

Publications

Andrew C.R. Martin

February 7, 2018

- [1] K.R. Abhinandan and A.C.R. Martin. Analyzing the ‘degree of humanness’ of antibody sequences. *J. Mol. Biol.*, 369:852–862, 2007.
- [2] K.R. Abhinandan and A.C.R. Martin. Analysis and improvements to Kabat and structurally correct numbering of antibody variable domains. *Molecular Immunology*, 45:3832–3839, 2008.
- [3] K.R. Abhinandan and A.C.R. Martin. Analysis and prediction of VH/VL packing in antibodies. *Protein Engineering Design and Selection*, 23:689–697, 2010.
- [4] N.S. Al-Numair, L. Lopes, P. Syrris, L. Monserrat, P. Elliott, and A.C.R. Martin. The structural effects of mutations can aid in differential phenotype prediction of beta-myosin heavy chain (Myosin-7) missense variants. *Bioinformatics*, 32:2947–2955, 2016.
- [5] N.S. Al-Numair and A.C.R. Martin. The SAAP pipeline and database: tools to analyze the impact and predict the pathogenicity of mutations. *BMC Genomics (ISMB 2012 SNP-SIG Special Issue)*, 14(Suppl 3):S4, 2013.
- [6] L.C. Allcorn and A.C.R. Martin. SACS - a self-maintaining database of antibody crystal structures. *Bioinformatics*, 18:175–181, 2002.
- [7] A. Baresic and A.C.R. Martin. Compensated pathogenic mutations. *Biomolecular Concepts*, 2:281–292, 2011.
- [8] A. Baresic, L.E.M. McMillan, H.H. Rogers, J.M. Hurst, and A.C.R. Martin. Compensated pathogenic deviations: analysis of structural effects. *Journal of Molecular Biology*, 396:19–30, 2010.
- [9] A. Cavallo and A.C.R. Martin. Mapping SNPs to protein sequence and structure data. *Bioinformatics*, 21:1443–1450, 2005.
- [10] J.C. Cheetham, S. Roberts, A.C.R. Martin, and A.R. Rees. Molecular modelling of antibody combining sites. *Protein Engineering*, 1:232–233, 1987.

- [11] D. Churamani, M. Boulware, L. Ramakrishnan, T. Geach, A.C.R. Martin, V. Vacquier, J. Marchant, L. Dale, and S. Patel. Molecular characterisation of a novel cell surface ADP-ribosyl cyclase from the sea urchin. *Cellular Signalling*, 20:2347–2355, 2008.
- [12] D. Churamani, M.J. Boulware, T.J. Geach, A.C.R. Martin, G.W. Moy, Y.-H. Su, V.D. Vacquier, J.S. Marchant, L. Dale, and S. Patel. Molecular and functional characterization of a novel intracellular ADP-ribosyl cyclase. *PLoS ONE*, 2(8):e797, 2007.
- [13] A.V.J. Collis, A.R. Brouwer, and A.C.R. Martin. Analysis of the antigen combining site - correlations between length and sequence composition of the hypervariable loops and the nature of the antigen. *J. Mol. Biol.*, 325:337–354, 2003.
- [14] D.W. Corne and A.C.R. Martin. Artificial intelligence in bioinformatics. *Computers and Chemistry*, 26:1–3, 2001. Special issue edited by Martin and Corne.
- [15] A.L. Cuff, R.W. Janes, and A.C.R. Martin. Analysing the ability to retain sidechain hydrogen-bonds in mutant proteins. *Bioinformatics*, 22:1464–1470, 2006.
- [16] A.L. Cuff and A.C.R. Martin. Analysis of void volumes in proteins and application to stability of the p53 tumour suppressor protein. *J. Mol. Biol.*, 344:1199–1209, 2004.
- [17] S.V.V. Deevi and A.C.R. Martin. An extensible automated protein annotation tool: standardizing input and output using validated XML. *Bioinformatics*, 22:291–296, 2006.
- [18] S. Ferdous and A.C.R. Martin. Exploration of conformational B-cell epitopes: components to peptide-based vaccines. *F1000Research*, 5:2142, 2016.
- [19] S. Ferdous and A.C.R. Martin. AbDb: Antibody structure database - a database of PDB derived antibody structures. *Database*, submitted.
- [20] H.M. Fooks, A.C.R. Martin, D.N. Woolfson, R.B. Sessions, and E.G. Hutchinson. Amino acid pairing preferences in parallel beta-sheets in proteins. *J. Mol. Biol.*, 356:32–44, 2006.
- [21] D.St.J. Gregory, A.C.R. Martin, J.C. Cheetham, and A.R. Rees. The prediction and characterization of metal binding sites in proteins. *Protein Engineering*, 6:29–35, 1993.
- [22] D.St.J. Gregory, D. Staunton, A.C.R. Martin, J.C. Cheetham, J.T. Pedersen, and A.R. Rees. Antibody combining sites - prediction and design. *Biochemical Society Symposium*, 57:147–155, 1990.

- [23] R. Harvey, M. Zambon, A.C.R. Martin, and W.S. Barclay. Restrictions to the adaptation of influenza A virus H5 haemagglutinin to the human host. *Journal of Virology*, 78:502–507, 2004.
- [24] B. Henderson and A.C.R. Martin. Bacterial virulence in the moonlight: Multitasking bacterial moonlighting proteins are virulence determinants in infectious disease. *Infection and Immunity*, 79:3476–91, 2011.
- [25] B. Henderson and A.C.R. Martin. Bacterial moonlighting proteins and bacterial virulence. *Current Topics in Microbiology and Immunology*, 358:155–213, 2013.
- [26] B. Henderson and A.C.R. Martin. Protein moonlighting: A new factor in biology and medicine. *Biochem. Soc. Trans.*, 42:1671–1678, 2014.
- [27] A. Hirtreiter, G.E. Damska, A. Cheung, D. Klose, D. Grohmann, E. Vojnic, A.C.R. Martin, P. Cramer, and F. Werner. Spt4/5 stimulates transcription elongation through the RNA polymerase clamp coiled coil motif. *Nucleic Acids Research*, 38:4040–4051, 2010.
- [28] J.M. Hurst, L.E.M. McMillan, C.T. Porter, A. Allen, J. Fakorede, and A.C.R. Martin. The SAAPdb web resource: a large scale structural analysis of mutant proteins. *Human Mutation*, 30:616–624, 2009.
- [29] J.M.G. Izarzugaza, A. Baresic, L.E.M. McMillan, C. Yeats, A. Clegg, C.A. Orengo, A.C.R. Martin, and A. Valencia. An integrated approach to the interpretation of single amino acid polymorphisms within the framework of CATH and Gene3D. *BMC Bioinformatics*, 10 Suppl 8:S5–S5, 2009.
- [30] J.M.G. Izarzugaza, L.E.M. Hopcroft, A. Baresic, C.A. Orengo, A.C.R. Martin, and A. Valencia. Characterization of pathogenic germline deviations in human protein kinases. *BMC Bioinformatics*, 12 Suppl.4:S1, 2011. Special Issue - Proceedings of the European Conference on Computational Biology (ECCB) 2010 Workshop: Annotation, interpretation and management of mutation (AIMM-2010).
- [31] T. Jackson, B.A. Morris, A.C.R. Martin, D.F.V. Lewis, and P.G. Sanders. Molecular modelling and site-directed mutagenesis on a bovine anti-testosterone monoclonal antibody. *Protein Engineering*, 5:343–350, 1992.
- [32] N. Jayaram, P. Bhowmick, and A.C.R. Martin. Germline VH/VL pairing in antibodies. *Protein Engineering Design and Selection*, 25:523–530, 2012.
- [33] N. Jayaram, D. Usvyat, and A.C.R. Martin. Evaluating tools for transcription factor binding site prediction. *BMC Bioinformatics*, 2016.
- [34] S. Jones, A.C.R. Martin, M. Karmirantzou, R.A. Laskowski, C. Orengo, and J.M. Thornton. Protein domains, folds and functions. In G. Gilliland and H. Berman, editors, *Transactions of the American Crystallography Association*, volume 32, ‘Structural Informatics’. American Crystallographic Association, 1997.

- [35] J.K. Kalsi, A.C.R. Martin, Y. Hirabayashi, M. Ehrenstein, C.M. Longhurst, C. Ravirajan, M. Zvelebil, D. Stollar, J.M. Thornton, and D.A. Isenberg. Functional and modelling studies of the binding of human monoclonal anti-DNA antibodies to DNA. *Molecular Immunology*, 33:471–483, 1996.
- [36] J.K. Kalsi, A.C.R. Martin, and D.A. Isenberg. Structure-function relation of anti-DNA antibodies. *Lupus*, 4:245–248, 1995.
- [37] S.M. Kipriyanov, G. Moldenhauer, A.C.R. Martin, O.A. Kupriyanova, and M. Little. Two amino acid mutations in an anti-human CD3 single chain Fv antibody fragment that affect the yield on bacterial secretion, but not the affinity. *Protein Engineering*, 10:445–453, 1997.
- [38] J. Krauss, M.A.E. Arndt, A.C.R. Martin, H. Liu, and S.M. Rybak. Specificity grafting of human antibody frameworks selected from a phage display library: generation of a highly stable humanized anti-CD22 single chain fv fragment. *Protein Engineering*, 16:753–759, 2003.
- [39] C.H.Y. Kwok, S.W.N. Au, A.C.R. Martin, and V.M.S. Lam. G6PDdb: An integrated database of glucose-6-phosphate dehydrogenase (G6PD) mutations. *Human Mutation*, 19:217–224, 2002.
- [40] S.E.A. Leigh, Y.P. Lee, R.A. Whittall, N. Dawson, S. Das, A.C.R. Martin, C.A. Orenge, and S.E. Humphries. Update and analysis of the UCL pro-protein convertase subtilisin/kexin type9 gene (PCSK9) variant database. *Atherosclerosis*, 235:E98, 2014.
- [41] Z. Liu, D. Song, A. Kramer, A.C.R. Martin, T. Dandekar, J. Schneider-Mergener, E.K.F. Bautz, and S. Duebel. Fine mapping of the antigen-antibody interaction of scFv215, a recombinant antibody inhibiting RNA polymerase II from *drosophila melanogaster*. *Journal of Molecular Recognition*, 12:103–111, 1999.
- [42] R.M. MacCallum, A.C.R. Martin, and J.M. Thornton. Antibody-antigen interactions: Contact analysis and binding site topography. *J. Mol. Biol.*, 262:732–745, 1996.
- [43] A.C.R. Martin. MoG: Molecular graphics for the Commodore Amiga. *Journal of Molecular Graphics*, 11:53–55, 1993.
- [44] A.C.R. Martin. Modelling antibodies: Approach and perspective. *Lupus*, 3:365–366, 1994.
- [45] A.C.R. Martin. Accessing the Kabat antibody sequence database by computer. *PROTEINS: Structure, Function and Genetics*, 25:130–133, 1996.
- [46] A.C.R. Martin. Model already exists for fair use of gene data. *Nature*, 406:933, 2000.

- [47] A.C.R. Martin. A practical introduction to the simulation of molecular systems. *Computers and Chemistry*, 24:239–240, 2000.
- [48] A.C.R. Martin. Process for storing data, 2000. US Patent US2004030502 application priority date 14 March 2000.
- [49] A.C.R. Martin. Ups and downs of protein topology; rapid comparison of protein structure. *Protein Engineering*, 13:829–837, 2000.
- [50] A.C.R. Martin. Can we integrate bioinformatics data on the internet? *Trends in Biotechnology*, 19:327–328, 2001.
- [51] A.C.R. Martin. Modelling molecular structures. *Computers and Chemistry*, 25:309–310, 2001.
- [52] A.C.R. Martin. Protein sequence and structure analysis of antibody variable domains. In S. Duebel and R. Kontermann, editors, *Antibody Engineering Lab Manual*. Springer-Verlag, Heidelberg, 2001.
- [53] A.C.R. Martin. Comparative modelling. In C.A. Orengo, D.T. Jones, and J.M. Thornton, editors, *Bioinformatics*. Bios Scientific Publishers, Oxford, 2002. ISBN: 1859960545.
- [54] A.C.R. Martin. Internet technologies for bioinformatics. In C.A. Orengo, D.T. Jones, and J.M. Thornton, editors, *Bioinformatics*. Bios Scientific Publishers, Oxford, 2002. ISBN: 1859960545.
- [55] A.C.R. Martin. PDBSprotEC: A web-accessible database linking PDB chains to EC numbers via SwissProt. *Bioinformatics*, 20:986–988, 2004.
- [56] A.C.R. Martin. Mapping PDB chains to UniProtKB entries. *Bioinformatics*, 21:4297–4301, 2005.
- [57] A.C.R. Martin. Protein sequence and structure analysis of antibody variable domains. In S. Duebel and R. Kontermann, editors, *Antibody Engineering Lab Manual Volume 2 (2nd Edition)*. Springer-Verlag, Heidelberg, 2010. ISBN-10: 3642011462, ISBN-13: 978-3642011467.
- [58] A.C.R. Martin. Structural biology of moonlighting - lessons from antibodies. *Biochem Soc Trans*, 42:1704–1708, 2014.
- [59] A.C.R. Martin. Viewing multiple sequence alignments with the Javascript sequence alignment viewer (JSAV). *F1000Research*, 3:249, 2014.
- [60] A.C.R. Martin. Anna Tramontano - in memorium, 2017. Obituary for the Antibody Society.
- [61] A.C.R. Martin. An introduction to the protein molecule. In B. Henderson, M.A. Fares, and A.C.R. Martin, editors, *Protein Moonlighting in Biology and Medicine, the Biological and Biomedical Consequences of Protein Moonlighting*. Wiley-Blackwell, Hoboken, New Jersey, 2017. Chapter 1. ISBN-10: 1118952081; ISBN-13: 978-1118952085.

- [62] A.C.R. Martin. Recommendation: Accurate structure prediction of CDR H3 loops enabled by a novel structure-based C-terminal constraint (Weitzner B.D., Gray J.J.), 2017.
- [63] A.C.R. Martin. Recommendation: Improving B-cell epitope prediction and its application to global antibody-antigen docking (Krawczyk K, Liu X, Baker T, Shi J, Deane C.M.), 2017.
- [64] A.C.R. Martin. The structural basis of protein moonlighting. In B. Henderson, M.A. Fares, and A.C.R. Martin, editors, *Protein Moonlighting in Biology and Medicine, the Biological and Biomedical Consequences of Protein Moonlighting*. Wiley-Blackwell, Hoboken, New Jersey, 2017. Chapter 4. ISBN-10: 1118952081; ISBN-13: 978-1118952085.
- [65] A.C.R. Martin and J. Allen. Bioinformatics tools for antibody engineering. In S. Duebel, editor, *Handbook of Therapeutic Antibodies Vol 1, Technologies*. Wiley-VCH, Weinheim, 2007. ISBN-10: 3-527-31453-9.
- [66] A.C.R. Martin and J. Allen. Bioinformatics tools for antibody engineering. In S. Duebel and J. Reichert, editors, *Handbook of Therapeutic Antibodies Vol 1, Technologies (2nd Edition)*. Wiley-Blackwell, Weinheim, 2014. ISBN-10: 3527329374, ISBN-13: 978-3527329373.
- [67] A.C.R. Martin and A. Baresic. Structural impact of SNPs. In G.K. Roberts, editor, *Encyclopedia of Biophysics*. Springer-Verlag, Berlin Heidelberg, 2013. ISBN 978-3-642-16711-9.
- [68] A.C.R. Martin, A. Baresic, and N. Al-Numair. Structural impact of SNPs. In G.K. Roberts, editor, *Encyclopedia of Biophysics*. Springer-Verlag, Berlin Heidelberg, forthcoming edition, in press. ISBN 978-3-642-16711-9.
- [69] A.C.R. Martin, J.C. Cheetham, and A.R. Rees. Modelling antibody hypervariable loops: A combined algorithm. *Proceedings of the National Academy of Science*, 86:9269–9272, 1989.
- [70] A.C.R. Martin, J.C. Cheetham, and A.R. Rees. Molecular modelling of antibody combining sites. *Methods in Enzymology*, 203:121–153, 1991.
- [71] A.C.R. Martin, A.M. Facchiano, A.L. Cuff, T. Hernandez-Boussard, M. Olivier, P. Hainaut, and J.M. Thornton. Mutation data and structural analysis of the p53 tumour-suppressor protein. *Human Mutation*, 19:149–164, 2002.
- [72] A.C.R. Martin, M.W. MacArthur, and J.M. Thornton. Assessment of comparative modelling in CASP2. *PROTEINS: Structure, Function and Genetics*, Suppl. 1:14–28, 1997.
- [73] A.C.R. Martin, R.M. MacCallum, and J.M. Thornton. Analysis and modelling of antibodies. *Immunology*, 86 Suppl 1:95, 1995.

- [74] A.C.R. Martin, C.A. Orengo, E.G. Hutchinson, S. Jones, M. Karmirantzou, R.A. Laskowski, J.B.O. Mitchell, C. Taroni, and J.M. Thornton. Protein folds and functions. *Structure*, 6:875–884, 1998.
- [75] A.C.R. Martin and A.R. Rees. Extracting human antibody sequences from public databases for antibody humanization: high frequency of species assignment errors. *Protein Engineering Design and Selection*, 29:403–408, 2016.
- [76] A.C.R. Martin and J.M. Thornton. Structural families of loops in homologous proteins: Automatic classification, modelling and application to antibodies. *J.Mol.Biol*, 263:800–815, 1996.
- [77] A.C.R. Martin, K. Toda, H.J. Stirk, and J.M. Thornton. Long loops in proteins. *Protein Engineering*, 8:1093–1101, 1995.
- [78] L.E.M. McMillan and A.C.R. Martin. Automatically extracting functionally equivalent proteins from SwissProt. *BMC Bioinformatics*, 9:418, 2008.
- [79] E. Merelli, G. Armano, N. Cannata, F. Corradini, M. d’Inverno, A. Doms, P. Lord, A. Martin, L. Milanese, S. Moeller, M. Schroeder, and M. Luck. Agents in bioinformatics, computational and systems biology. *Briefings in Bioinformatics*, 8:45–59, 2007.
- [80] R. Nan, I. Farabella, F.F. Schumacher, A. Miller, J. Gor, A.C.R. Martin, D.T. Jones, I. Lengyel, and S.J. Perkins. Zinc binding to the tyr402 and his402 allotypes of complement factor H: possible implications for age-related macular degeneration. *J. Mol. Biol*, 408:714–735, 2011.
- [81] T. Northey, A. Baresic, and A.C.R. Martin. IntPred: a structure-based predictor of protein-protein interaction sites. *Bioinformatics*, 34:223–229, 2017.
- [82] C.A. Orengo, A.C.R. Martin, G. Hutchinson, S. Jones, Jones. D.J., A.D. Michie, M.B. Swindells, and J.M. Thornton. Classifying a protein in the CATH database of domain structures. *Acta Crystallographica*, D54:1155–1167, 1998.
- [83] C.A. Orengo, F.M. Pearl, Bray J.E., A.E. Todd, A.C.R. Martin, L. Lo Conte, and J.M. Thornton. The CATH database provides insights into protein structure/function relationships. *Nucleic Acids Research*, 27:275–279, 1999.
- [84] T. Osborne, M. Heath, A.C.R. Martin, J. Pankowski, K. Hudson-Edwards, and J. Santini. Cold-adapted arsenite oxidase from a psychrotolerant *polaromonas* species. *Metallomics*, 5:318–324, 2013.
- [85] F. Pearl, A.E. Todd, J.E. Bray, A.C.R. Martin, A.A. Salamov, M. Suwa, M.B. Swindells, J.M. Thornton, and C.A. Orengo. Using the CATH domain database to assign structures and functions to the genome sequences. *Biochem. Soc. Trans*, 28:269–275, 2000.

- [86] C.T. Porter and A.C.R. Martin. BiopLib and BiopTools - a C programming library and toolset for manipulating protein structure (application note). *Bioinformatics*, 31:4017–4019, 2015.
- [87] C.T. Ravirajan, M.A. Rahman, L. Papadaki, M. Griffiths, J. Kalsi, A.C.R. Martin, M.R. Ehrenstein, D.S. Latchman, and D.A. Isenberg. Genetic structural and functional properties of a human IgG anti-DNA antibody. *European Journal of Immunology*, 28:339–350, 1998.
- [88] C.T. Ravirajan, M.A. Rahman, L. Papadaki, M.H. Griffiths, J. Kalsi, A.C.R. Martin, M.R. Ehrenstein, D.S. Latchman, and D.A. Isenberg. Correction: Genetic, structural and functional properties of an IgG DNA-binding monoclonal antibody from a lupus patient with nephritis (*European Journal of Immunology* 28(1998)339-350). *European Journal of Immunology*, 29:3052, 1999.
- [89] M. Reczko, A.C.R. Martin, H. Bohr, and S. Suhai. Prediction of hypervariable CDR-H3 loop structures in antibodies. *Protein Engineering*, 8:389–395, 1995.
- [90] A.R. Rees, A.C.R. Martin, J.C. Cheetham, and D. Webster. Prediction of three-dimensional structure of antibody combining sites., 1989.
- [91] A.R. Rees, A.C.R. Martin, S. Roberts, and J.C. Cheetham. Combining sites and epitopes defined by molecular modelling, protein engineering and NMR. In C. Craik, R. Fletterick, C.R. Matthews, and J. Wells, editors, *Proceedings of the UCLA Symposia on Molecular and Cellular Biology: Protein and Pharmaceutical Engineering*, pages 35–54. Liss, New York, 1989. ISBN: 047156771X, 9780471567714.
- [92] A.R. Rees, A.C.R. Martin, D.M. Webster, J.C. Cheetham, , and S. Roberts. Antibody combining sites: Prediction and design. *Biophysical J*, 57:A384, 1990. (Thirty-Fourth Annual Meeting of the Biophysical Society, February 18-22, 1990 Baltimore Convention Center Baltimore, Maryland).
- [93] S. Rybak, J. Krauss, M. Arndt, and A.C.R. Martin. Specificity grafting of a murine antibody onto a human framework, 2003. US Patent 7,456,260. Issued 25 Nov 2008. (Priority date 17 June 2002).
- [94] J.W. Saldanha, A.C.R. Martin, and O.J.P. Leger. A single backmutation in the human kIV framework of a previously unsuccessfully humanized antibody restores the binding activity and increases the secretion in *cos* cells. *Molecular Immunology*, 36:709–719, 1999.
- [95] M.B. Swindells, C.T. Porter, M. Couch, J. Hurst, K.R. Abhinandan, J.H. Nielsen, G. Macindoe, J. Hetherington, and A.C.R. Martin. abYsis: Integrated antibody sequence and structure - management, analysis and prediction. *Journal of Molecular Biology*, 429:356–364, 2017.

- [96] P. Thullier, O. Huish, T. Pelat, and A.C.R. Martin. The humanness of macaque antibody sequences. *Journal of Molecular Biology*, 396:1439–1450, 2010.
- [97] E. Usifo, S.E.A. Leigh, R.A. Whittall, N. Lench, A. Taylor, C. Yeats, C.A. Orengo, A.C.R. Martin, J. Celli, and S.E. Humphries. Low density lipoprotein receptor gene familial hypercholesterolemia variant database: update and pathological assessment. *Annals of Human Genetics*, 76:387–401, 2012.
- [98] F. Zuccotto, A.C.R. Martin, R.A. Laskowski, I. Gilbert, and J.M. Thornton. Dihydrofolate reductase: a potential drug target in trypanosomes and Leishmania. *Journal of Computer Aided Molecular Design*, 12:241–257, 1998.