

THOMAS LEON BLUNDELL

Published Work: ~476 Publications, ~30 in Nature, Science etc

1. Sridharan S, Howard N, Kerbarh O, Błaszczak M, Abell C, Blundell TL (2010) Crystal Structure of Escherichia coli Enterobactin-specific Isochorismate Synthase (EntC) Bound to its Reaction Product Isochorismate: Implications for the Enzyme Mechanism and Differential Activity of Chorismate-utilizing Enzymes. *Journal of Molecular Biology* doi:10.1016/j.jmb.2010.01.019
2. Sibanda BL, Chirgadze D, Blundell TL (2010) Crystal Structure of DNA-PKcs Reveals a Large Open-Ring Cradle Comprised of HEAT Repeats. *Nature* 7;463(7277):118-21.
3. Blundell TL, Bolanos-Garcia VM (2009) Targeting protein interactions of p53 for therapeutic intervention: Success in a frustrated landscape. *Cell Cycle* 8:22, 3631-3635; November 15, 2009;
4. Reis NM, Chirgadze DY, Blundell TL, Mackley MR (2009). The effect of protein-precipitant interfaces and applied shear on the nucleation and growth of lysozyme crystals. *Acta Cryst. D* 65, 1127-1139 [doi:10.1107/S0907444909031527]
5. Worth CL, Gong S, Blundell TL. (2009) Structural and functional constraints in the evolution of protein families. *Nat Rev Mol Cell Biol.* 2009 Oct;10(10):709-20. Epub 2009 Sep 16. Review. PMID: 19756040
6. Gong S, Worth CL, Bickerton GR, Lee S, Tanramluk D, Blundell TL.(2009) Structural and functional restraints in the evolution of protein families and superfamilies. *Biochem Soc Trans.* 2009 Aug;37(Pt 4):727-33. Review. PMID: 19614584
7. Lee S, Brown A, Pitt W, Higuero A, Gong S, Bickerton G, Schreyer A, Tanramluk D, Baylay A, Blundell T. (2009) Structural interactomics: informatics approaches to aid the interpretation of genetic variation and the development of novel therapeutics. *Molecular BioSystems* doi: 10.1039/B906402H
8. Higuero AP, Schreyer A, Bickerton GRJ, Pitt WR, Groom CR, Blundell TL (2009) Atomic Interactions and Profile of Small Molecules Disrupting Protein-Protein Interfaces: the TIMBAL Database. *Chemical Biology & Drug Design.* 74, 457 - 467
9. Gong S, Worth C, Bickerton G, Lee S, Tanramluk D, Blundell T. Structural and functional restraints in the evolution of protein families and superfamilies. *Biochemical Society transactions* 37 (Pt 4) , 727-33 (2009)
10. Hung AW, Silvestre HL, Wen S, Ciulli A, Blundell TL, Abell C. (2009) Application of Fragment Growing and Fragment Linking to the Discovery of Inhibitors of Mycobacterium tuberculosis Pantothenate Synthetase. *Angewandte Chemie* DOI: 10.1002/anie.200903821
11. Truman, A.W., Dias, M.V., Wu, S., Blundell, T.L., Huang, F., Spencer, J.B. (2009) Chimeric glycosyltransferases for the generation of hybrid glycopeptides. *Chem Biol* 16, 676 – 685
12. Lee S, Blundell TL (2009) Ulla: a program for calculating environment-specific amino acid substitution tables. *Bioinformatics.* PMID: 19417059
13. Lee S, Blundell TL (2009) BIPA: a database for protein-nucleic acid interaction in 3D structures. *Bioinformatics.* PMID: 19357098
14. Tanramluk D, Pitt WR, Schreyer A, Blundell TL (2009) On the Origins of Enzyme Inhibitor Selectivity and Promiscuity: A Case Study of Protein Kinase Binding to Staurosporine. *Chem Biol Drug Des*
15. Karmali AM, Blundell TL and Furnham N (2009) Model-building strategies for low-resolution X-ray crystallographic data. *Acta Crystallographica Section D: Biological Crystallography* 65, 121-127

16. Schreyer, A. & Blundell (2009) T. Credo: A protein-ligand interaction database for drug discovery. *Chem Biol Drug Des* 73: 157–167
17. Victor M. Bolanos-Garcia, Tomomi Kiyomitsu, Sheena D'Arcy, Dimitri Y. Chirgadze, J. Günter Grossmann, Dijana Matak-Vinkovic, Ashok R. Venkitaraman, Mitsuhiro Yanagida, Carol V. Robinson, Tom L. Blundell (2009) The Crystal Structure of the N-Terminal Region of BUB1 Provides Insight into the Mechanism of BUB1 Recruitment to Kinetochores. *Structure* 17, 105-116
18. Forman, J.R., Worth, C.L., Bickerton, G.R.J., Eisen, T., & Blundell, T.L.(2009) Structural bioinformatics mutation analysis reveals genotype-phenotype correlations in von Hippel-Lindau disease and suggests molecular mechanisms of tumourigenesis. *Proteins: Structure, Function, and Bioinformatics* 77, 84-96
19. Gore,S.P., and T.L. Blundell (2008) *OPSAX Optimal side-chain packing in proteins and crystallographic refinement*, *J App Cryst.* 41, 319-328
20. Worth CL, Blundell TL (2008) Satisfaction of hydrogen-bonding potential influences the conservation of polar sidechains *Proteins: Structure, Function and Bioinformatics*
21. Cheng TMK , Blundell TL, Fernandez-Recio J (2008) Structural assembly of two-domain proteins by rigid-body docking . *BMC Bioinformatics*, 9:441doi:10.1186/1471-2105-9-441
22. Ciulli, A, Scott, D.E., Ando, M., Reyes, F., Saldanha, S.A., Tuck, K.L., Chirgadze, D.Y., Blundell, T.L. and Abell, C. (2008) Inhibition of Mycobacterium tuberculosis pantothenate synthetase by analogues of the reaction intermediate. *ChemBiochem.* 9, 2606-2611
23. Gong S, Blundell TL (2008) Discarding Functional Residues from the Substitution Table Improves Predictions of Active Sites within Three-Dimensional Structures. *PLoS Computational Biology* 4(10): e1000179 doi:10.1371/journal.pcbi.1000179
24. Montalvao RW, Cavalli A, Salvatella X, Blundell TL & Vendruscolo M (2008): Structure Determination of Protein-Protein Complexes Using NMR Chemical Shifts: Case of an Endonuclease Colicin;Immunity Protein Complex. *Journal of the American Chemical Society* 130, 15990-15996
25. Nunez-Miguel R, Sanders J, Chirgadze D Y, Blundell TL, Furmaniak W, Rees Smith B (2008) FSH and TSH binding to their respective receptors: similarities, differences and implication for glycoprotein hormone specificity. *Journal of Molecular Endocrinology* 41, 145–164
26. Goodger SJ, Robinson CJ, Murphy KJ, Gasiunas N, Harmer NJ, Blundell TL, Pye DA, Gallagher JT (2008) Evidence that heparin saccharides promote FGF2 mitogenesis through two distinct mechanisms. *J Biol Chem* 283(19) 09 May 2008
27. Furnham N., de Bakker P.I.W, Gore S., Burke D.F. and Blundell T.L. (2008) Comparative modelling by restraint-based conformal sampling. *BMC Structural Biology* 8:7 1186/1472-6807-8-7
28. Worth CL and Blundell TL. (2007) Estimating the effects of SNPs on protein structure: loss of protein interactions and stability as indicators of mis-function and disease-association. *Current Topics in Biochemical Research*, **9**, 53-62.
29. Cheng, T., Blundell, T.L., Fernandez-Recio, J. (2007) pyDock: electrostatics and desolvation for effective scoring of rigid-body protein-protein docking *Proteins* 68, 503-515.
30. Blundell TL (2007) In *Proceedings of the International Belstein Workshop: Molecular Interactions: Bringing Chemistry to Life* Ed Hicks MG and Kettner C
31. Blundell TL (2007) New Dimensions of Structural Proteomics: Exploring Chemical and Biological Space. *Structure* **15**, 1342-1343.
32. Worth C.L., Bickerton G.R.J, Schreyer A., Forman, J.R., Cheng T.M.K., Lee S., Gong S., Burke D.F. and Blundell T.L. (2007) A structural bioinformatics approach to the analysis of nonsynonymous single nucleotide polymorphisms (n SNPs) and their relation to disease. *Journal Bioinformatics & Computational Biology* **5**, 1297 - 1318
33. Li Y, Chirgadze DY, Bolanos-Garcia VM, Sibanda BL, Davies OW, Ahnesorg P, Jackson SP, Blundell TL (2007) Crystal structure of human XLF/Cernunnos reveals unexpected

- differences from XRCC4 with implications for NHEJ. *EMBO Journal* 27(1):290-300
34. Ciulli A, Blundell TL, Abell C (2007) Discovery and Extrapolation of Fragment Structures towards Drug Design. RSC Monograph : Computational and Structural Approaches to Drug Discovery: Protein-Ligand Interactions' Ed R Stroud pp
 35. Harmer NJ, King JD, Palmer CM, Preston A, Maskell DJ, Blundell TL. (2007) Cloning, expression, purification and preliminary crystallographic analysis of the short-chain dehydrogenase enzymes WbmF, WbmG and WbmH from *Bordetella bronchiseptica*. *Acta Crystallogr Sect F Struct Biol Cryst Commun.* 63,711-5.
 36. King JD, Harmer NJ, Preston A, Palmer CN, Rejzek M, Field RA, Blundell TL, Maskell DJ J. (2007) Predicting Protein Function from Structure—The Roles 2 of Short-chain dehydrogenase/Reductase Enzymes in 3 *Bordetella* O-antigen Biosynthesis. *J. Mol. Biol.* 374, 749–763
 37. Burke DF, Worth CL, Prego EM, Cheng T, Smink LJ, Todd JA and Blundell TL (2007) Bioinformatic analysis of non-synonymous SNPs *BMC Bioinformatics*, 8:301
 38. Sanders J, Chirgadze DY, Sanders P, Baker S, Sullivan A, Bhardwaja A, Bolton J, Reeve M, Nakatake N, Evans M, Richards R, Powell M, Nunez Miguel R, Blundell TL, Furmaniak J, Rees Smith B (2007) Crystal Structure of the TSH Receptor in Complex with a Thyroid-Stimulating autoantibody *THYROID* 17, 395-410
 39. Gore SP, Karmali AM and Blundell TL (2007) RapperTK : a versatile engine for discrete restraint-based conformational sampling of macromolecules *BMC Structural Biology* 7:13
 40. Kerbarh O, Ciulli A, Chirgadze D, Blundell TL and Abell C (2007) Nucleophile Selectivity of Chorismate-Utilizing Enzymes. *ChemBioChem* 8, 1–3
 41. Ciulli A, Lobley C, Tuck KL, Smith AG, Blundell TL and Abell C (2007) pH-tuneable binding of 2_′-phospho-ADP-ribose to ketopantoate reductase: a structural and calorimetric study. *Acta Cryst. D*63, 171–178
 42. Ciulli A, Chirgadze DY, Smith AG, Blundell TL, Abell C. (2007) Crystal structure of *Escherichia coli* ketopantoate reductase in a ternary complex with NADP⁺ and pantoate bound: substrate recognition, conformational change, and cooperativity. *J Biol Chem.* 282:8487-97.
 43. Smith RE, Lovell SC, Burke DF, Montalvao RW, Blundell TL (2007) Andante: Reducing side-chain rotamer search space during comparative modeling using environment-specific substitution probabilities. *Bioinformatics* 2007; doi: 10.1093/bioinformatics/btm073
 44. Worth CL, Burke DF, Blundell TL.(2006) Estimating the effects of single nucleotide polymorphisms on protein structure: how good are we at identifying likely disease associated mutations? *Proceedings of “Molecular Interactions—Bringing Chemistry to Life.”* pp 11–26
 45. Blundell TL, Fernández-Recio J. (2006) Cell biology: brief encounters bolster contacts. *Nature.* 444:279-80.
 46. Chelliah V, Blundell TL. (2006) Quantifying structural and functional restraints on amino acid substitutions in evolution of proteins. In "Oleg Borisovich Ptitsyn: Personality, Scientist, Teacher, Friend" (Eds. V.E. Bychkova, A.V. Finkelstein) University Publishing House, Moscow., pp. 135-148,
 47. Bolanos-Garcia VM, Fernandez-Recio J, Allende JE and Blundell TL (2006) Identifying interaction motifs in CK2b – a ubiquitous kinase regulatory subunit. *Trends in Biochemical Sciences* 31, 654-661
 48. Chelliah V, Blundell TL, Fernández-Recio, J. (2006) Efficient Restraints for Protein-Protein Docking by Comparison of Observed Amino Acid Substitution Patterns with those Predicted from Local Environment. *J.Mol.Biol.* 357, 1669-1682
 49. Ryu EK, Cho KJ, Kim JK, Harmer NJ, Blundell TL, Kim KH (2006) Expression and purification of recombinant human Fibroblast growth factor receptor in *Escherichia coli*. *Science Direct Protein Expression and Purification* 49: 15–22
 50. N. Furnham, A.S. Dore, D.Y. Chirgadze, P.I.W. de Bakker, M.A. DePristo, T.L. Blundell

- (2006) Knowledge-based Real-space Explorations for Low Resolution Structure Determination. *Structure*. 14: 1313-1320
51. Ciulli A, Williams G, Smith AG, Blundell TL and Abell C (2006) Probing Hot Spots at Protein-Ligand Binding Sites: A Fragment-Based Approach Using Biophysical Methods. *J. Med. Chem.* 49: 4992 – 5000
 52. Hoskins J, Lovell S and Blundell TL (2006) An algorithm for predicting protein-protein interaction sites: abnormally exposed amino acid residues and secondary structure elements. *Protein Science*. 15:1017-1029
 53. Kerbath O, Chirgadze D, Blundell TL, and Abell C (2006) Crystal Structures of *Yersinia enterocolitica* Salicylate Synthase and its Complex with the Reaction Products Salicylate and Pyruvate. *J. Mol. Biol* 357, 524-534.
 54. Blundell TL, Sibanda BL, Montalvao RW, Brewerton S, Vijayalakshmi C, Worth CL, Harmer NJ, Davies O and Burke D. (2006). Structural biology and bioinformatics in drug design: opportunities and challenges for target identification and lead discovery. *Phil. Trans. R. Soc. B*. 361, 413-423.
 55. Furnham N, Blundell TL, DePristo MA, Terwilliger T (2006) Is one solution sufficient? *Nature Structural Molecular Biology*. 13, 184-185
 56. Popovic B, Tang X, Chirgadze DY, Huang F, Blundell TL, Spencer JB. (2006) Crystal structures of the PLP- and PMP-bound forms of BtrR, a dual functional aminotransferase involved in butirosin biosynthesis. *Proteins*. 65(1):220-30.
 57. P.I.W. de Bakker, N. Furnham, T.L. Blundell, M.A. DePristo (2006) Conformer generation under restraints. *Current Opinion in Structural Biology*. 16: 160-165
 58. Gherardi E, Sandin S, Petoukhov MV, Finch J, Youles ME, Ofverstedt L-G, Miguel RN, Blundell TL, Vande Woude GF, Skoglund U, Svergun DI (2006) Structural basis of hepatocyte growth factor/scatter factor and MET signalling. *Proc Natl Acad Sci USA* 103:4046-4051
 59. Dore, A.S., Furnham, N., Davies, O.R., Sibanda, B.L., Chirgadze, D.Y., Jackson, S.P., Pellegrini, L., and Blundell, T.L. (2006). Structure of an Xrcc4-DNA ligase IV yeast ortholog complex reveals a novel BRCT interaction mode. *DNA Repair (Amst)* 5, 362-368.
 60. Miguel RN, Chen S, Nikfarjam L, Kominami S, Carpenter B, Pra CD, Betterle C, Zanchetta R, Nakamatsu T, Powell M, Hewer R, Blundell TL, Smith BR, and Furmaniak J (2005) Analysis of the interaction between human steroid 21-hydroxylase and various monoclonal antibodies using comparative structural modelling. *European Journal of Endocrinology* 153, 949-961.
 61. Montalvao RW, Smith RE, Lovell SC, Blundell TL. (2005) CHORAL: a differential geometry approach to the prediction of the cores of protein structures *Bioinformatics* 2005, 21(19):3719-3725
 62. Robinson CJ, Harmer NJ, Goodger SJ, Blundell TL, Gallagher JT. (2005) Cooperative dimerization of fibroblast growth factor 1 (FGF1) upon a single heparin saccharide may drive the formation of 2 : 2 : 1 FGF1:FGFR2c:heparin ternary complexes. *J Biol Chem* 2005, 280(51):42274-42282
 63. Chelliah V, Blundell TL and Mizuguchi K (2005) Functional Restraints on the Patterns of Amino Acid Substitutions: Application to Sequence–Structure Homology Recognition. *Structure, Function, and Bioinformatics* 61: 722-731.
 64. Bolanos-Garcia VM, Beaufils S, Renault A, Grossmann JG, Brewerton S, Lee M, Venkitaraman A, Blundell TL (2005) The Conserved N-Terminal Region of the Mitotic Checkpoint Protein BUBR1: A Putative TPR Motif of High Surface Activity. *Biophys J*, 89, 2640-9.
 65. Miguel RN, Sanders J, Blundell TL, Smith BR, Furmaniak J. (2005) Comparative modeling of the thyrotropin receptor *Thyroid* 2005, 15(7):746-747
 66. Chelliah V and Blundell TL (2005). Quantifying structural and functional restraints on amino acid substitutions in evolution of proteins. *Biochemistry (Moscow)*. 70, 835-840.

67. Carafoli F, Chirgadze DY, Blundell TL & Gherardi E (2005) Crystal Structure of the β -Chain of Hgfl/Msp. *FEBS Journal* 272 (2005) 5799–5807
68. Loble, C. M., Ciulli, A., Whitney, H. M., Williams, G., Smith, A. G., Abell, C., and Blundell, T. L. (2005). The Crystal Structure of Escherichia coli Ketopantoate Reductase with NADP+ Bound. *Biochemistry* 44, 8930-8939.
69. Coxon KM, Chakauya E, Ottenhof HH, Whitney HM, Blundell TL, Abell C, Smith AG. (2005) Pantothenate biosynthesis in higher plants. *Biochem Soc Trans* 2005, 33(Pt 4):743-746
70. Cubellis MV, Caillez F, Blundell TL, Lovell SC. (2005) Properties of polyproline II, a secondary structure element implicated in protein-protein interactions. *Proteins* 2005, 58(4):880-892
71. DePristo M, de Bakker PIW, Johnson RJK & Blundell TL (2005) Crystallographic Refinement by Knowledge-Based Exploration of Complex Energy Landscapes. *Structure*, 13, 1311–1319
72. Congreve M, Murray CW and Blundell TL (2005) Structural Biology and Drug Discovery. *Drug Discovery Today* 10, 895-907
73. Gore S, Burke DF and Blundell TL (2005) PROVAT: A tool for Voronoi Tessellation Analysis of Macromolecular structures. *Bioinformatics* 21(15):3316-7
74. Ehebauer MT, Chirgadze DY, Arias AM, Hayward P & Blundell TL (2005) High-resolution crystal structure of the human Notch 1 ankyrin domain. *Biochem. J.* 392, 13-20
75. Blundell TL (2005). New Strategies for structure-guided design of AIDS antivirals. *Progress in Biophysics and Molecular Biology.* 88 191-192.
76. Blundell TL. (2005) The developing art of protein crystallisation: new advances from improved knowledge automaton and miniaturisation. *Progress in Biophysics and Molecular Biology* 88 283-284.
77. Harmer NJ, Sivak JM, Amaya E, Blundell TL (2005) Crystal structure of the X. tropicalis Spred1 EVH1 domain suggests a fourth distinct peptide-binding mechanism within the EVH1 family A. *FEBS Letters* 579, 1161–1166
78. Messenger NJ, Kabitschke C, Andrews R, Grimmer D, Núñez Miguel R, Blundell TL, Smith JC, Fiona C. Wardle (2005) Functional Specificity of the Xenopus T-Domain Protein Brachyury Is Conferred by Its Ability to Interact with Smad1. *Developmental Cell* 8, 1–12. 1.15 Å
79. Chelliah V, Chen L, Blundell TL, Lovell SC (2004) Distinguishing Structural and Functional Restraints in Evolution in Order to Identify Interaction Sites. *J. Mol. Biol.* 342, 1487-504
80. Sanders J, Jeffreys J, Depraetere H, Evans M, Richards T, Kiddie A, Brereton K, Premawardhana LDKE, Chirgadze DY, Nunez Miguel R, Blundell TL, Furmaniak J and Rees Smith B. (2004) Characteristics of a human monoclonal autoantibody to the thyrotropin receptor: sequence structure and function. *Thyroid* 14(8), 560-570.
81. Bertrand L, Sayed MFR, Pei X-Y, Parisini E, Dhanaraj V, Bolanos-Garcia VM, Allende JE, Blundell TL (2004) Structure of the regulatory subunit of CK2 in the presence of a p21WAF1 peptide shows the flexibility of the acidic loop. *Acta Cryst. D* 60, 1698-1704.
82. Harmer NJ, Pellegrini L, Chirgadze D, Fernandez-Recio J, Blundell TL (2004) The crystal structure of fibroblast growth factor (FGF) 19 reveals novel features of the FGF family and offers a structural basis for its unusual receptor affinity. *Biochemistry* 43, 629-40.
83. Harmer NJ, Ilag LL, Mulloy B, Pellegrini L, Robinson CV, Blundell TL (2004). Towards a resolution of the stoichiometry of the fibroblast growth factor (FGF)-FGF receptor-heparin complex. *Journal of Molecular Biology* 339, 821-34
84. Blundell TL, Patel S (2004) High-throughput X-ray crystallography for drug discovery. *Current Opinion in Pharmacology.* 4, 490-496
85. González B, Pajares MA, Martínez-Ripoll M, Blundell TL and Sanz-Aparicio J. (2004) Crystal structure of rat liver betaine homocysteine s-methyltransferase reveals new

- oligomerization features and conformational changes upon substrate binding. *Journal of Molecular Biology*. 338 771-782
86. DePristo MA, De Bakker PI, Blundell TL (2004) Heterogeneity and inaccuracy in protein structures solved by x-ray crystallography. *Structure (Camb)* 12, 831-8
 87. Badasso MO, Dhanaraj V, Wood SP, Cooper JB and Blundell TL (2004) Crystallization and X-ray analysis of the Y75N mutant of *Mucor pusillus* pepsin complexed with inhibitor. *Acta Cryst. (2004)*. D60, 770-772
 88. Brewerton SC, Dore AS, Drake AC, Leuther KK, Blundell TL. (2004) Structural analysis of DNA-PKcs: modelling of the repeat units and insights into the detailed molecular architecture. *J Struct Biol.* 145, 295-306
 89. Ottenhof HA, Ashurst JA, Whitney HM, Saldanha A, Schmitzberger F, Gweon HS, Blundell TL, Abell C and Smith AG (2003) Organisation of the pantothenate (vitamin B5) biosynthesis pathway in higher plants. *The Plant Journal* 37, 61-72
 90. Schmitzberger F, Kilkenny ML, Lobley CM, Webb ME, Vinkovic M, Matak-Vinkovic D, Witty M, Chirgadze DY, Smith AG, Abell C and Blundell TL (2003) *The EMBO Journal* 22, 6193-6204.
 91. Lo T, Pellegrini L, Venkitaraman AR and Blundell TL. (2003) Sequence fingerprints in BRCA2 and RAD51: implications for DNA repair and cancer. *DNA Repair* 2. 1015-1028
 92. Deane, C and Blundell, T (2003). Protein Comparative modelling and drug discovery. *The Practice of Medicinal Chemistry.* 27, 445-458.
 93. Owen D, Lowe PN, Nietlispach D, Brosnan CE, Chirgadze DY, Parker PJ, Blundell TL, Mott HR (2003) Molecular dissection of the interaction between the small G proteins Rac1 and RhoA and Protein Kinase C Related Kinase 1 (PRK1). *J. Biol. Chem.* 278: 50578 - 50587
 94. Gherardi E, Youles MY, Miguel RN, Blundell TL, Iamele L, Gough J, Bandyopadhyay A, Hartmann G, Butler JG (2003) Functional map and domain structure of the MET, the product of the c- met protooncogene and receptor for hepatocyte growth factor scatter factor, receptor. *Proc. Natl. Acad. Sci (USA)* 100, 12039-12044
 95. Miguel, R.N., Sanders, J., Jeffreys, J., Depraetere, H., Blundell, T., Furmaniak and J., Rees Smith, B (2003). Thyrotropin Receptor Cleavage Domain and Tissue Inhibitor Thyroid, 13, 665-666.
 96. von Delft F, Inoue T, Saldanha SA, Ottenhof HH, Schmitzberger F, Birch LM, Dhanaraj V, Witty M, Smith AG, Blundell TL, Abell C. (2003) "Structure of *E. coli* Ketopantoate Hydroxymethyl Transferase Complexed with Ketopantoate and Mg(2+), Solved by Locating 160 Selenomethionine Sites." *Structure* 11, 985-96.
 97. Schmitzberger F, Smith AG, Abell CA, and Blundell TL (2003) Comparative Analysis of the *E. coli* Ketopantoate Hydroxymethyltransferase Crystal Structure Confirms that It Is a Member of the ($\alpha\beta$)₈ Phosphoenolpyruvate/Pyruvate Superfamily. *J. Bacteriol.* 185, 4163-4171
 98. Yu DS, Sonoda E, Takeda S, Huang CLH, Pellegrini L, Blundell TL and Venkitaraman AR (2003) Dynamic control of RAD51 in the nucleus of living cells by self-association and interaction with BRCA2. *Mol Cell.* 12, 1029-1041.
 99. Evans PC, Smith TS, Lai MJ, Williams MG, Burke DF, Heyninck K, Kreike MM, Beyaert R, Blundell TL, Kilshaw PJ. (2003) *J Biol Chem.* 278(25):23180-6.
 100. Vinayagam A, Sh J, Pugalenthig, Meenakshi B, Blundell TL and Sowdhamini R (2003) DBASE2.0: updated domain database with improved methods for the identification of structural domains. *BIOINFORMATICS* 19, 1-6.
 101. Shin DS, Pellegrini L, Daniels D, Yelent B, Craig L, Tsurata H, Yu D, Hitomi C, Arvai AS, Blundell TL, Venkitaraman AR and Tainer JA (2003) Full-length archaeal Rad51 structure and mutants: mechanisms for RAD51 assembly and control by BRCA2. *EMBO J.* 2003 22 4566-76
 102. DePristo MA, de Bakker PIW, Lovell SC, Blundell TL (2003) Ab Initio Construction of Polypeptide Fragments: Efficient Generation of Accurate, Representative

- Ensembles. *PROTEINS: Structure, Function, and Genetics* 51, 41–55
103. M.A. DePristo, P.I.W. de Bakker, R.P. Shetty, T.L. Blundell (2003) Discrete restraint-based protein modeling and the C α -trace problem. *Protein Science*. 12: 2032-2046
 104. De Bakker PIW, DePristo MA, Burke DF, Blundell TL (2003) Ab Initio Construction of Polypeptide Fragments: Accuracy of Loop Decoy Discrimination by an All-Atom Statistical Potential and the AMBER Force Field With the Generalized Born Solvation Model. *PROTEINS: Structure, Function, and Genetics* 51, 21–40.
 105. R.P. Shetty, P.I.W. de Bakker, M.A. DePristo, T.L. Blundell (2003) Advantages of finegrained side chain conformer libraries. *Protein Engineering*. 16: 963-969
 106. Patel S, Martinez-Ripoll M, Blundell TL and Albert A (2002) Structural Enzymology of Li⁺ sensitive/MG2 dependent Phosphatases. *J. Mol. Biol.* 320, 1087-1094.
 107. Pomes A, Chapman MD, Vailes LD, Blundell TL and Dhanaraj V (2002) Cockroach Allergen Bla g 2 Structure, Function, and Implications for Allergic Sensitization. *Am J Respir Crit Care Med* 165, 391-397.
 108. Gonzalez B, Pajares MA, Too H-P, Garrido F, Blundell TL and Sanz-Aparicio J (2002) Betaine-homocysteine S-methyltransferase is one of the three. Crystallization and preliminary X-ray study of recombinant betaine-homocysteine S-methyltransferase from rat liver. *Acta Cryst.* (2002). D 58, 1507-1510.
 109. Pellegrini L, Yu DS, Lo T, Anand S, Lee M, Blundell TL, Venkitaraman AR (2002) Insights into DNA recombination from the structure of a RAD51-BRCA2 complex. *Nature* 420, 287-293
 110. Blundell TL, Abell C, Cleasby A, Hartshorn MJ, Tickle IJ, Parasini E and Jhoti. (2002) High-throughput X-ray crystallography for drug discovery. *Drug Design, Cutting Edge Approaches*. Ed Darren Flower. Royal Society Chemistry, 53- 59.
 111. Pellegrini L, Burke DF and Blundell TL (2002) Activation mechanism of fibroblast growth factor receptor tyrosine kinase revealed by crystal structure of fibroblast growth factor receptor ectodomain bound to fibroblast growth factor and heparin. In *Insulin and related proteins structure to function and pharmacology*. 189-200.
 112. Harmer NJ, Chirgadze D, Kim K-H, Pellegrini L, Blundell TL (2002) The structural biology of growth factor receptor activation. *Biophysical Chemistry* 100, 545 – 553
 113. Watanabe K, Chirgadze DY, Lietha D, de Jonge H, Blundell TL and Gherardi E (2002). A new crystal form of the NK1 splice variant of HGF/SF demonstrates extensive hinge movement and suggests that the NK1 dimer originates by domain swapping. *J.Mol.Biol* 319, 283-288.
 114. Williams MG, Shirai H, Shi J, Nagendra HG, Mueller J, Mizuguchi K, Miguel RN, Lovell SC, Innis CA, Deane CM, Chen L, Campillo N, Burke DF, Blundell TL and Bakker PIW (2001) Sequence-structure homology recognition by iterative alignment refinement and comparative modelling. *Proteins* 45(5), 92-97.
 115. Blundell, T.L., Bolanos-Garcia, V., **Chirgadze, D.Y.**, Harmer, N.J., Lo, T., Pellegrini, L., Sibanda, L.B. (2002) Asymmetry in the multiprotein systems of molecular biology (2002) *Structural Chemistry* **13** (3-4), 405-412.
 116. Patel S, Blundell TL (2002) Crystal Structure of an Enzyme Displaying both Inositol-Polyphosphate 1-Phosphatase and 3'-Phosphoadenosine-5'-Phosphate Phosphatase Activities: A Novel Target for Lithium Therapy. *J. Mol. Biol.* 315, 677-686.
 117. Blundell, T.L., Jhoti, H. and Abell, C. (2002). High-Throughput crystallography for lead discovery in drug design. *Nature Reviews Drug Discovery*. 1, 45-54.
 118. Martinez-Martin M, Siddle K and Blundell TL. (2001). The use of structural genomics and protein superfamilies in drug discovery: prediction that the binding site of the insulin receptor ectodomain lies at the concave face of A α -helix. *Royal Society Chemistry Medicinal Chemistry, into the millennium*. 25-31.
 119. Himpel S, Panzer P, Eirimbter K, Czajkowska H, Sayed M, Packman LC, Blundell TL, Kentrup H, Grotzinger J, Joost H-G, Becker W (2001) Identification of the

- autophosphorylation sites and characterisation of their effects in the protein kinase DYRK1A *Biochem. J.* 359, 497-505.
120. Matak-Vinkovic, D., Vinkovic, M., Saldanha S.A., Ashurst, J.L., von Delft, F., Inoue, T., Nunez Miguel, R., Smith, A.G., Blundell, T.L. and Abell, C. (2001) Crystal structure of *Escherichia coli* ketopantoate reductase at 1.7Å resolution and insight into the enzyme mechanism. *Biochemistry* 2001, 14493-14500.
 121. Martin-Martinez, M., Blundell, T.L., Burke, D., Dhanaraj, V., Mizuguchi, K., Molina, F., Sayed, M., Shi, J., Sibanda, L.B. and Williams, M. (2001) Genomics, Protein Superfamilies and Drug Discovery. "Medicinal Chemistry Into the Millennium" Editors: M.M. Campbell and I.S. Blagbrough, Royal Society of Chemistry Special Publication, 264, pp 266-282.
 122. Nagendra, H.G., Harrington, A.E., Harmer, N.J., Pellegrini, L., Blundell, T.L. and Burke, D.F. (2001). Sequence analyses and comparative modeling of fly and worm fibroblast growth factor receptors indicate that the determinants for FGF and heparin binding are retained in evolution. *FEBS Letters* 501, 51-58.
 123. Leitha D, Chirgadze DY, Mulloy B, Blundell TL, Gherardi E (2001) Crystal structures of NK1 heparin complexes reveal the basis for NK1 activity and enable engineering of potent agonists and the MET receptor. *EMBO J.* 20, 5543-5555
 124. Sibanda BL, Critchlow†S, Begun J, Pei XY, Jackson SP, Blundell TL, Pellegrini L (2001) Insight into the mechanism of DNA end joining from the structure of an Xrcc4 dimer in complex with DNA ligase IV. *Nature Structural Biology* 8, 1015-1019
 125. De Bakker P, Bateman A, Burke DF, Miguel RN, Mizuguchi K, Shi J, Shirai H, Blundell TL, (2001) HOMSTRAD: adding sequence information to structure-based alignments of homologous protein families. *BIOINFOMATICS* 17, 748-749.
 126. Shirai H, Shi J, Blundell TL, Mizuguchi K (2001) Structural Bioinformatics as an Approach to Genomics-based Drug Discovery *Global Outsourcing Review* 3, 48-53
 127. Mendes J, Nagarajaram H, Soares CM, Blundell TL, and Carrondo MA (2001) Incorporating Knowledge-based Biases into an Energy-based Side-chain Modelling Method: Application to Comparative Modelling of Protein Structure. *Biopolymers* 59, 72-86.
 128. Shi J, Blundell TL, and Mizuguchi K (2001) FUGUE: Sequence-structure Homology Recognition Using Environment-specific Substitution Tables and Structure-dependent Gap Penalties. *J. Mol. Biol.* 310, 243-257.
 129. Deane CM, Kaas Q and Blundell TL (2001) SCORE: predicting the core of protein models. *BIOINFOMATICS* 17, 541-550.
 130. Carvin D., Islam SA, Sternberg M., Blundell TL (2001) The preparation of heavy-atom derivatives of protein crystals for use in multiple isomorphous replacement and anomalous scattering. *International tables for Crystallography, Volume F. Crystallography of Biological macromolecules.* Dordrecht: Kluwer Academic publishers. Editors: Rossmann MG and Arnold E. pp 247- 262
 131. Shirai H, Blundell TL, & Mizuguchi K (2001) A novel family of enzymes that catalyse the modification of guanidine groups. *Trends Biochem. Sci.* 26, 465-468.
 132. von Delft F, Lewendon A, Dhanaraj V, Blundell TL, Abell C & Smith A (2001) The crystal structure of *E. coli* Pantothenate Synthase confirms it as a member of the cytidyltransferase superfamily. *Structure* 9, 439-450.
 133. Deane CM, and Blundell TL (2001) CODA: A combined algorithm for predicting the structurally variable regions of protein models. *Protein Science* 10, 599-612.
 134. Blundell TL, Burke DF, Chirgadze D, Dhanaraj D, Hyvonen M, Innis A, Parisini E, Pellegrini L, Sayed M and Sibanda BL (2000). Protein-protein interactions in receptor activation and intracellular signalling. *Biol. Chem.* 381, 955-959.
 135. Blundell TL and Mizuguchi K (2000) Structural genomics: an overview. *Prog. Biophys. Molec. Biol.* 73, 289-295.

136. Pellegrini L., Burke D.F., von Delft F., Mulloy B., Blundell TL (2000) Crystal Structure of fibroblast growth factor receptor ectodomain bound to ligand and heparin. *Nature* 407, 1029-1034
137. Innis CA, Shi JY, & Blundell TL (2000) Evolutionary trace analysis of TGF- β and related growth factors: implications for site directed mutagenesis. *Prot. Eng.* 13, 839-847.
138. Mizuguchi K and Blundell TL (2000) Analysis of conservation and substitutions of secondary structure elements within protein superfamilies. *Bioinformatics* 16, 1111-1119.
139. Albert A, Yenush L, Gil-Mascarell MR, Rodriguez PL, Patel S, Martinez-Ripoll M, Blundell TL, Serrano R (2000) X-ray structure of yeast Hal2p, a major target of lithium and sodium toxicity and identification of framework interactions determining cation sensitivity. *Journal of Molecular Biology* 295, 927-938.
140. Albert A, Blundell TL, Dhanaraj V, Donate LE, Groves M, Guruprasad K, Nugent PG, Orprayoon P, Pitts JE, Rufino S, Srinivasan N, Williams M and Wilsher J (2000) Site-directed mutagenesis, biochemical characterisation, and X-ray analysis of chymosins with substituted single amino acid substitutions and loop replacements. *Aspartic Proteinases*. 23, 169-177.
141. Deane, CM and Blundell TL (2000) Examination of the Less favoured Regions of the Ramachandran plot. *Indian Academy of Sciences*. 16 196-208
142. M. O. Badasso, J. A. Read, V. Dhanaraj, J. B. Cooper, S. P. Wood, T. L. Blundell, T. Dreyer, and J. Winther. (2000) Purification, co-crystallization and preliminary X-ray analysis of the natural aspartic proteinase inhibitor IA3 complexed with saccharopepsin from *saccharomyces cerevisiae*. *Acta Cryst. D*, 56, 915-917
143. Burke DF, Deane CM and Blundell TL (2000) Browsing the SLoop database of structurally classified loops connecting elements of protein secondary structure. *Bioinformatics*: 16, 513-519.
144. Deane CM, and Blundell TL (2000) A novel exhaustive search algorithm for predicting the conformation of polypeptide segments in proteins. *Proteins: Structure, Function and Genetics*. 40, 135-144.
145. Deane, C. M., Allen, F. H., Taylor, R. & Blundell, T. L. (1999). Carbonyl-carbonyl interactions stabilize the partially allowed Ramachandran conformations of asparagine and aspartic acid. *Protein Eng* 12(12), 1025-8
146. Walker AR, Davison PA, Bolognesi-Winfield AC, James CM, Srinivasan N, Blundell TL, Esch JJ, Marks MD and Gray JC (1999) The transparent testa glabra1 locus, which regulates trichome differentiation and anthocyanin biosynthesis in arabidopsis, encodes a WD40 repeat protein. *The Plant Cell*. 11, 1337-1349.
147. Marino-Buslje C, Martin-Martinez M, Mizuguchi K, Siddle K and Blundell TL (1999) The insulin receptor: from protein sequence to structure. *Biochemical Society Transactions* 27. 715-726.
148. Mizuguchi K, Dhanaraj V, Blundell TL and Murzin AG (1999) N-ethylmaleimide-sensitive fusion protein (NSF) and CDC48 confirmed as members of the double-psi β -barrel aspartate decarboxylase/formate dehydrogenase family. *Structure* 7, R215-R216.
149. Burke DF, Deane CM, Nagarajaram HA, Campillo N, Martin-Martinez M, Mendes J, Molina F, Perry J, Reddy BVB, Soares CM, Steward RE, Williams M, Carrondo MA, Blundell TL, Mizuguchi K. (1999) An Iterative structure-assisted approach to sequence alignment and comparative modeling. *Proteins, Structure, Function, and Genetics Suppl.* 3, 1-6.
150. G. Pavlovsky, M. G. Williams, Q. Z. Ye, D. F. Ortwine, C. F. Purchase, 2nd, A. D. White, V. Dhanaraj, B. D. Roth, L. L. Johnson, D. Hupe, C. Humblet, and T. L. Blundell. (1999) X-ray structure of human stromelysin catalytic domain complexed with nonpeptide inhibitors: implications for inhibitor selectivity. *Protein Sci.* 8, 1455-1462
151. Arias CA, Martin-Martinez M, Blundell TL, Arthur M, Courvalin P, Reynolds PE (1999) Characterization and modelling of VanT: a novel membrane-bound, serine racemase

- from vancomycin-resistant *Enterococcus gallinarum* BM4174. *Molecular Microbiology*. 31 no 6, 1653-1664.
152. Reddy BVB, Nagarajaram HA, Blundell TL (1999) Analysis of interactive packing of secondary structural elements in α/α units in proteins. *Protein Science*. 8, 573-586.
 153. Srinivasan N, Antonelli M, Jacob G, Korn I, Romero F, Jedlicki A, Dhanaraj V, Sayed M F-R, Blundell TL, Allende CC, Allende JE (1999) Structural interpretation of site-directed mutagenesis and specificity of the catalytic subunit of protein kinase CK2 using comparative modelling. *Protein Engineering*. 12, 119-127.
 154. Korn I, Gutkind S, Srinivasan N, Blundell TL, Allende CC, Allende JE (1999) Interactions of protein kinase CK2 subunits. *Molecular and Cellular Biochemistry*. 191, 75-83.
 155. Chirgadze, D.Y., Hepple, J.P., Zhou, H., Byrd, R.A., Blundell, T.L. & Gherardi, E. (1999). Crystal structure of the NK1 fragment of HGF/SF suggests a novel mode for growth factor dimerization and receptor binding. *Nature Structural Biology* 6, 72-79.
 156. Castillo, R.M., Mizuguchi, K., Dhanaraj, V., Albert, A., Blundell, T.L. & Murzin, A.G. (1999). A six-stranded double-psi α barrel is shared by several protein superfamilies. *Structure* 7, 1-11.
 157. Nagarajaram H, Reddy BVB and Blundell TL (1999) Analysis and prediction of inter-strand packing distances between α -sheets of globular proteins *Protein engineering* 12, 1055-1062
 158. Groves, M.R., Dhanaraj, V., Badasso, M., Nugent, P., Pitts, J.E., Hoover, D.J. & Blundell, T.L. (1998). A 2.3 Å resolution structure of chymosin complexed with a reduced bond inhibitor shows that the active site β -hairpin flap is rearranged when compared with the native crystal structure. *Protein Engineering* 11, 833-840.
 159. Rodionov, M.A. & Blundell, T.L. (1998). Sequence and structure conservation in a protein core. *Proteins* 33, 358-366.
 160. Snook, C.F., Woolley, G.A., Oliva, G., Pattabhi, V., Wood, S.P., Blundell, T.L. & Wallace, B.A. (1998) The structure and function of antiameobin 1, a proline-rich membrane-active polypeptide. *Structure* 6, 783-792.
 161. Marino-Buslje, C., Mizuguchi, K., Siddle, K., Blundell, T. (1998). A third fibronectin type III domain in the extracellular region of the insulin receptor family. *FEBS Letters* 441, 331-336.
 162. Sowdhamini, R., Burke, D.F., Deane, C., Huang, J-F., Mizuguchi, K., Nagarajaram, H.A., Overington, J.P., Srinivasan, N., Steward, R.E. & Blundell, T.L. (1998). Protein three-dimensional structural databases: domains, structurally aligned homologues and superfamilies. *Acta Cryst D54*, 1168-1177.
 163. Pellegrini L, Commander P, Mulloy B, Martin-Martinez M, Blundell TL, Burke DF (1998) The role of heparin in the complex formation between fibroblast growth factor 2 and its high affinity receptor: comparative modelling and biochemical studies. *Biochemical Soc. Trans* 26, 545-549.
 164. Islam, S.A., Carvin, D., Sternberg, M.J.E. & Blundell, T.L. (1998). HAD, a data bank of heavy-atom binding sites in protein crystals: A resource for use in multiple isomorphous replacement and anomalous scattering. *Acta Cryst D54*, 1199-1206.
 165. Mizuguchi, K., Deane, C.M., Blundell, T.L., Johnson, M.S. & Overington, J.P. (1998). JOY: protein sequence-structure representation and analysis. *BIOINFORMATICS* 14, 617-623.
 166. Mizuguchi, K., Deane, C.M., Blundell, T.L. and Overington, J.P. (1998) HOMSTRAD: A database of protein structure alignments for homologous families. *Protein Science* 7, 2469-2471.
 167. Mizuguchi, K., Parker, J.S., Blundell, T.L. & Gay, N.J. (1998). Getting Knotted: a model for the structure and activation of Spatzle. *TIBS* 23, 239-242.
 168. Sowdhamini, R., Burke, D., Huang, J-F., Mizuguchi, K., Nagarajaram, H.A.,

- Srinivasan, N., Steward, R.E and Blundell, T.L. (1998). CAMPASS: A Database Of Structurally Aligned Protein Superfamilies. *Structure* 6, 1087-1094.
169. Chirgadze, D.Y., Hepple, J., Byrd, R.A., Sowdhamini, R., Blundell, T.L and Gherardi, E. (1998) Insights into the structure of hepatocyte growth factor/scatter factor (HGF/SF) and implications for receptor activation. *FEBS Letters* 430: 126-129
170. Brotherton, D.H., Dhanaraj, V., Wick, S., Brizuela, L., Domaille, P.J., Voyanik, E., Xu, X., Parisini, E., Smith, O.B., Archer, S.J., Serrano, M., Brenner, S.L., Blundell, T.L. and Laue, E.D. (1998) Crystal structure of the complex of the cyclin D-dependent kinase Cdk6 bound to the cell cycle inhibitor p19INK4d. *Nature* 395, 244-250
171. Loew, A., Ho Y-K., Blundell, T.L. and Bax (1998) Phosducin induces a structural change in transducin $\beta\gamma$. *Structure* 6, 1007-1019
172. Cordeiro M, Lowther T, Dunn BM, Guruprasad K, Blundell TL, Pais MS, Brodelius PE (1998) Substrate specificity and molecular modelling of aspartic proteinases (Cyprosin) from flowers of *Cynara cardunculus* subsp. *flavescens* cv. *Cardoon* *Advances In Experimental Medicine And Biology* 436, 473-479.
173. Domingos A, Xue ZT, Guruprasad K, Clemente A, Blundell TL, Pais MS, Brodelius PE (1998) An aspartic proteinase from flowers of *Centaurea calcitrapa* - Purification, characterization, molecular cloning, and modelling of its three-dimensional structure. *Advances In Experimental Medicine And Biology* 436, 465-472.
174. Blundell, T.L., Guruprasad, K., Albert, A., Williams, M., Sibanda, B.L and Dhanaraj, V. (1998) The Aspartic Proteinases: an historical overview. *Advances In Experimental Medicine And Biology* 436, 1-13.
175. Olsen, V., Guruprasad, K., Cawley, N.X., Chen, H.C., Blundell, T.L and Loh, P. (1998) Cleavage efficiency of the novel aspartic proteinase yapsin 1 (Yap3p) enhanced for substrates with arginine residues flanking the P1 sites: correlation with electronegative active-site pockets predicted by molecular modelling. *Boichemistry* 37: 2768-2777.
176. Albert, A., Dhanaraj, V., Genschel, U., Khan, G., Ramjee, M.K., Pulido, R., Sibanda, B.L., von Delft, F., Witty, M., Blundell, T.L., Smith, A.G and Abel, C. (1998) Crystal structure of aspartate decarboxylase at 2.2Å resolution provides evidence for an ester in protein self-processing. *Nature Structural Biology* 5(4): 289-293.
177. Burke, D., Wilkes, D., Blundell, T.L. and Malcolm, S. (1998) Fibroblast growth factor receptors: lessons from the genes. *TIBS* 23, 59-62.
178. Williams, M.G., Wilsher, J., Nugent, P., Mills, A., Dhanaraj, V., Fabry, M., Sedláček, J., Uusitalo, J.M., Penttilä, M.E., Pitts, J. and Blundell, T.L. (1997) Mutagenesis, biochemical characterization and X-ray structural analysis of point mutants of bovine chymosin. *Protein Engineering* 10, 991-997
179. Bax, B., Blundell, T.L., Murray-Rust, J. and McDonald N.Q. (1997) Structure of mouse 7S NGF: a complex of nerve growth factor with four binding proteins. *Structure*. 5: 1275-1285.
180. Gherardi, E., Hartmann, G., Hepple, J., Chirgadze, D.Y., Srinivasan, N. and Blundell, T.L. (1997) Domain structure of hepatocyte growth factor/scatter factor (HGF/SF) *Ciba Found. Symp.* 212, 84-93.
181. Rufino, S.D., Donate, L.E., Canard, L.H.J. and Blundell, T.L. (1997) Predicting the conformational class of short and medium size loops connecting regular secondary structures: Application to comparative modelling. *J.Mol.Biol.* 267, 352-367.
182. Aguilar, C.F., Badasso, M., Dreyer, T., Cronin, N.B., Newman, M.P., Cooper, J.B., Hoover, D.J., Wood, S.P., Johnson, M.S. and Blundell, T.L. (1997) The 3-D structure at 2.4Å resolution of glycosylated proteinase A from the lysosome-like vacuole of *Saccharomyces cerevisiae*. *J.Mol.Biol.* 4, 899-915.
183. Topham, C.M., Srinivasan, N. and Blundell, T.L. Prediction of the stability of protein mutants based on structural environment-dependent amino acid substitution and propensity tables. (1997) *Protein Engineering*.10: 7-21.

184. Blundell, T.L., Guruprasad, K., Albert, Armando., Williams, M., Sibanda, B.L. and Dhanaraj, D. Aspartic proteinases: From the first X-ray photos of pepsin crystals to hundreds of 3-D structures. (1997) *Current Science*. 72: 483-489.
185. Donate, L.E., Rufino, S.D., Canard, L.H.J. and Blundell, T.L.* (1996) Conformational analysis and clustering of short and medium size loops connecting regular secondary structures: A database for modelling and prediction. *Protein Science*. 5, 2600-2616.
186. Aguilar, CF, Badasso M, Dreyer T, Cronin NB, Newman MP, Cooper, JB, Hoover D.J., Wood, S.P., Johnson, M.S. and Blundell, T.L. The three-dimensional structure at 2.4Å resolution of glycosylated proteinase A from the lysosome-like vacuole of *Saccharomyces cerevisiae*. 1997 *J.Mol.Biol.* 4, 899-915.
187. Srinivasan N & Blundell TL (1996) Insights on the structures of functional modules in protein kinase C family. *Molecular Biology Intelligence Units* (eds. PJ Parker & LV Dekker)
188. Blundell TL (1996). Structure-based drug design. 1996 *Nature*. 384S: 23-26
189. Louie GV, Brownlie PD, Lambert R, Cooper JB, Blundell TL, Wood SP, Malashkevich N, Hadener A, Warren M & Jordan PM. The 3-D Structure of *Escherichia coli* PBDG deaminase at 1.76Å resolution. (1996) *Proteins* 25, 48-78
190. Blundell TL and Srinivasan N. Symmetry, stability, and dynamics of multidomain and multicomponent protein systems. (1996) *Proc. Natl. Acad. Sci. USA*. 93. 233-241
191. Srinivasan N, Guruprasad K, and Blundell TL (1996) Comparative modelling of proteins in *Protein Structure Prediction* ed: M.J.E. Sternberg. Oxford University Press. Oxford 111-138
192. Dhanaraj V, Ye Q-Z, Johnson LL, Hupe DJ, Ortwine F, Dunbar JB, Rubin JR, Pavlosvsky A, Humblet C & Blundell TL (1996) Designing inhibitors of the metalloproteinase superfamily: comparative analysis of representative structures. *Drug Design and Discovery* 13: 3-14
193. Zhu Z-Y & Blundell TL (1996) The use of amino acid patterns of classified helices and strands in secondary structure prediction. *J. Mol. Biol.* 2: 261-276
194. Sowdhamini R, Rufino S & Blundell TL (1996) A database of globular protein structural domains: clustering of representative family members into similar folds. *Folding and Design* 1, 209-220
195. Srinivasan N, Rufino SD, Pepys MB, Wood SP and Blundell TL (1996) Lectin fold: Yesterday, today and tomorrow. *ChemTracts - Biochemistry and Molecular Biology* 6: 149-164
196. Dhanaraj V, Ye Q-Z, Johnson LL, Hupe DJ, Ortwine DF, Dunbar JB, Rubin JR, Pavlovsky A, Humblet C and Blundell TL (1996) X-ray structure of a hydroxamate inhibitor complex of stromelysin catalytic domain and its comparison with members of the zinc metalloproteinase superfamily. *Structure* 4: 375-386
197. Guruprasad K, Blundell TL, Xie S, Green J, Szafransk B, Nagel RJ, McDowell K, Baker CB & Roberts RM (1996) Comparative modelling and analysis of amino acid substitutions suggests that the family of pregnancy-related glycoproteins includes both active and inactive aspartic proteinases. *Protein Engineering* 9: 849-856
198. Srinivasan N, Waterfield MD and Blundell TL (1996) Comparative analysis of the regions binding by-subunits in Ga and PH domains. *Biochem.Biophys.Res. Communications* 220: 697-702
199. Nugent PG, Albert A, Oprayoon P, Wilsher J, Pitts JE, Blundell TL and Dhanaraj V (1996) Protein engineering loops in aspartic proteinases: site-directed mutagenesis, biochemical characterisation and X-ray analysis of chymosin with a replaced loop from rhizopuspepsin. *Protein Engineering* 9: 885-893.
200. Srinivasan N, Bax B, Blundell TL & Parker PJ. (1996) Structural aspects of the functional modules in human protein kinase-Ca deduced from comparative analyses.

- Proteins; Structure, Function and Genetics 26: 217-235.
201. Inrona M, Alles VV, Castellano M, Picardi G, Degioia L, Bottazzi B, Srinivasan N, Blundell TL, Hamilton TA & Mantovani A. (1996) Cloning of mouse PTX3, a new member of the pretraxin gene family expressed at extrahepatic sites. *Blood* 87: 1862-1872
 202. Blundell TL & Zhu Z-Y (1995) The α -helix as seen from the protein tertiary structure: a 3-D structural classification. *Biophysical Chemistry* 55: 167-184
 203. Patthy L & Blundell TL (1995) Sequences and Topology (Editorial Overview) *Current Opinion in Structural Biology* 1: 1-3
 204. Sowdhamini R, Rufino SD & Blundell TL (1995) The construction and uses of protein domain topologies and templates. *Chem Tracts* 5: 291-306
 205. Guruprasad L, Dhanaraj V, Timm D, Blundell TL, Gout I and Waterfield M D (1995) The crystal structure of the N-terminal SH3 domain of Grb2. *J. Mol. Biol.* 248: 856-866
 206. Rao-Naik C, Guruprasad G, Batley B, Rapundalo S, Hill J, Blundell TL, Kay J and Dunn BM (1995) Exploring the Binding Preferences/specificity in the Active site of Human Cathepsin E. *Proteins* 22:168-181
 207. Sowdhamini R, Srinivasan N, Guruprasad K, Rufino S, Dhanaraj V, Wood SP, Emsley J, White HE & Blundell TL (1995) Protein 3-D structure and molecular recognition: a story of soft locks and keys. *Pharmaceutica Acta Helveticae.* 69:185-192
 208. Aguilar CF, Dhanaraj V, Guruprasad K, Dealwis C, Badasso M, Cooper JB, Wood SP and Blundell TL (1995) Comparisons of the 3-D structures, specificities and glycosylation of renins, yeast proteinase A and cathepsin D. *Aspartic Proteinases: Structure, Function, Biology, and Biomedical Implications.* Ed. K Takahashi, Plenum Press p155-165
 209. Dhanaraj V, Pitts J, Nugent P, Orprayoon P, Cooper JB, Blundell TL, Uusitalo J and Pentilla M (1995) Protein Engineering of surface loops: Preliminary X-ray analysis of the CHY155-156RHI mutant. *Aspartic Proteinases: Structure, Function, Biology, and Biomedical Implications.* Ed. K Takahashi, Plenum Press p95-99
 210. Rufino R, Srinivasan N, Sowdhamini R, Murray-Rust J, Donate LE, May ACW, Guruprasad K, Dhanaraj V, Sibanda BL and Blundell TL (1995) Structure-based design of proteins: learning from evolution by comparative analyses of protein families. *Perspectives in Protein engineering and Complimentary Technologies.* Ed: MJ G & Roger Epton Mayflower Worldwide Ltd 1-8
 211. Guruprasad K, Dhanaraj V, Groves M and Blundell TL (1995) Aspartic proteinases: The structure and functions of a versatile superfamily of enzymes. *Supplement to Journal of computer-aided molecular design* 2:329-341
 212. Sowdhamini R, Rufino SD and Blundell TL (1995) The construction and use of protein domain topologies and templates. *Chemstracs* 5:291-306
 213. Guruprasad K, Dhanaraj V, Groves M & Blundell TL (1995) Aspartic proteinases: The structure and functions of a versatile superfamily of enzymes. *Prospectives in Drug Discovery & Design* Pub ESCOM
 214. Timm D, Guruprasad L, Bax B & Blundell TL (1995) Protein three-dimensional structure and drug design: some examples from intracellular components of the signal transduction pathway. *European Journal of Medicinal Chemistry* 30:605s-620s Ed: Jean-Claude Muller. Publisher: Elsevier
 215. Guruprasad L, Dhanaraj V, Timm D, Blundell TL, Gout I and Waterfield M D (1995) The crystal structure of the N-terminal SH3 domain of Grb2. *JMB* 248:856-866
 216. Sowdhamini R and Blundell TL (1995) An Automatic method involving cluster analysis of secondary structures for the identification of domains in proteins. *Protein Science* 4:506-521
 217. McDonald NQ, Murray-Rust J and Blundell TL (1994) The first structure of a receptor tyrosine kinase domain: a further step in understanding the molecular basis of insulin action. *Structure* (1995) 3:1-6

218. Donate LE, Gherardi E, Srinivasan N, Sowdhamini R, Aparicio S and Blundell TL (1994) Molecular evolution and domain structure of plasminogen-related growth factors. *Protein Science* 3:2378-2394
219. Bradshaw RA, Murray-Rust J, Ibanez CF, McDonald NQ, Lapatto R and Blundell TL (1994) NGF: structure/function relationships. *Protein Science* 3:1901-1913
220. Brownlie P, Lambert R, Louie GV, Jordan PM, Blundell TL, Warren MJ, Cooper JB & Wood SP (1994) The 3D structures of mutants of PBDG: towards understanding of the structural basis of acute intermittent porphyria. *Protein Science* 3:1644-1650
221. Timm D, Kamran S, Gout I, Guruprasad L, Waterfield M & Blundell TL (1994) Crystal Structure of the pleckstrin homology domain from dynamin. *Natural Structural Biology* 1:782-788
222. Srinivasan N, White HE, Emsley J, Wood SP, Pepys MB and Blundell TL (1994) Comparative analyses of pentraxins: implications for protomer assembly and ligand binding. *Structure* 2:1017-1027
223. Narasimha L, Singh J, Humblet C, Guruprasad K & Blundell TL (1994) Snail and spider toxins share a similar tertiary structure and 'cystine motif'. *Structural Biology*.1:850-852
224. Donnelly D, Findlay JBC & Blundell TL (1994) The evolution and structure of Aminergic G protein-coupled receptors. *Receptors and Channels*. 3:61-78
225. Whittle PJ & Blundell TL (1994) Protein Structure-Based Drug Design. *Ann.Rev.Biophys.Biomol.Struct.*23:349-375
226. Guruprasad K, Tormakangas K, Kerniven J & Blundell, TL (1994) Comparative modelling of barley-grain aspartic proteinase: a structural rationale for observed hydrolytic specificity. *FEBS letters* 352:131-136
227. Sali A & Blundell TL (1994) Comparative protein modelling by satisfaction of spatial restraints. *Protein Structure by Distance Analysis*. Ed:H Bohr & s Brunak. IOS Press
228. Blundell TL (1994) Realising our potential from the science base: Technology interaction and the food industry in the UK. *Trends in Food Science & Technology* 5:101-104
229. Lambert R, Brownlie PD, Woodcock SC, Louie GV, Cooper JC, Warren MJ, Jordan PM, Blundell TL & Wood SP (1994) Structural Studies on porphobilinogen deaminase. *Ciba Foundation Symposium* 180 Ed Wiley, Chichester. p97-110.
230. Blundell, TL. (1994) Problems and solutions in protein engineering - towards rational design. *Trends in Biotechnology*. 12:145-148
231. May AC, Johnson MJ, Rufino SD, Wako H, Zhu Z-y, Sowdhamini R, Srinivasan N, Rodionov MA & Blundell TL (1994) The recognition of protein structure and function from sequence: adding value to genome data *Phil.Soc.R.Soc.Lond.B*. 344:373-381
232. Pitts JE, Dhanaraj V, Dealwis CG, Mantafounis D, Nugent P, Oprayoon P, Cooper JB, Newman N & Blundell TL (1994) Multidisciplinary cycles for protein engineering: site-directed mutagenesis and X-ray structural studies of aspartic proteinases. *J.Scnd.Clin.Biochem*. 321-330
233. Newman RH, Carpenter E, Freemont PS, Blundell TL and Parker P (1994) Microcrystals of B1 isozyme of protein kinase C: an electron microscopy study. *Biochemical Journal* 298: 391-393
234. Dhanaraj V, Nugent P, Pitts JE, Cooper JB & Blundell TL. (1994) Structure-based design of enzymes. *Proceedings of the 6th European Congress on Biotechnology, Florence, Italy*. Ed: L Alberghina, L Frontali, P Sensi. Elsevier Science BV.
235. Donnelly D, Overington JP & Blundell TL (1994) The prediction and orientation of α -helices from sequence alignments: the combined use of environment-dependent substitution tables, Fourier transform methods and helix capping rules. *Prot.Eng.* 7:645-653258.
236. Frazao C, Topham C, Dhanaraj V and Blundell TL (1994) Comparative modelling of

- human renin: a retrospective evaluation of the model with respect to the X-ray crystal structure. *Pure & Appl.Chem.* 66:43-50.
237. Rufino SD and Blundell TL (1994) Structure-based identification and clustering of protein families and superfamilies. *J. of Computer-Aided Molecular Design* 8:5-27
238. Dealwis CG, Frazao C, Badasso M, Cooper JB, Tickle IJ, Driessen H, Blundell TL, Murakami K, Miyazaki H, Sueiras-Diaz J, Jones DM and Szelke (1994) X-ray analysis at 2.0Å resolution of mouse submaxillary renin complexed with a decapeptide inhibitor CH-66, based on the 4-16 fragment of rat angiotensinogen. *JMB* 236:342-360.
239. Edwards Y, Johnson M, Moss DS and Blundell TL (1994) The effects of local environments on the pattern of amino acid substitution in homologous protein structure: the role of side-chain to main-chain van Der Waals interactions. *Techniques in Protein Chemistry V: Protein Society. Academic Press Inc* p405-411
240. Johnson M S, Srinivasan N, Sowdhamini R and Blundell TL (1994) Knowledge-based protein modeling. *Critical Reviews in Biochemistry and Molecular Biology* CRC Press 29:1-70
241. Blundell TL (1994) Metalloproteinase super-families and drug design. *Nature Structural Biology* 1:73-75
242. Emsley J, White HE, O'Hara BP, Oliva G, Srinivasan N, Tickle IJ, Blundell TL, Pepys MB & Wood SP (1994) The 3D structure of pentameric human serum amyloid P component defined at 2Å resolution reveals a lectin-like fold and calcium-mediated ligand binding. *Nature* 367:338-249.
243. Wako H and Blundell TL (1994) Use of amino acid environment-dependent substitution tables and conformational propensities in structure prediction from aligned sequences of homologous proteins; Paper II. Secondary structures. *JMB* 238:693-708
244. Wako H and Blundell TL (1994) Use of amino acid environment-dependent substitution tables and conformational propensities in structure prediction from aligned sequences of homologous proteins Paper I. Solvent accessibility classes. *JMB* 238:682-692
245. Johnson MS, Blundell TL. Sequence patterns that characterise protein families with a common fold. (1993) *Methods in Protein Sequence Analysis*. Ed: K Imahori & F Sakiyama, Plenum Press, NY pp 245-251
246. Blundell, T.L, Ruffle, S.V, Donnelly, D and Nugent J.H.A. A three-dimensional model of the Photosystem II reaction centre of *Pisum sativum*. (1993) *Photosynthesis Research* 34:287-300
247. Dhanaraj V, Dealwis C, Bailey D, Cooper JB and Blundell TL. The 3-D structures of inhibitor complexes of monomeric aspartic proteinases. (1993) Ed: Francesc X Avilés, *Innovations in Proteases and their Inhibitors*. Pub: Walter de Gruyter, Berlin, New York 1993 141-159
248. Blundell, T.L. Structural Biology and diabetes mellitus: Molecular pathogenesis and rational drug design. (1993) *Diabetologia*. 35: S69-S76
249. Blundell, TL. (1993) New scientific opportunities for a sustainable agriculture. *J.Roy.Ag.Soc.Eng.* 154:19-28
250. Murray-Rust J, McDonald NQ, Blundell TL, Hosang M, Oefner C, Winkler F & Bradshaw RA. Topological similarities in TGF-β2, PDGF-BB and NGF define a superfamily of polypeptide growth factors. *Structure Current Biology*(1993) 1:153-159
251. Overington JP, Zhu Z-Y, Sali A, Johnson MS, Sowdhamini R, Louie GV & Blundell TL. (1993) Molecular recognition in protein families: A database of aligned three-dimensional structures of related proteins. *Biochemical Society Transactions*, 597-604
252. Blundell TL. (1993) Structural correlations of families of homologous proteins. In "Structure Correlation" Ed: Bürgi H and Dunitz J: pp1-7
253. Sali A & Blundell TL. (1993) Comparative modelling by satisfaction of spatial restraints. *J. Mol. Biol.* 234: 779-815
254. Reddy BVB & Blundell TL. Packing of Secondary Structural Elements in Proteins:

- Analysis and Prediction of Inter-Helix Distances. *JMB* (1993) 233:464-479
255. Doolittle RF & Blundell TL. Sequence and topology unit and diversity all over again. *Current Opinion in Structural Biology* (1993) 3:377-378
 256. Najmudin S, Nalini V, Driessen H, Slingsby C, Blundell TL, Moss D S and Lindley P F. (1993) Structure of the Bovine eye Lens Protein gammaB(gammaII)-Crystallin at 1.47Å. *Acta Cryst. D49*: 223-233
 257. Blundell TL and Johnson MS (1993) Catching a Common Fold. *Protein Science* 2:877-883
 258. Scarborough PE, Gurprasad K, Topham C, Richo GR, Conner GE, Blundell TL and Dunn BM Exploration of subsite binding specificity of human cathepsin D through kinetics and rule-based molecular binding. *Protein Science* 2:264-276
 259. Badasso M, Wood SP, Aguilar C, Cooper JB, Blundell TL & Dreyer T (1993) Crystallization and crystallographic characterisation of aspartic proteinase-A from Baker's yeast and its complexes with inhibitors *JMB* 232:701-703
 260. Aguilar CF, Newman MP, Sanz Aparicio J, Cooper JB, Tickle IJ & Blundell TL (1993) The use of protein homologues in the rotation function. *Acta Cryst. A49*:306-315
 261. Topham CM, McLeod A, Eisenmenger F, Overington JP, Johnson MS & Blundell TL (1993) Fragment Ranking in Modelling Protein Structure. *JMB* 229:194-220
 262. Bradshaw R, Blundell TL, Lapatto R, McDonald NQ & Murray-Rust J (1993) Nerve Growth Factor Revisited. *TIBS* 18:48-52
 263. Bailey D, Cooper JB, Veerapandian B & Blundell TL (1993) X-ray crystallographic studies of complexes of pepstatin A and a statine-containing human renin inhibitor with endothiapepsin. *Biochemistry Journal* 289: 363-371
 264. Hoffrén, AM, Saloheimo M, Thomas P, Overington J, Johnson MS, Knowles JKC & Blundell TL (1993) Modelling of the lignin peroxidase LIII of *Phlebia radiata*: Use of sequence template generated from a three-dimensional structure. *Protein Engineering* 6:177-182
 265. N Srinivasan & Blundell TL (1993) An evaluation of the performance of an automated procedure for comparative modelling of protein tertiary structure. *Protein Engineering* 6:501-512
 266. Donnelly D, Overington J, Ruffle S, Nugent J & Blundell TL (1993) Modelling a-helical transmembrane domains: the calculation and use of substitution tables for lipid-facing residues. *Protein Science* 2:55-70
 267. Newman N, Watson F, Roychowdhury P, Jones H, Badasso M, Cleasby A, Wood SP, Tickle IJ, Blundell TL (1993) X-ray analyses of aspartic proteinases V: structure and refinement at 2.0Å resolution of the aspartic proteinase from *mucor pusillus*. *Journal Molecular Biology*. 230:260-283
 268. Johnson M, Overington J & Blundell TL (1993) Alignment and searching for common protein folds using a Data Bank of structural templates. *JMB* 231:735-752
 269. Ruffle SV, Donnelly D, Blundell TL, Nugent JHA (1992) A three-dimensional model of the photosystem-II reaction centre of *pisumsativum*. *Photosynthesis Research* 34:287-300
 270. Ibanez CF, Ebendal T, Barbany G, Murray-Rust J, Blundell TL (1992) Disruption of the low affinity receptor-binding site of NGF allows neuronal survival and differentiation by binding to the trk gene product. *Cell* 69: 329-341
 271. Panayotou G, Bax B, Gout I, Federwisch M, Wroblowski B, Dhand R, Fry MJ, Blundell TL, Wollmer A and Waterfield MD (1992) Interactions of the p85 subunit of PI 3-kinase and N-terminal SH2 with a PDGF receptor phosphorylation site: structural features and analysis of conformational changes. *EMBO Journal* 11: 4261-4272
 272. Cooper J, Blundell TL, Quail W, Frazao C, Foundling S I, Humblet C, Lunney EA, Lowther WT, & Dunn BM (1992) X-ray crystallographic analysis of inhibition of endothiapepsin by cyclohexyl renin inhibitors. *Biochemistry* 31:8142-8150.

273. Blundell TL, Hubbard R, Weiss MA (1992) Structural biology and diabetes mellitus: molecular pathogenesis and rational drug design. *Diabetologia* 35:S69-S76
274. Louie GV, Brownlie PD, Lambert R, Cooper JB, Blundell, TL, Wood SP (1992) Structure of porphobilinogen deaminase reveals a flexible multidomain polymerase with a single catalytic site, *Nature* 359: 33-39
275. Dhanaraj, V, Dealwis C, Frazao C, Badasso M, Sibanda L, Tickle IJ, Cooper JB, Newman M, Aguilar C, Wood SP, Blundell TL, Hobart PM, Geoghegan KF, Ammirati MJ, Danley DE, O'Connor BA and Hoover DJ (1992) Molecular recognition and drug design: the structural basis of specificity and human and mouse renins defined by X-ray analyses of peptide inhibitor complexes. *Molecular Recognition RSC volume Special publications No 111*
276. Jordan PM, Warren MJ, Mgbeje BIA, Wood SP, Cooper JB, Louie G, Brownlie P, Lambert R and Blundell TL (1992) Crystallization and preliminary X-ray investigation of *Escherichia coli* porphobilinogen deaminase. *J.Mol.Biol.* 224:269-271
277. Dhanaraj V, Dealwis C, Frazao C, Badasso M, Sibanda BL, Tickle IJ, Cooper JB, Driessen HPC, Newman M, Aguilar C, Wood SP, Blundell TL, Hobart PM, Geoghegan K, Ammirati MJ, Danley DE, O'Connor BA and Hoover DJ. (1992) X-ray analyses of peptide inhibitor complexes define the structural basis of specificity for human and mouse renins. *Nature* 357:466-472
278. Blundell TL (1992). Patterns of sequence and 3-D structure variation in families of homologous proteins: Lessons for tertiary templates and comparative modelling. *Patterns of Proteins Sequence and Structure.* 7:189-205
279. Blundell TL and Doolittle R (1992) Sequence and topology-an inverse approach to the old folding problem. *Current Opinion in Structural Biology* 2:381-383
280. Murray-Rust J, McLeod A, Blundell TL and Wood SP (1992) Structure and evolution of insulins: implications for receptor binding. *Bioessays* 14:1-7
281. Sali A, Veerapandian B, Cooper JB, Moss DS, Hofmann T and Blundell TL (1992) Domain flexibility in aspartic proteinases. *Proteins* 12: 158-170.
282. Overington J, Donnelly, D, Johnson M S, Sali A, Blundell TL (1992) Environment-specific amino acid substitution tables: Tertiary templates and prediction of protein folds *Protein Science.* 2, 216-226.
283. Veerapandian B, Cooper J B, Sali A, Blundell, T L, Rosati RL, Dominy BW, Damon DB and Hoover, D. J. (1992) Direct observation by X-ray analysis of the tetrahedral 'Intermediate' of aspartic proteinases. *Protein Science* 1:322-328
284. Blundell TL, Cooper JB, Sali A and Zhu ZZ (1992) Comparisons of the sequences, 3-D structures and mechanisms of pepsin-like and retroviral aspartic proteinases. *Advances in Experimental Medicine and Biology* 306:443-453
285. Badasso M, Frazao, C, Sibanda, BL, Dhanaraj V, DeAlwis C, Cooper J B, Wood SP, Blundell TL, Murakami K, Miyazaki H, Hobart PM, Geoghegan K F, Ammirati M J, Lanzetti A J, Danley D E, O'Connor BA, Hoover DJ, Sueiras-Diaz J, Jones DM and Szelke M (1992) Crystallization and preliminary X-ray analysis of complexes of peptide inhibitors with human recombinant and mouse submandibular renins. *J.Mol.Biol* 223: 447-453
286. Lunney EA, Humblet CC, Repine JT, Blundell TL, Cooper JB and Sibanda BL (1991) Molecular Modelling of renin Inhibitor P2 substituents. *Ibid.* p274-281
287. Hoover DJ, Veerapandian B, Cooper J, Damon DB, Dominy BW, Rosati RL and Blundell TL (1991) X-ray analysis of a difluorostatone renin inhibitor bound as the tetrahedral hydrate to the aspartic protease endothiapepsin. *Structure & Function of the Aspartic Proteinases.* Wd:BM Dunn, Plenum Press, NY. p269-273
288. Hoffran A, Saloheimo M, Thomas P, Overington J, Johnson MS, Blundell TL (1991) Modelling the lignin peroxidase L111 of *Phlebia radiata* using a knowledge-based approach. *J.Chim.Phys;* 88: 2659-2662
289. Aguilar C, Bailey D, Badasso M, Blundell T L, Dhanaraj V, Dealwis C, Hemmings

- H, Frazao C, Newman M, Sali A, Tickle IJ, Wilderspin A and Wood SP (1991) New Insights into cellular and viral proteinase structures and the design of inhibitors. Workshop on Innovations of Proteases & their Inhibitors. 266, 21
290. Carvin D, Suhail A I, Sternberg M J E and Blundell TL (1991) Establishment of a heavy-atom databank for protein structures Proceedings of the CCP4 Meeting, Daresbury Laboratory, UK, 150-162
291. Newman M, Safro M, Frazao C, Khan G, Zdanov A, Tickle IJ, Blundell TL and Andreeva N (1991) X-ray analyses of aspartic proteinases IV: Structure and refinement at 2.2Å resolution of bovine chymosin. *J. Mol. Biol.* 222: 1295-1309
292. Blundell TL (1991) Comparative analysis of protein 3-D structures and an approach to the inverse folding problem. *Protein Conformation* 161:28-51
293. McDonald N, Lapatto R, Murray-Rust J, Gunning J, Wlodawer A and Blundell TL (1991) New Protein fold revealed by a 2.3Å resolution crystal structure of nerve growth factor. *Nature* 345: 411-414
294. McDonald NQ and Blundell TL (1991) Crystallization and characterization of the high molecular weight form of Nerve Growth Factor (7S NGF). *J. Mol. Biol.* 219:595-601
295. Blundell TL, Cooper J, Donnelly D, Driessen H, Edwards Y, Eisenmenger F, Frazao C, Johnson M, Niefind K, Newman M, Overington J, Sali A, Slingsby C, Nalinin V and Zhu ZZ (1991) Patterns of sequence variation in families of homologous proteins. *Methods in Proteins Sequence Analysis* Jornvall/Hoog/Gustavsson (eds) Birkhauser Verlag Basel.
296. Slingsby C, Bax B, Lapatto R, Bateman OA, Driessen H, Lindley PF, Moss DS, Najmudin, S. and Blundell T L (1991) Molecular interactions of crystallins in relation to optical properties. *Presbyopia Research Stark*. Plenum Press, New York
297. Slingsby C, Bax B, Lapatto R, Bateman OA, Driessen H, Lindley PF, Moss DS, Najmudin S and Blundell TL (1991) Molecular interactions of crystallins in relation to optical properties. *Presbyopia Research: From Molecular Biology to Visual Adaptation*, Ed. by G. Obrecht & L. W:41-48. Plenum
298. Lapatto R, Nalini V, Bax B, Driessen H, Lindley P, Blundell TL and Slingsby C. (1991) High resolution structure of an oligomeric eye lens α -crystallin. *Journal Molecular Biology* 222:1067-1083
299. Pitts J, Cooper JB and Blundell TL (1991) Three-dimensional structures and engineering of proteinases for the food industry: modification of specificity, pH optimum and stability. *Protein Engineering* 106-115
300. Zhu ZZ, Sali A and Blundell TL (1991) A variable gap penalty function and feature weights for protein 3-D structure comparisons. *Protein Engineering* 5:43-51
301. Hoover DJ, Damon DB, Rosati RL, Dominy BW, Veerapandian B, Cooper JB and Blundell TL (1990) A model for the tetrahedral intermediate in the catalytic mechanism of aspartic proteinases: synthesis of a sub-nanomolar difluorostatone renin inhibitor and X-ray analysis at 2.0Å resolution of its hydrate complexed with endothiapepsin
302. Johnson MS, Sutcliffe MJ and TL Blundell (1990) Molecular anatomy: phyletic relationships derived from three-dimensional structures of proteins. *J. of Molecular Evolution* 30:43-59
303. Wilderspin A, Gaskin D, Lapatto R, Blundell TL, Hemmings A, Overington J, Pitts J, Wood S, Zhu Z, Pearl L, Danley D, Geoghegan K, Hawrylik S, Lee SE, Shield K, Hobart P, Merson J, Whittle P and Blundell TL (1990) The three-dimensional structure and evolution of HIV-I protease. *Retroviral Proteases* 79-91
304. Blundell TL, Carney Devon, Hubbard Tim, Johnson Mark J, McLeod Alasdair, Overington John P, Sali Andrej, Sutcliffe Michael J, Thomas Pamela and Blundell TL (1990) Knowledge-based protein modelling and design of novel molecules *Proc. of Braunschweig Symposium on Biotechnology*
305. Sali A, Veerapandian B, Cooper JB, Moss DS, Hofmann T and T L Blundell (1990) Rigid body movement and conformational differences in aspartic proteinases. *Structure and*

Function of the Aspartic Proteinases 269-273

306. Bax B, Lapatto R, Nalini V, Driessen H, Lindley P, Mahdevan D, and Blundell TL (1990) X-ray analysis of bB2-crystallin and evolution of oligomeric lens proteins and C Slingsby. *Nature*: 347, 776-780
307. Strop P, Sedlacek J, Stys J, Kaderabkova Z, Blaha I, Pavlickova L, Pohl J, Fabry M, Kostka V, Newman M, Frazao C, Shearer A, Tickle I J and Blundell TL (1990) Engineering enzyme sub-site specificity: preparation, kinetic characterisation and X-ray analysis at 2.0Å resolution of Val111Phe site-mutated calf chymosin. *Biochemistry* 29, 9863-9871
308. Topham CM, Thomas P, J P Overington, M S Johnson, F Eisenmenger and T L Blundell) and Blundell TL (1990) An assessment of COMPOSER: a rule-based approach to modelling protein structure *Biochem. Soc. Trans.* 57, 1-9
309. Sali A, Overington JP, Johnson MS and T L Blundell (1990) From comparisons of protein sequences and structures to protein modelling and design *Trends Biochem. Sci.* 15, 235-240.
310. Blundell TL, Lapatto R, Wilderspin A, Hemmings A, Hobart Peter M, Danley D, Whittle P and Blundell TL (1990) The three-dimensional structure of HIV-proteinase and the design of antiviral agents for the treatment of AIDS. *Trends Biochem Sci.* 15, 425-430
311. Veerapandian B, Cooper JB, Sali A and T L Blundell (1990) X-ray analysis of aspartic proteinases. part 111: the three-dimensional structure of endothiapep-sin complexed with a transition-state isostere inhibitor of renin at 1.6Å resolution *J. Mol. Biol.* 216, 1017-1029
312. Overington J, Sali Andrej and T L Blundell TL (1990) Tertiary structural constraints on protein evolutionary diversity: templates, key residues and structure prediction. *Proc. Roy. Soc. B* 241, 132-145
313. Blundell TL, Johnson Mark S and John P Overington (1990) Knowledge-based protein modelling and the design of novel molecules. *Protein design and the development of new therapeutics and vaccines* (Hook and Poste, eds.) Plenum 10:209-227
314. Donnelly D, Johnson MS, Saunders J and Blundell TL (1990) An analysis of the periodicity of conserved residues in sequence alignments of G-protein coupled receptors *FEBS*, 251, 109-116
315. Waterfield MD, Greenfield C, Hiles I, Federwisch M, Wollmer A, McDonald N and Blundell TL (1990) The use of optical techniques to detect conformational changes associated with the interaction of epidermal growth factors and its receptor. *Advances in Second Messenger and Phosphoprotein Re-search* 24, 301-306
316. Blundell TL, McDonald N, Murray-Rust J, McLeod A, Wood S (1990) Three-dimensional structure models for EGF and insulin receptor interactions and signal transduction. *NATO ASI* 29, 187-195
317. Husain J, Blundell TL, Cooper S, Pitts JE, Tickle IJ, Wood SP, Hraby VJ, Buku A, Fischman AJ, Wyssbrod HR, Mascarenhas Y and Blundell TL (1990) The conformation of deamino-oxytocin: X-ray analysis of the 'dry' and 'wet' forms. *Phil.Trans.Roy. Soc.* 327, 625-654.
318. Cooper JB, Khan G, Taylor G, Tickle I J and Blundell T L (1990) X-ray analyses of aspartic proteinases: the structure of hexagonal pepsin at 2.3Å resolution *J. Mol. Biol.* 214, 199-222
319. Pitts J, Mantafounis D, Elliot G, Newman N, Frazao C, Wilderspin A, Gaskin D, Hemmings A, Lapatto R and Blundell TL (1990) Multidisciplinary cycles for protein engineering and receptor-based drug design. *Protein Structure function* 57-70
320. Sali A and Blundell TL (1989) Definition of general topological equivalence in protein structures. *J. Mol. Biol.* 212, 403-428
321. Johnson MS, Sali A and Blundell TL (1989) Phylogenetic relationships from three-dimensional protein structures *MTh. Enzymology* 183, 670-690
322. Sali A, Veerapandian B, Cooper JB, Foundling SI, Hoover DJ and Blundell TL

- (1989) High-resolution X-ray diffraction study of the complex between endothiapepsin and an oligopeptide inhibitor: the analysis of the inhibitor binding and the description of the rigid body shift in the enzyme. *EMBO Journal* 8, 2179-2188.
323. Lapatto R, Blundell TL, Hemmings A, Overington J, Wilderspin A, Wood S, Merson JR, Whittle PJ, Danley DE, Geoghegan KF, Hawrylik SJ, Lee SE, Scheld K G, Hobart PM and Blundell TL (1989) X-ray analysis of HIV-1 proteinase at 2.7Å resolution confirms structural homology among re-troviral enzymes *Nature* 342, 299-302
324. Greenfield C, Hiles I, Waterfield MD, Frederwisch M, Wollmer A, McDonald N and Blundell TL (1989) Epidermal Growth Factor binding induces a conformational change in the external domain of its receptor. *EMBO Journal* 8, 4115-4123.
325. McDonald N, Murray-Rust J, and Blundell TL (1989) Structure-function relationships of growth factors and their receptors. *Brit. Med. Bul.* 45, 554-569
326. Blundell TL and Pearl LP (1989) A second front against AIDS *Nature* 337, 396-397
327. Blundell TL, Jenkins JA, Sewell BT, Pearl LH, Cooper JB, Tickle IJ, Wood SP, Veerapandian B and Blundell TL (1989) X-ray analysis of aspartic proteinases: The three-dimensional structure at 2.1Å resolution of endothiapepsin. *J. Mol. Biol.* 211, 919-941
328. Cooper JB, Foundling SI, Boger J, Jupp RA, Kay J and Blundell TL (1989) X-ray studies of aspartic proteinase-statine inhibitor complexes. *Biochemistry* 28, 8596-8603.
329. Blundell TL (1989) The three-dimensional structure of aspartic proteinase and their inhibitors: Lessons for drug design. *Nova Acta Leopoldina* 57-58
330. Blundell TL, Elliot G, Gardner SP, Hubbard T, Islam S, Johnson M, Mantafounis D, Murray Rust P, Overington J, Pitts JE, Sali A, Sibanda BL, Singh J, Sternberg, MJE, Sutcliffe MJ, Thornton, JM, and Travers P (1989) Protein engineering and design *Phil. Trans. Royal Society* B324, 447- 460
331. Sibanda BL, Thornton JM and Blundell TL (1989) The conformation of B-hairpins in protein structure: a systematic classification with applications to modelling by homology, electron density fitting and protein engineering *J. Mol. Biol.* 206,759-777
332. Slingsby C, Driessen HPC, White H, Mylvaganam S, Najmudin S, Bax B, Bibby MA, Lindley PF, Moss DS and Blundell TL (1988) Molecular interactions of crystallins in relation to cataract. (1988)UCLA Symposia on Molecular & Cellular Biology 88, 417-426, Alan R Liss, Inc
333. Akrigg D, Bleasby AJ, Dix NIM, Findlay JBC, North ACT, Parry-Smith D, Wootton JC, Gardner SP, Hayes F, Islam S, Sternberg MJE, Thornton JM, Tickle IJ and Blundell TL (1988) A protein sequence/structure database. *Nature* 335, 745-746
334. Slingsby C, Driessen H, Mahadevan D, Bax B and Blundell T L (1988) Evolutionary and functional relationships between the basic acidic B-crystallins *Exp. Eye Res.* 46, 375-403
335. Baker EN, Cutfield JF, Cut-field SM, Dodson EJ, Dodson GG, Crowfoot Hodgkin D M, Hubbard RE, Isaacs NW, Reynolds CD, Sakabe K, Sakabe N, Vijayan NM and Blundell TL (1988) The structure of 2-Zn pig insulin crystals at 1.5Å resolution *Phil Trans. R. Soc. Lond.* B319, 369-456
336. Blundell TL, Carney D, Gardner S, Hayes F, Howlin B, Hubbard T, Overington J, Singh D, Sibanda BL, Sutcliffe M (1988) Knowledge-based protein modelling and design; 18th Sir Hans Krebs Lecture *Eur. J. Biochem.* 173, 513-520
337. Wood SP, Oliva G, O'Hara BP, White H, Perkins SJ, Sardharwalla I, Pepys B and Blundell (1988) A pentameric form of human serum amyloid P component: Crystallization, X-ray diffraction and neutron scattering studies *J. Mol. Biol.* (1988) 202, 23-30
338. Cooper JB and Foundling SI and Blundell TL (1988).A rational approach to the design of antihypertensives: X-ray studies of complexes between aspartic proteinases and aminoalcohol renin inhibitors *Topics in Medicinal Chemistry* (1988) Ed. P R Leeming. *Royal Soc. Chem.* 308-313
339. Sali A, Veerapandian B, Cooper JB, Foundling IS, Hoover D and Blundell TL (1988)

- High resolution X-ray diffraction study of the complex between endothiapepsin and an azahomostatine oligopeptide inhibitor
340. Johnson MS, Sutcliffe MJ and Blundell, TL (1988) Molecular Anatomy: Phyletic relationships derived from the three-dimensional structures of proteins. *J. Mol. Evol.* (1990) 30, 43-49.
 341. Baudys M, Foundling S, Pavlik M, Blundell TL, Kostka V (1988) Protein Chemical Characterization Of Mucor-Pusillus Aspartic Proteinase - Amino-Acid Sequence Homology With The Other Aspartic Proteinases, Disulfide Bond Arrangement And Site Of Carbohydrate attachment. *FEBS Lett.* 235, 271-274
 342. Sergeev YV, Chirgadze YN, Mylvaganam SE, Driessen H, Slingsby C and Blundell, TL. and Blundell (1988) Surface interactions of gamma-crystallins in the crystal medium in relation to their association in the eye lens. *Proteins* 4, 137-147.
 343. Mylvaganam SE, Slingsby C, Lindley, P and Blundell, TL (1987) Preliminary X-ray studies of adult turkey delta-crystallin: evidence of a space group transition. *Acta Cryst B*43, 580-582
 344. Akrigg D, Bleasby AJ, Dix NIM, Findlay JBC, North ACT, Parry-Smith D, Wootton JC, Blundell TL, Gardner SP, Hayes F, Islam S, Sternberg MJE, Thornton JM, Tickle IJ, Murray-Rust P (1988) A protein sequence/structure database. *Nature* 335, 745-746.
 345. Hubbard TJP and Blundell TL (1987) Comparisons of solvent-inaccessible cores of homologous proteins: definitions useful for protein modeling. *Protein Engineering*, 1, 159-171
 346. Sibanda BL, Sternberg MJE, Thornton JM and Blundell TL (1987) Knowledge-based prediction of protein structures and the design of novel molecules *Nature*, 326, 347-352
 347. Foundling SI, Cooper J, Watson FE, Cleasby A, Pearl LH, Sibanda BL, Hemmings A, Wood S P, Valler MJ, Norey CG, Kay J, Boger J, Dunn BM, Leckie BJ, Jones DM, Atrash N, Hallett A, Szelke M and Blundell TL (1987) High resolution X-ray analyses of renin inhibitor-aspartic proteinase complexes *Nature*, 327, 349-352
 348. Cooper JB, Foundling SI, Hemmings A, Watson FE, Sibanda BL, Jones DM, Hallett A, Atrash B, Szelke M and Blundell TL (1987) Inhibitors of aspartic proteinases and their relevance to the design of antihypertensive agents. *Biochemical Society Transactions* 751-754
 349. Sergeev Yu V, Chirgadze Yu N, Driessen H, Slingsby C, Lindley P and Blundell T L and (1987) The key role of residue 103 in the surface interactions of gamma-crystallins. *Molekularnaya Biologiya* 21, 377-381
 350. Jhoti H, McLeod AN, Ishi-zaki H, Nagasawa H, Suzuki A and Blundell TL (1987) Prothoracicotropic hormone has an insulin-like tertiary structure. *FEBS* 219, 419-425
 351. Bajaj M, Waterfield MD and Blundell TL(1987) Structure-function studies of growth-factor receptors "Membrane Receptors, Dynamics and Energetics" (1987) ed. K W A Wirtz. *NATO ASI Series A: Life Sciences Vol. 133*, 127-134
 352. Foundling SI, Cooper J, Watson FE, Pearl LH, Hemmings A, Wood SP, Hallet A, Jones DM, J Sueiras, Atrash B, Szelke M and Blundell TL (1987) Crystallographic studies of reduced bond inhibitors complexed with an aspartic proteinase *Journal of Cardiovascular Pharmacology* S59-S68
 353. Cooper J, Foundling SI and Blundell TL (1987) On the rational design of renin inhibitors: X-ray studies of aspartic proteinases complexed with transition-state analogues. *Biochemistry* 26, 5585
 354. Sutcliffe M J, Hayes F and Blundell TL (1987) Knowledge-based modelling of homologous proteins, part II: rules for replacement of sidechains. *Protein Engineering* 1, 384 - 391
 355. Sutcliffe MJ, Hannef I, Carney D and Blundell TL (1987) Knowledge-based modelling of homologous proteins, part I: three-dimensional frameworks de-rived from the

- simultaneous superposition of multiple structures *Protein Engineering*, 1, 377-384
356. Cooper J, Found-ling S, Hemmings A and Blundell TL (1987) The structure of a synthetic pepsin inhibitor complexed with endothiapepsin *Eur. J. Biochem.* 169, 215-221
357. Bajaj M, Waterfield MD, Schlessinger J, Taylor WR and Blundell TL (1987) On the tertiary structure of the extracellular domains of the epidermal growth factor and insulin receptors. *Biochemica et Biophysica Acta* 916, 220-226
358. Luchin SV, Zinovieva RD, Tomarev SI, Dolgilevich SM, Gause GG Jr., Bax B, Dreissen H and Blundell TL (1987) Frog lens BA1-crystallin: the nucleotide sequence of the cloned cDNA and computer graphics modelling of the three-dimensional structure. *Biochemica et Biophysica Acta* 916, 163-171
359. Pitts JE, Wood SP, Tickle IJ, Trehearne AM, Mascarenhas Y, Li JY, Hussain J, Cooper, S and Blundell TL (1987) X-ray analysis of deaminooxytocin: conformational flexibility and receptor binding. *Biological Organisation: Macromolecular Interaction at High Resolution* 289-306
360. Safro MG, Andreeva S and Blundell TL (1987) Role of peripheral interactions in the specificity of chymosin. 21, 1582-1589
361. Treharne AC, Wood SP, Tickle IJ, Pitts JE, Husain J, Glover IJ, Cooper S and Blundell TL (1986) X-ray analysis of polypeptide hormones at <1Å resolution: anisotropic thermal motion and secondary structure of pancreatic polypeptide and deamino-oxytocin *Crystallography in Molecular Biology*, Ed. D Moras, J Drenth, B Stranberg, D Suck and K Wilson. NATO ASI Series A: Life Science 153-165
362. Barlow DJ, Edwards MS, Sibanda BL, Sternberg MJE, Taylor WR, Thornton JM and Blundell TL (1986) The analysis of homologous tertiary structures and the design of novel proteins *Protein Engineering* 29-40
363. Blundell TL (1986) Diversity and invariance in the evolution of protein tertiary structure. *Chemica Scripta* 26B, 213-219
364. Summers LJ, Slingsby C, Dunnen den JT, Moormann RJM, Shoenmakers JGG and Blundell TL (1986) Structural variation in mammalian gamma-crystallins based on computer graphics analyses of human, rat and calf sequences *Exp. Eye Res.* 43, 77-92
365. Wistow G, Summers L and Blundell (1986) Evidence for a structural relationship between protein S, A development specific protein of *Myxococcus xanthus*, and the $\beta\gamma$ -crystallins of the vertebrate lens. *Eurage G Duncan*, ed. 189-201
366. Bajaj M, Horuk R, Pitts JE, Wood SP, Gowan LK, Schwabe C, Wollmer A, Gliemann J, Gammeltoft S and Blundell TL (1986) Coypu insulin: Primary structure, conformation and biological properties of a hystricomorph rodent insulin. *Biochem. J.* 238, 345-351.
367. Sibanda BL, Hemmings A, Foundling SF, Tickle IJ, Pearl LH, Wood SP and Blundell TL (1986) A rational approach to the design of renin inhibitors *Molecular Graphics and Drug Design* Eds. A S V, G C K Roberts and M L Tute 324-333.
368. Summers LJ, Gause GG, Tomarev SI and Blundell TL (1986) A computer graphics model of from gamma-crystallin based on the three-dimensional structure of calf gamma-II crystallin. *FEBS Letters* 208, 11- 16.
369. Singh J, Thornton J, Burley SK, Petsko GA and Blundell TL (1986) Knowledge-based design of novel peptides. *Peptides* (1986) Ed. D. Theodoropoulos *Aromatic Interactions. Science* Vol. 234, 1005
370. Griffin JF, Langs DA, Smith GD, Van Roey PM, Tickle IJ, Bedarkar S and Blundell TL (1986) The crystal structures of (Met5) enkephalin and a third form of (Leu5) enkephalin *Proc. Nat. Acad. Sci.* 83, 3272-3276.
371. Barlow D, Sibanda BL, Thornton JM, Taylor WR, Tickle IJ, Sternberg MJE, Pitts JE, Haneef I Hem-mings AM and Blundell TL (1986) Three-dimensional structural aspects of the design of new protein molecules. (1986) *Phil. Trans. Roy. Soc.*, A317, 333-334.
372. Wood SP, Tickle IJ, Treharne AC, Pitts JE, Mascarenhas Y, Li J-Y, Husain J,

- Cooper J, Hrubby VJ, Wyssbrod HR, Buku A, Fischmann AJ and Blundell TL (1986) Crystal structure analysis of deamino-oxytocin: conformational flexibility and receptor binding. *Science* 232, 633-636
373. Sternberg JE and Blundell TL (1985) Computer-aided design in protein engineering. *Trends in Biotechnology* 3, 228-235.
374. Hemmings AM, Foundling SI, Sibanda BL, Wood SP, Pearl LH and Blundell TL (1985) Energy calculations on aspartic proteinases: human renin, enthothiaepsin and its complex with an angiotensinogen fragment analogue, H-142. *Biochem. Soc. Trans.* (1985) 13 1036-1040
375. Dafgard E, Bajaj M, Honegger A, Pitts JE, Wood SP and Blundell TL (1985) The conformation of insulin-like growth factors: relationships with insulins. *J. Cell Sci.* 3, 53-64.
376. Glover ID, Moss DS, Tickle IJ, Pitts JE, Haneef I, Wood SP, and Blundell TL (1985) Anisotropic thermal motion and polypeptide secondary structure studied by X-ray analysis at 0.98Å resolution. *Adv. Biophys.* 20, 1-12.
377. Sibanda BL, Hemmings AM and Blundell TL (1985) Computer graphics modelling and the subsite specificities of human and mouse renins. in *Aspartic proteinases and their inhibitors*. Ed: V Kostka. Walter de Gruyter & Co., Berlin/New York, 339-349.
378. SI, Wood SP, Pearl LH, Watson FE, Hallett A, Jones DM, Atrash B, Szelke M, Leckie BJ, Beattie S, Dunn BM, Valler MJ, Rolph CE, Kay J Blundell TL (1985) Inhibition of aspartic proteinases by transition state substrate analogues in Aspartic proteinases and their inhibitors. (1985) Walter de Gruyter & Co., Berlin/New York, 467-478
379. Summers LJ Wistow GJ and Blundell TL (1985) Myxococcus xanthus spore coat protein S may have a similar structure to vertebrate lens Bgamma-crystallins. *Nature* 316, 771-773.
380. Summers LJ, Slingsby C, White H, Narebor M, Moss DS, Miller LR, Mahadevan D, Lindley PF, Driessen HP, Dunnen den JT, Moormann RJ, Van Leen RW, Shoenmakers JGC and Blundell TL (1984) The molecular structures and interactions of bovine and human gamma-crystallins in Human Cataract Formation. (1984) Pitman Press, Bath, UK, 219-236.
381. Aulabaugh A, Niemczura WP, Gibbons WA and Blundell TL (1984) A study of the interactions between residues in the C-terminal half of calmodulin by one- and two-dimensional NMR methods and computer modelling *Eur. J. Biochem.* 143, 409-418.
382. Bajaj M, Wood SP and Blundell TL (1984) Evolution in the insulin family: molecular clocks that tell the wrong time *Proc. Biochem. Soc.* 49, 45-54.
383. Tickle IJ, Sibanda BL, Pearl LH, Hemmings AM and Blundell TL (1984) Protein crystallography, interactive computer graphics and drug design *X-ray Crystallography and Drug Design*. Clarendon Press, Oxford, UK, 427-44.
384. Summers LJ, Moss D, Lindley PF, Slingsby C, Wistow GJ, Narebor M, Bartunik H, Bartels K and Blundell TL (1984) X-ray studies of the lens specific proteins: the crystallins. in *Peptide and Protein Reviews* Marcel Dekker Inc., New York, USA, 147-168.
385. Slingsby C, Inana G, Piatigorsky J, Norman B and Blundell TL (1984) Gene and protein structure of a B-crystallin polypeptide in murine lens: relationship of exons and structural motifs. *Nature* 302, 310-315.
386. Pearl LH and Blundell TL (1984) The active site of aspartic proteinases. *FEBS Letters* 174, 96-101
387. Honegger A and Blundell TL (1984) A computer graphics study of insulin-like growth factors and their receptor interactions in Insulin-like growth factors/somatomedins: basic chemistry, biology and clinical importance. Walter de Gruyter & Co., New York, 93-113
388. Glover ID, et al, and Blundell TL (1984) Conformational studies on the pancreatic polypeptide hormone family. *Eur. J. Biochem.* 142, 379-385.
389. Sternberg MJE, Travers P, Bodmer WF and Blundell TL (1984) Structural and evolutionary analysis of HLA-D-region products. *Nature* 301, 235-238.

390. Bajaj M and Blundell TL (1984) Evolution and the tertiary structure of proteins. *Ann. Rev. Biophys. Bioeng.* 13, 453-492.
391. Barlow D, Borkakoti N, Thornton J and Blundell TL (1983) Solvent-induced distortions and the curvature of alpha-helices. *Nature* 306, 281-283.
392. Wistow G, Turnell B, Summers L, Slingsby C, Moss D, Miller L, Lindley P and Blundell TL (1983) X-ray analysis of the eye lens protein gamma-II crystallin at 1.9A. *J. Mol. Biol.* 170 175-202.
393. Sibanda BL, Pearl L and Blundell TL (1983) Three-dimensional structure, specificity and catalytic mechanism of renin. *Nature* 304, 273-275.
394. Bedar-kar S, Humbel RE and Blundell TL (1983) Tertiary structures, receptor binding and antigenicity of insulin-like growth factors. *Fed. Proc.* 42, 2592-2597.
395. Busetta B, Tickle IJ and Blundell TL (1983) DOCKER, an interactive program for simulating protein receptor and substrate interactions. *J. Appl. Cryst.* 16, 432-437.
396. Blundell TL (1983) The conformation of glucagon, in *Handbook of Experimental Pharmacology*, Vol. 66 (1983) Springer-Verlag, Berlin 37-56
397. Strassburger W, Wollmer A, Pitts JE, Glover ID, Tickle IJ, Steffens GJ, Gunzler WA, Otting F, Flohe L and Blundell TL (1983) Adaptation of plasminogen activator sequences to known protease structures. *FEBS Letters* 157, 219-223.
398. Bajaj M, Pitts JE, Wood SP, Tatnell MA, Falkmer S, Emdin SO, Gowan LK, Crow H, Schwabe C, Wollmer A, Strassburger W and Blundell TL (1983) Dogfish insulin: primary structure, conformation and biological properties of an elasmobranchial insulin. *Eur. J. Biochem.* (1983) 135, 535-542
399. Glover I, Haneef I, Pitts JE, Wood SP, Moss D, Tickle I and Blundell TL (1983) Conformational flexibility in small globular hormone: X-ray analysis of avian pancreatic polypeptide at 0.98A resolution. *Biopolymers* 22, 293-304.
400. Bedarkar S, Gowan LK, C Schwabe and Blundell TL (1982) Relaxin - a member of the insulin family? in *Biology of Relaxin and its Role in the Human*. Excerpta Medica, Amsterdam, 14-21.
401. Gowan LK, McDonald JK, Schwabe C and Blundell TL (1982) On the three-dimensional structure of relaxin. *Ann. NY Acad. Sci.* 22-23.
402. Blundell TL (1982) Recent developments in the crystallography of globular proteins. *NATO Advance Study Institutes Series A45*, 45-61
403. Gunning J, Bedarkar S, Taylor GL, Blundell TL, Wlodawer A, Hodgson KO, Shooter EM, Fourme R, Gaberand B, Williams R (1982) Conformational studies of polypeptide growth factors: IGF and NGF. *Cell Function and Differentiation*, Alan R Liss, Inc., NY, pp 221-230.
404. Pitts JE, Wood SP and Blundell TL (1981) The conformation and molecular biology of pancreatic hormones and homologous growth factors. *Crit. Revs. Biochem.* 13, 141-213.
405. Glover ID and Blundell TL (1982) Three-dimensional structure-function relationships in pancreatic hormones *Topics in Molecular Pharmacology*, Elsevier Science Publishers BV, Amsterdam, The Netherlands, pp123-149.
406. Pitts JE, Tickle IJ, Wood SP and Blundell TL (1981) Crystal structure analysis of the avian pancreatic polypeptide at 1.37A resolution. *Kristallografiya* 27, 97-106.
407. Wood SP and Blundell TL (1981) The conformation, flexibility and dynamics of polypeptide hormones. *Ann. Rev. Biochem.* 51, 123-154.
408. Strassburger W, Glatter U, Wollmer W, Feischauer J, Mercola DA, Glover ID, Pitts JE, Tickle IJ, Wood SP and Blundell TL (1981) Calculated tyrosyl circular dichroism of proteins: absence of tryptophan and cystine interferences in avian pancreatic polypeptide. *FEBS Lett.* 139, 295-299.
409. Wistow G, Slingsby C, Driessen H, de Jong W, Bloemendal H and Blundell TL (1981) Eye-lens proteins: the three-dimensional structure of B-crystallin predicted from monomeric gamma-crystallin. *FEBS Letters* 133, 9-16.

410. Gunning J and Blundell TL (1981) Crystal structure analysis of the larger peptide hormones. *The Peptides* 4, 55-84.
411. Pitts JE, Tickle IJ, Wood SP, Wu C-W and Blundell TL (1981) X-ray analysis (1.4Å resolution) of avian pancreatic polypeptide: small globular protein hormone. *Proc. Nat. Acad. Sci. USA* 78, 4175-4179.
412. Pitts JE, Tickle IJ, Wood SP and Blundell TL (1981) The conformation and receptor binding of pancreatic hormones. *Trans Biochem. Soc.* 9, 31-32.
413. Blundell TL, Lindley P, Miller L, Moss DS, Slingsby C, Tickle IJ, Turnell WG and Wistow G (1981) The molecular structure and stability of the eye lens: X-ray analysis of gamma-crystallin II *Nature* 289, 771-777.
414. Horuk R and Blundell TL (1981) A monomeric insulin from the casiragua: molecular and model building using computer graphics. *Hoppe-Seyler's S Physiol. Chem.* 362, 727-733.
415. Blundell TL (1981) Protein-protein recognition and assembly, in structural aspects of recognition and assembly in biological macromolecules, *Balaban ISS*, 281-286
416. Bedarkar S, Gowan L, Reinig JW, Schwabe C and Blundell TL (1981) On the primary and tertiary structure of relaxin from the sand tiger shark. *FEBS Letters* 129, 80-82.
417. Pitts JE, Wood SP, Horuk R, Bedarkar S and Blundell TL (1980) Pancreatic hormone storage granules: the role of metal ions and polypeptide oligomers), in *insulin: chemistry, structure and function of insulin and related hormones*, Walter de Gruyter and Co., pp 673-682.
418. Pitts JE, Wood SP, Hearn L, Tickle IJ, Wu C, F Robinson ICA and Blundell TL (1980) Crystallisation and preliminary crystallographic data of a porcine neurophysin 1-Tyr-Phe-NH₂ complex *FEBS Letters* 121, 41-43.
419. Narebor ME, Slingsby C, Lindley PF and Blundell TL (1980) Preliminary X-ray crystallographic study of the turkey lens protein gamma-crystallin, *J. Mol. Biol.* 143, 223-225.
420. Horuk R, Wood SP, Lazarus NR, Neville RWJ and Blundell TL (1980) The use of hystricomorph insulins in defining the insulin-receptor interactions, *Actualites de Chimie Therapeutique* 7, 15-25.
421. Horuk R, Lazarus NR, Neville RWJ, Stone D, Wollmer A and Blundell TL (1980) A monomeric insulin from the porcupine (*Hystrix cristata*), an Old World hystricomorph. *Nature* 286, 822-824.
422. Sewell BT, Tickle IJ, Slingsby S, Moss DS, Lindley PF, Turnell WG, Wistow GJ, Jenkins JA and Blundell TL (1980) Structural evidence for gene duplication and fusion in the evolution of proteins, in *Biomolecular structure, conformation, function and evolution Vol.1: Diffraction and related studies*, Pergamon Press, pp251-256.
423. Jones HB, Khan MG, Taylor GA, Sewell BT, Pearl LH, Wood SP and Blundell TL (1980) The active site of acid proteinase. In *Enzyme regulation and mechanism of action*, Pergamon Press, 281-288.
424. Blundell TL (1980) Insulin and glucagon receptors (with L Kuehn) in *cellular receptors, hormones and neurotransmitters*. John Willey & Sons Ltd 281-288.
425. Blundell TL and Humbel RE (1980) Hormone families: pancreatic hormones and homologous growth factors. *Nature* 287, 781-787.
426. Blundell TL (1980) Chemistry, structure and function of insulin and related hormones, *FEBS Letters* 109, 167-170
427. Pitts JE, Tickle IJ, Wood SP and Blundell TL (1979) X-ray analysis and the conformation of pancreatic polypeptide. In *Peptides: structure and biological function* Pierce Chemical Co. Rockford, USA, pp. 1011-1016
428. Sewell BT, Blundell TL and McLachlan AD (1979) Four-fold structural repeat in the acid proteases. *Biochem. Biophys. Acta* 580, 24-31
429. Khan G, Sewell T, Tickle IJ, Wood EA, Jenkins JA, Roy-Chowdhury P and Blundell

- TL (1979) The three-dimensional structures of acid proteinases *FEBS Lett.* 52, 81-94
430. Hearn L, Tickle IJ, Palmer RA, Morgan BJ, Smith GD, Griffin E and Blundell TL (1979) Crystal structure of (Leu⁵) enkephalin *Science* 205, 220-225
431. Blundell TL (1979) Conformation and molecular biology of polypeptide hormones: glucagon, *Trends in Biochem. Sci.* 80-83
432. Blundell TL (1979) Conformation and molecular biology of polypeptide hormones: insulin, insulin-like growth factor and relaxin, *Trends Biochem. Sci.* 51-54
433. Bedarkar S, Tickle IJ, Wood SP, Dockerill S and Blundell TL (1978) Polypeptide hormone-receptor interactions: the structure and receptor binding of insulin and glucagon, in *Molecular interactions and activity in proteins*, *Excerpta Medica*, 105-121
434. Bedarkar S, Tickle IJ, Turnell WG, Wood SP and Blundell TL (1978) The evolution and devolution of insulin-like activity and zinc binding in the structurally homologous polypeptides. *Biomolecular Structure* (1978) Pergamon Press
435. Lindley PF, Moss DS, Slingsby C, Tickle IJ, Turnell WG and Blundell TL (1978) The low resolution structure analysis of the lens protein gamma-crystallin. *Acta Cryst.* B34, 3653-3657.
436. Tang J, James MNG, Hsu IN, Jenkins JA and Blundell TL (1978) Structural evidence for gene duplication in the evolution of acid proteinases *Nature* 271, 618-621.
437. Bedarkar S, Blundell TL, Rindernecht E and Humbel RE (1978) Insulin-like growth factor: a model for the tertiary structure accounting for its immuno-reactivity and receptor binding *Proc. Nat. Acad. Sci. USA* 75, 108-184.
438. Wood SP, Tickle IJ, Wollmer A, Steiner DF and Blundell TL (1978) Insulin polymorphism: some physical and biological properties of rat insulins *Arch. Biochem. Biophys.* 186, 175-183.
439. Dockerill S, Pitts JE, Wood SP, Tickle IJ and Blundell TL (1977), Glucagon and pancreatic hormone III: X-ray analysis, conformation and receptor binding. *Proc. 11th FEBS meeting, Copenhagen* 45, 149- 258.
440. Jenkins JA, Tickle IJ, Sewell T, Ungaretti L, Wollmer A and Blundell TL (1977) X-ray analysis and circular dichroism of the acid protease from *Endothia parasitica* and chymosin. In *Acid Proteases*, ed. J. Tang, Plenum Publishing NY, pp43-60.
441. Bedarkar S, Dockerill D, Pitts JE, Tickle IJ, Wood SP and Blundell TL (1977) The conformation and molecular biology of pancreatic and homologous hormones, *Mol. Endocrinol.* 15-26.
442. Symmetrical features in polypeptide hormone-receptor interactions (with C R Beddell, G C Shep-ey, K Sasaki, S Dockerill and P J Goodford), *Int. J. Peptide Res.* (1977) 9 15-26
443. Subramanian E, Swan IDA, Liu M, Davies DR, Jenkins JA, Tickle IJ and Blundell TL (1977) Homology among acid proteases: comparison of crystal structure at 3A resolution of acid proteases from *Rhizopus chinensis* and *Endothia parasitica* *Proc. Nat. Acad. Sci. USA* 74, 556-559.
444. Bedarkar S, Turnell WG, Schwabe C and Blundell TL (1977) Relaxin has conformational homology with insulin, *Eur. J Biochem.* 270, 449-451.
445. Wood SP, Pitts JE, Tickle IJ, Jenkins JA and Blundell TL (1977) Purification, crystallisation and preliminary X-ray studies on avian pancreatic polypeptide, *Eur. J Biochem.* 270, 449-451.
446. Friesen H, Bran-denbug D, Diaconescu C, Gattner H, Naithani N, Nowak J, Zahn H, Dockerill S, Wood SP and Blundell TL (1977) Structure-function relationships of insulins modified in the A1 region in *Peptides*, eds. M. Goodman and J Meienhofer John Wiley & Sons, 136-140.
447. Blundell TL and Johnson LN (1976) *Protein Crystallography* Academic Press, pp 565
448. Blundell TL and Wood SP (1976) *Membrane receptors for peptide hormones*, New

Scientist 72, 670-671.

449. Sasaki K, Dockerill S, Adamiak DA, Tickle IJ, Wood SP and Blundell TL (1976) The relation of structure to storage and receptor binding of glucagon *Metabolism* 25, 1331-1336.
450. Pullen RA, Lindsay DG, Tickle IJ, Wood SP, Brandenburg D, Zahn H, Gliemann J, Gammeltoft S and Blundell TL (1976) On the receptor binding region of insulin *Nature* 259, 369-373.
451. Adamiak DA, Tickle IJ, Blundell TL and Kosturkiewicz K (1975) The structure of the rubidium salt of N-(Purin-6-ylcarbonyl)-L-threonine tetrahydrate, a hypermodified base in the anticodon loop of some tRNAs *Acta Cryst. B* 31, 1242-1246.
452. Blundell TL and Wood SP (1975) Is the evolution of insulin Darwinian or due to selectively neutral mutation? *Nature* 257, 197-203.
453. Jenkins JA, Tickle IJ, Ungaretti L and Blundell TL (1975) X-ray analysis and circular dichroism of the acid proteinase from *Endothia parasitica* *J. Mol. Biol.* 99 583-590.
454. Brunori M, Curti B, Bolognesi M, Coda A, Fumagalli M, Ungaretti L and Blundell TL (1975) Studies on metmyoglobin from *Aplysia Limacina*, *J. Mol. Biol.* 97, 665-666.
455. Blundell TL (1975) Glucagon, *New Scientist* 662-664
456. Sasaki K, Dockerill S, Adamiak DA, Tickle IJ and Blundell TL (1975) X-ray analysis of glucagon and its relationship to receptor binding *Nature* 257, 751-757.
457. Wood SP, Wollmer A, Neville R, Lazarus N and Blundell TL (1975) Studies on guinea pig and chinchilla insulins *Eur. J. Biochem.* 55, 531-542
458. Pullen RA, Jenkins JA, Tickle IJ, Wood SP and Blundell TL (1975) The structure and flexibility of polypeptide hormones: X-ray studies of insulin, glucagon and human placental lactogen *Cell. Mol. Biochem.* 8, 5-20.
459. Blundell TL, Dodson GG, Mercola D (1972) Insulin, in *Peptides* (1974)
460. Blundell TL, Dodson GG, Mercola D and Hodgkin DC (1972) Structure of insulin and its relationship to activity, *Diabetes* (1972) 21, 192-301
461. Blundell TL, Dodson GG, Mercola D, and Hodgkin DC (1972) The structure, chemistry and biological activity of insulin, *Adv. Prot. Chem.* 26, 279-402.
462. Blundell TL, Cutfield JF, Dodson GG, Dodson E, Mercola D and Hodgkin DC (1972) The structure and function of zinc insulin, *Acta Vitaminologica et Enzymologica* 5-6
463. Blundell TL, and Powell HM (1972) The coordination of the dimethylthallium ion in the crystal and molecular structure of 1,10-phenanthroline-dimethylthallium(II) perchlorate (with H M Powell) *Proc. Roy. Soc. Lon.* A331, 161- 169
464. Blundell TL, Cutfield JF, Dodson GG, Dodson E, Mercola D, and Hodgkin DC (1972) The arrangement in three dimensions of the atoms in insulin molecules and crystals, in "Insulin Action" Academic Press, NY and London, 1-28
465. Blundell TL, Cutfield JF, Dodson GG, Dodson E, Mercola D and Hodgkin DC (1971) Conformation of insulin, in *Structure and activity relationship of protein and polypeptide hormones* *Excerpta Medica* 161, 231-238
466. Blundell TL and Powell HM (1971) The crystal and molecular structure of [Co(QP)C1]BPh QP=tris(o-diphenylphosphinophenyl)phosphine) *J. Appl. Cryst.* B27, 2304-2310.
467. Blundell TL, Cutfield JF, Cutfield SM, Dodson GG, Dodson EJ, Hodgkin DC, Mercola D, Vijayan M (1971) Atomic positions in 2-Zinc insulin crystals *Nature* 231, 506-511.
468. Blundell TL, Cutfield JF, Dodson GG, Dodson E, Mercola D and Hodgkin DC (1971) The crystal structure of rhombohedral 2-Zinc insulin, *Cold Spring Harbour Symposium* 36, 233-241.
469. Blundell TL, Cutfield JF, Dodson GG, Dodson E, Mercola D and Hodgkin DC (1971) The structure and biology of insulin *Biochem. J.* 125, 50-51.
470. Blundell TL, Dodson GG, Dodson E, Vijayan M and Hodgkin DC (1971) X-ray analysis and the structure of insulin. The Gregory Pincus Memorial Lecture, Recent

- Progress in Hormone Research 27, 1-40.
471. Blundell TL, Dodson GG, Dodson E, Vijayan M and Hodgkin DC (1971) The structure of a protein hormone insulin *Contemp. Phys.* 12, 209-228.
 472. Adams MJ, Blundell TL, Dodson GG, Dodson E, Vijayan M, Baker EN, Harding MM, Hodgkin DC, Rimmer B, Sheats S. (1969) Structure of rhombohedral 2-Zinc insulin crystals *Nature* 224, 491-495.
 473. Blundell TL, Dodson GG, Dodson E, Vijayan M and Hodgkin, DC (1969) Low resolution structure of insulin. *Acta Cryst.* A25, 5184-5191
 474. Blundell, TL and Powell, HM (1967) The crystal and molecular structure of [Pd(TPAS)Cl]ClO₄C₆H₆[TPAS o-phenylenebis-(o-dimethylarsinophenyl methylarsine)]: the stereochemistry of a pentacoordinate palladium complex ion *J. Chem. Soc.* 1650-1657.
 475. Blundell TL, Powell HM and Venanzi LM (1967) A distorted trigonal bipyramidal co-ordination of cobalt in tris-(o-diphenylphosphinophenyl) phosphinochlorocobalt(II) tetraphenylborate *Chem. Comm.* 21, 763-69
 476. Blundell TL and Powell HM (1967) An unusual co-ordination of thallium in the crystal structure of dimethyl-1, 10-phenanthroline-thallium perchlorate *Chem. Comm.* 21, 54-
 477. Blundell TL, Kilbourn BT and Powell HM (1965) The molecular structures of Bis-(o-dimethylarsinophenyl) methylarsinecopper-manganese penta-carbonyl triphenylgermanium-manganese pentacarbonyl, and triphenylphosphinegold-cobalt tetra-carbonyl. *Chem. Comm.* 19, 444-445

Selected publications on general topics

1. Blundell TL (1982) Trust and gullibility in science, *Trends Biochem. Sci.* 352-353.
2. Blundell TL (1990) Designer drugs head the market place. *New Scientist* 1720, 61-64
3. Blundell TL (1991) Agricultural Research: Sixty Years of Achievement. *Science in Parliament* 48.
4. Blundell TL (1992) Agricultural Research in the Real World. *Science in Parliament* 49:23-24
5. Blundell TL. (1995) Structural Molecular Biology and Drug Discovery. Leon Goldberg Memorial Lecture. *Fd Chem.Toxic* 33:979-992 Publisher Elsevier
6. Blundell, TL. (1996) Women in the Biosciences. *The Biochemist.* August/September.
7. Blundell, T.L. (1998). The funding for small and large biological science in Europe. *The Royal Society*, 15-21.
8. Blundell TL (1998) Academia Industry Research Networks for the Future. Forty third Fawley Lecture, University of Southampton Press. pp1-19
9. Blundell TL (1999) Future Challenges for Environmental Policies. *Science in Parliament.* 56, 4-5.
10. Blundell TL (1999) Preface for *The Development of Modern Agriculture: British Farming since 1931.* Macmillan (London), pp1-5
11. Blundell TL (1999) Future challenges for environmental policies. *Journal of the Institution of Environmental Sciences.* 8, 7-8.