayton LK, Abraham S, Harrison SC, Reinherz EL. The human immunodeficiency virus gp120 binding site on CD4: delineation by quantitative equilibrium and kinetic binding studies of mutants in conjunction with a high-resolution CD4 atomic structure. *J Exp Med*. 1992 Aug 1; 176(2) : 507-17.
- [32] Wu H, Myszka DG, Tendian SW, Brouillette CG, Sweet RW, Chaiken IM, et al. Kinetic and structural analysis of mutant CD4 receptors that are defective in HIV gp120 binding. *Proc Natl Acad Sci U S A*. 1996 Dec 24; 93(26) : 15030-5.
- [33] Ryu SE, Truneh A, Sweet RW, Hendrickson WA. Structures of an HIV and MHC binding fragment from human CD4 as refined in two crystal lattices. *Structure*. 1994 Jan 15; 2(1) : 59-74.
- [34] Zhou T, Xu L, Dey B, Hessel AJ, Van RD, Xiang SH, et al. Structural definition of a conserved neutralization epitope on HIV-1 gp120. *Nature*. 2007; 445(7129) : 732-7.
- [35] Montessori V, Press N, Harris M, Akagi L, Montaner JS. Adverse effects of antiretroviral therapy for HIV infection. *CMA*. 2004 Jan 20; 170(2) : 229-38.
- [36] Blay WM, Kasprzyk T, Misher L, Richardson BA, Haigwood NL. Mutations in envelope gp120 can impact proteolytic processing of the gp160 precursor and thereby affect neutralization sensitivity of human immunodeficiency virus type 1 pseudoviruses. *J Virol*. 2007 Dec; 81(23) : 13037-49.
- [37] Park EJ, Vujcic LK, Anand R, Theodore TS, Quinnan CV. Mutations in both gp120 and gp41 are responsible for the broad neutralization resistance of variant human immunodeficiency virus type 1 MN to antibodies directed at V3 and non-V3 epitopes. *J Virol*. 1998; 72(9) : 7099-107.
- [38] Borkow G, Lara HH, Lapidot A. Mutations in gp41 and gp120 of HIV-1 isolates resistant to hexa-arginine neomycin B conjugate. *Biochem Biophys Res Commun*. 2003 Dec 26; 312(4): 1047-52.
- [39] Hermann FG, Egerer L, Brauer F, Gerum C, Schwalbe H, Dietrich U, et al. Mutations in gp120 contribute to the resistance of human immunodeficiency virus type 1 to membrane-anchored C-peptide maC46. *J Virol*. 2009 May; 83(10) : 4844-53.
- [40] Johnson VA, Calvez V, Gunthard HF, Paredes R, Pillay D, Shafer R, et al. 2011 update of the drug resistance mutations in HIV-1. *Top Antivir Med*. Nov; 19(4) : 156-64.

- [41] Fauci AS. HIV and AIDS: 20 years of science. *Nat Med*. 2003 Jul; 9(7) : 839-43.
- [42] Citterio P, Rusconi S. Novel inhibitors of the early steps of the HIV-1 life cycle. *Expert Opin Investig Drugs*. 2007 Jan; 16(1) : 11-23.
- [43] U.S. Food and Drug Administration. 2009 May 05. "Approved antiretroviral drugs for pediatric treatment of HIV infection." [online]. Available <http://www.fda.gov/ForConsumers/ByAudience/ForPatientAdvocates/HIVandAIDSActivities/ucm118951.htm> (2011 June 09).
- [44] Hughes CA, Robinson L, Tseng A, MacArthur RD. New antiretroviral drugs: a review of the efficacy, safety, pharmacokinetics, and resistance profile of tipranavir, darunavir, etravirine, rilpivirine, maraviroc, and raltegravir. *Expert Opin Pharmacother*. 2009 Oct; 10(15) : 2445-66.
- [45] Kuritzdes DR. HIV-1 entry inhibitors: an overview. *Curr Opin HIV AIDS*. 2009; 4(2) : 82-7.
- [46] Sedgwick SG, Smerdon SJ. The ankyrin repeat: a diversity of interactions on a common structural framework. *Trends Biochem Sci*. 1999 Aug; 24(8) : 311-6.
- [47] Wiehe K, Peterson MW, Pierce B, Mintseris J, Weng Z. Protein-protein docking: overview and performance analysis. *Methods Mol Biol*. 2008; 413 : 283-314.
- [48] Smith GR, Sternberg MJ. Prediction of protein-protein interactions by docking methods. *Curr Opin Struct Biol*. 2002 Feb; 12(1) : 28-35.
- [49] Chen R, Li L, Weng Z. ZDOCK: an initial-stage protein-docking algorithm. *Proteins*. 2003 Jul 1; 52(1) : 80-7.
- [50] Chen R, Weng Z. A novel shape complementarity scoring function for protein-protein docking. *Proteins*. 2003 May 15; 51(3) : 397-408.
- [51] Chen R, Weng Z. Docking unbound proteins using shape complementarity, desolvation, and electrostatics. *Proteins*. 2002 May 15; 47(3) : 281-94.
- [52] Gabb HA, Jackson RM, Sternberg MJ. Modelling protein docking using shape complementarity, electrostatics and biochemical information. *J Mol Biol*. 1997; 272(1) : 106-20.
- [53] Pierce B, Weng Z. ZRANK: reranking protein docking predictions with an optimized energy function. *Proteins*. 2007; 67(4) : 1078-86.

- [54] Li L, Chen R, Weng Z. RDOCK: refinement of rigid-body protein docking predictions. *Proteins*. 2003 Nov 15; 53(3) : 693-707.
- [55] Macindoe G, Mavridis L, Venkatraman V, Devignes MD, Ritchie DW. HexServer: an FFT-based protein docking server powered by graphics processors. *Nucleic Acids Res*. 2010 Jul; 38 : W445-9.
- [56] Ritchie DW, Kemp GJ. Protein docking using spherical polar Fourier correlations. *Proteins*. 2000 May 1; 39(2) : 178-94.
- [57] Clackson T, Ultsch MH, Wells JA, de Vos AM. A hot spot of binding energy in a hormone-receptor interface. *Science*. 1995; 267(5196) : 383-6.
- [58] Bogan AA, Thorn KS. Anatomy of hot spots in protein interfaces. *J Mol Biol*. 1998; 280(1) : 1-9.
- [59] Jones S, Thornton JM. Prediction of protein-protein interaction sites using patch analysis. *J Mol Biol*. 1997 Sep 12; 272(1) : 133-43.
- [60] Zhou HX, Qin S. Interaction-site prediction for protein complexes: a critical assessment. *Bioinformatics*. 2007; 23(17) : 2203-9.
- [61] Walker-Taylor A, Jones D.T. Computational methods for predicting protein-protein interactions. *Protein Reviews*. 2005; 3 : 89-114.
- [62] Marshall G, Vakser I. Protein-protein docking methods. *Protein Reviews*. 2005; 3 : 115-146.
- [63] Tsai CJ, Lin SL, Wolfson HJ, Nussinov R. Studies of protein-protein interfaces: a statistical analysis of the hydrophobic effect. *Protein Sci*. 1997;6(1) : 53-64.
- [64] Yan C, Wu F, Jernigan RL, Dobbs D, Honavar V. Characterization of protein-protein interfaces. *Protein J*. 2008; 27(1) : 59-70.
- [65] De S, Drishnadev O, Srinivasan N, Rekha N. Interaction preferences across protein-protein interfaces of obligatory and non-obligatory components are different. *BMC Struct Biol*. 2005; 5 : 15.
- [66] Jones S, Thornton JM. Principles of protein-protein interactions. *Proc Natl Acad Sci U S A*. 1996; 93(1) : 13-20.
- [67] Zhanhua C, Gan JG, Lei L, Sakhakar MK, Kanguane P. Protein subunit interfaces: heterodimers versus homodimers. *Bioinformation*. 2005; 1(2) : 28-39.

- [68] Lo Conte L, Chothia C, Janin J. The atomic structure of protein-protein recognition sites. *J Mol Biol.* 1999; 285(5) : 2177-98.
- [69] Bahadur RP, Zacharias M. The interface of protein-protein complexes: analysis of contacts and prediction of interactions. *Cell Mol Life Sci.* 2008; 65(7-8) : 1059-72.
- [70] Elsevier Health. 2002. "Amino Acids and Proteins." [online]. Available <http://www.elsevierhealth.com/media/us/samplechapters/9780323053716/Chapter%2002.pdf> (2012 June 09).
- [71] McKee T, McKee JR. "Amino Acids, Peptides, and Proteins." in BIOCHEMISTRY The Molecular Basis of Life, 5th ed. OXFORD UNIVERSITY PRESS, pp. 123-44, 2011.
- [72] Jones S, Thornton JM. Protein-protein interactions: a review of protein dimer structures. *Prog Biophys Mol Biol.* 1995; 63(1) : 31-65.
- [73] Glaser F, Steinberg DM, Vakser IA, Ben-Tal N. Residue frequencies and pairing preferences at protein-protein interfaces. *Proteins.* 2001; 43(2) : 89-102.
- [74] Fernández A, Ridgway SL, Scheraga HA. Amino acid residues at protein-protein interfaces: why is propensity so different from relative abundance? *J. Phys. Chem.* 2003; 107(36) : 9929-32.
- [75] Dong Q, Wang X, Lin L, Guan Y. Exploiting residue-level and profile-level interface propensities for usage in binding sites prediction of proteins. *BMC Bioinformatics.* 2007; 8 : 147.
- [76] Kyte J and Doolittle RF. A simple method for displaying the hydropathic character of protein. *J Mol Biol.* 1982; 157 (1) : 105-32.
- [77] Tuncbag N, Keskin O, Gursoy A. HotPoint: hot spot prediction server for protein interfaces. *Nucleic Acids Res.* 2010; 38 : W402-6.
- [78] Tuncbag N, Gursoy A, Keskin O. Identification of computational hot spots in protein interfaces: combining solvent accessibility and inter-residue potentials improves the accuracy. *Bioinformatics.* 2009; 25(12) : 1513-20.
- [79] Thorn KS, Bogan AA. ASEdb: a database of alanine mutations and their effects on the free energy of binding in protein interactions. *Bioinformatics.* 2001; 17(3) : 284-5.
- [80] Fischer TB, Arunachalam KV, Bailey D, Mangual V, Bakhru S, Russo R. The binding interface database (BID): a compilation of amino acid hot spots in protein interfaces. *Bioinformatics.* 2003; 19(11) : 1453-4.

- [81] Hubbard SJ, Thornton JM. 1993. Department of Biochemistry and Molecular Biology. London, University College.
- [82] Miller S, Lesk AM, Janin J, Chothia C. The accessible surface area and stability of oligomeric proteins. *Nature*. 1987; 328(6133) : 834-6.
- [83] Keskin O, Bahar I, Badretdinov AY, Ptitsyn OB, Jernigan RL. Empirical solvent-mediated potentials hold for both intra-molecular and inter-molecular inter-residue interactions. *Protein Sci*. 1998; 7(12) : 2578-86.
- [84] Kortemme T, Baker D. A simple physical model for binding energy hot spots in protein-protein complexes. *Proc Natl Acad Sci U S A*. 2002; 99(22) : 14116-21.
- [85] Lise S, Buchan D, Pontil M, Jones DT. Predictions of hot spot residues at protein-protein interfaces using Support Vector Machines. *PLoS One*. 2011; 6(2) : e16774.
- [86] Lise S, Archambeau C, Pontil M, Jones DT. Prediction of hot spot residues at protein-protein interfaces by combining machine learning and energy-based methods. *BMC Bioinformatics*. 2009; 10 : 365.
- [87] Neria E, Fischer S, Karplus M. Simulation of activation free energies in molecular systems. *Journal of Chemical Physics*. 1996; 105(5) : 1902-21.
- [88] Lazaridis T, Karplus M. Effective energy function for proteins in solution. *Proteins*. 1999; 35(2) : 133-52.
- [89] *Grolier Multimedia Encyclopedia*. 2012. "Histogram." *Grolier Multimedia Encyclopedia [online]*. Available <http://gme.grolier.com/article?Assetid=0138950-0> (2012 June 09).
- [90] Pollack HN, Huang S, Shen PY. Climate change record in subsurface temperatures: A global perspective. *Science*. 1998 Oct 9; 282(5387) : 279-81.
- [91] Filzmoser P, Hron K, Reimann C. Univariate statistical analysis of environmental (compositional) data: problems and possibilities. *Sci Total Environ*. 2009 Nov 15; 407(23) : 6100-8.
- [92] Weismuller P, Kratz C, Brandts B, Kattenbeck K, Trappe HJ, Ranke C. AV nodal pathways in the R-R interval histogram of the 24-hour monitoring ECG in patients with atrial fibrillation. *Ann Noninvasive Electrophysiol*. 2001; 6(4) : 285-9.

- [93] Kwok NM, Jia X, Wang D, Chen SY, Fang G, Ha QP. Visual impact enhancement via image histogram smoothing and continuous intensity relocation. *Computers & Electrical Engineering*. 2001; 37(5) : 681–94.
- [94] Brunelli R, Mich O. Histograms analysis for image retrieval. *Pattern Recognition*. 2001; 34(8) : 1625–1637.
- [95] Chodera JD, Swope WC, Pitera JW, Seok C, Dill KA. Use of the weighted histogram analysis method for the analysis of simulated and parallel tempering simulations. *J. Chem. Theory Comput*. 2007; 3(1) : 26–41.
- [96] Putheti RR, Okigbo R, Patil S, Advanapu M, Leburu R. Method development and validations: characterization of critical elements in the development of pharmaceuticals. *International Journal of Health Research*. 2008; 1(1) : 11-20.
- [97] Araujo P. Key aspects of analytical method validation and linearity evaluation. *J Chromatogr B Analyt Technol Biomed Life Sci*. 2009; 877(23) : 2224-34.
- [98] Hu Z, Ma B, Wolfson H, Nussinov R. Conservation of polar residues as hot spots at protein interfaces. *Proteins*. 2000; 39(4) : 331-42.
- [99] DeLano WL, Ultsch MH, de Vos AM, Wells JA. Convergent solutions to binding at a protein-protein interface. *Science*. 2000; 287(5456) : 1279-83.
- [100] DeLano WL. Unraveling hot spots in binding interfaces: progress and challenges. *Curr Opin Struct Biol*. 2002; 12(1) : 14-20.
- [101] Bock JR, Gough DA. Predicting protein--protein interactions from primary structure. *Bioinformatics*. 2001; 17(5) : 455-60.
- [102] Shulman-Peleg A, Shatsky M, Nussinov R, Wolfson. MultiBind and MAPPIS: web servers for multiple alignment of protein 3D-binding sites and their interactions. *Nucleic Acids Res*. 2008; 36 : W260-4.
- [103] Huo S, Massova I, Kollman PA. Computational alanine scanning of the 1:1 human growth hormone-receptor complex. *J Comput Chem*. 2002; 23(1) : 15-27.
- [104] Clackson T, Ultsch MH, Wells JA, de Vos AM. Structural and functional analysis of the 1:1 growth hormone:receptor complex reveals the molecular basis for receptor affinity. *J Mol Biol*. 1998; 277(5) : 1111-28.
- [105] Rajamani D, Thiel S, Vajda S, Camacho CJ. Anchor residues in protein-protein interactions. *Proc Natl Acad Sci U S A*. 2004; 101(31) : 11287-92.

- [106] Gonzalez-Ruiz D, Gohlke H. Targeting protein-protein interactions with small molecules: challenges and perspectives for computational binding epitope detection and ligand finding. *Curr Med Chem*. 2006; 13(22) : 2607-25.
- [107] Gao Y, Wang R, Lai L. Structure-based method for analyzing protein-protein interfaces. *J Mol Model*. 2004; 10(1) : 44-54.
- [108] Cukuroglu EA, Gursoy A, Keskin O. HotRegion: a database of predicted hot spot clusters. *Nucleic Acids Res*. 2012; 40 : D829-33.
- [109] Nimmanpipug P, Khampa C, Lee VS, Nangola S, Tayapiwattana C. Identification of amino acid residues of a designed ankyrin repeat protein potentially involved in intermolecular interactions with CD4: analysis by molecular dynamics simulations. *J Mol Graph Model*. 2011; 31 : 65-75.
- [110] Laskowski RA, MacArthur MW, Moss DS, Thornton JM. PROCHECK: A program to check the stereochemical quality of protein structures. *J. Appl. Crystallogr*. 1993; 26 : 283-91.