

Publications by Astbury Centre Members 2006

- Anstiss, M. & Nelson, A. (2006). Catalytic and stoichiometric approaches to the desymmetrisation of centrosymmetric piperazines by enantioselective acylation: a total synthesis of Dragmacidin A. *Org. Biomol. Chem.* 4, 4135-4143.
- Arscott, S., Gaudet, M., Brinkmann, M., Ashcroft, A. E. & Blossey, R. (2006). Capillary filling of miniaturized sources for electrospray mass spectrometry. *J. Phys.-Condes. Matter* 18, S677-S690.
- Barnes, K., Dobrzynski, H., Foppolo, S., Beal, P. R., Ismat, F., Scullion, E. R., Sun, L. J., Tellez, J., Ritzel, M. W. L., Claycomb, W. C., Cass, C. E., Young, J. D., Billeter-Clark, R., Boyett, M. R. & Baldwin, S. A. (2006). Distribution and functional characterization of equilibrative nucleoside transporter-4, a novel cardiac adenosine transporter activated at acidic pH. *Circulation Research* 99, 510-519.
- Barratt, E., Bronowska, A., Vondrasek, J., Cerny, J., Bingham, R., Phillips, S. & Homans, S. W. (2006). Thermodynamic penalty arising from burial of a ligand polar group within a hydrophobic pocket of a protein receptor. *J. Mol. Biol.* 362, 994-1003.
- Bentham, M., Mazaleyrat, S. & Harris, M. (2006). A cluster of arginine residues near the N-terminus of the HIV-1 Nef protein is required both for membrane association and CD4 down-modulation. *J. Gen. Virol.* 87, 563-571.
- Bentham, M., Mazaleyrat, S. & Harris, M. (2006). Role of myristoylation and N-terminal basic residues in membrane association of the human immunodeficiency virus type 1 Nef protein. *J. Gen. Virol.* 87, 563-571.
- Besong, G., Jarowicki, K., Kocienski, P. J., Sliwinski, E. & Boyle, F. T. (2006). Synthesis of (S)-(-)-N-acetylcolchinol using intramolecular biaryl oxidative coupling. *Org. Biomol. Chem.* 4, 2193-2207.
- Bingham, R. J., Dive, V., Phillips, S. E. V., Shirras, A. D. & Isaac, R. E. (2006). Structural diversity of angiotensin-converting enzyme - Insights from structure-activity comparisons of two Drosophila enzymes. *Febs J.* 273, 362-373.
- Boda, K. & Johnson, A. P. (2006). Molecular complexity analysis of *de novo* designed ligands. *Journal of Medicinal Chemistry* 49, 5869-5879.
- Boyne, J. R. & Whitehouse, A. (2006). gamma-2 Herpes virus post-transcriptional gene regulation. *Clin. Microbiol. Infect.* 12, 110-117.
- Boyne, J. R. & Whitehouse, A. (2006). Nucleolar trafficking is essential for nuclear export of intronless herpesvirus mRNA. *Proc. Natl. Acad. Sci. U. S. A.* 103, 15190-15195.
- Bracey, K. & Wray, D. (2006). Tubulin as a possible binding partner of the heag2 potassium channel. *Acta Pharmacologica Sinica* 27, 186-186.
- Bradford, J. R., Needham, C. J., Bulpitt, A. J. & Westhead, D. R. (2006). Insights into protein-protein interfaces using a Bayesian network prediction method. *J. Mol. Biol.* 362, 365-386.

- Bunka, D. H. J. & Stockley, P. G. (2006). Aptamers come of age - at last. *Nature Reviews Microbiology* 4, 588-596.
- Burgoyne, N. J. & Jackson, R. M. (2006). Predicting protein interaction sites: binding hot-spots in protein-protein and protein-ligand interfaces. *Bioinformatics* 22, 1335-1342.
- Carr, S. B., Makris, G., Phillips, S. E. V. & Thomas, C. D. (2006). Crystallization and preliminary X-ray diffraction analysis of two N-terminal fragments of the DNA-cleavage domain of topoisomerase IV from *Staphylococcus aureus*. *Acta Crystallographica Section F-Structural Biology and Crystallization Communications* 62, 1164-1167.
- Caryl, J. A. & Thomas, C. D. (2006). Investigating the basis of substrate recognition in the pC221 relaxosome. *Molecular Microbiology* 60, 1302-1318.
- Clare, D. K., Orlova, E. V., Finbow, M. A., Harrison, M. A., Findlay, J. B. C. & Saibil, H. R. (2006). An expanded and flexible form of the vacuolar ATPase membrane sector. *Structure* 14, 1149-1156.
- Clarke, D., Griffin, S., Beales, L., Gelais, C. S., Burgess, S., Harris, M. & Rowlands, D. (2006). Evidence for the formation of a heptameric ion channel complex by the hepatitis C virus p7 protein *in vitro*. *J. Biol. Chem.* 281, 37057-37068.
- Cobos, E. S. & Radford, S. E. (2006). Sulfate-induced effects in the on-pathway intermediate of the bacterial immunity protein Im7. *Biochemistry* 45, 2274-2282.
- Connell, S. D. & Smith, D. A. (2006). The atomic force microscope as a tool for studying phase separation in lipid membranes. *Mol. Membr. Biol.* 23, 17-28.
- Cooksey, J. P., Kocienski, P. J., Li, Y. F., Schunk, S. & Snaddon, T. N. (2006). Synthesis of the C1-C16 fragment of ionomycin using a neutral (eta(3)-allyl)iron complex. *Org. Biomol. Chem.* 4, 3325-3336.
- Cordy, J. M., Hooper, N. M. & Turner, A. J. (2006). The involvement of lipid rafts in Alzheimer's disease. *Mol. Membr. Biol.* 23, 111-122.
- Crampton, N., Bonass, W. A., Kirkham, J., Rivetti, C. & Thomson, N. H. (2006). Collision events between RNA polymerases in convergent transcription studied by atomic force microscopy. *Nucleic Acids Res.* 34, 5416-5425.
- Crampton, N., Bonass, W. A., Kirkham, J. & Thomson, N. H. (2006). Studying silane mobility on hydrated mica using ambient AFM. *Ultramicroscopy* 106, 765-770.
- Crampton, N., Thomson, N. H., Kirkham, J., Gibson, C. W. & Bonass, W. A. (2006). Imaging RNA polymerase-amelogenin gene complexes with single molecule resolution using atomic force microscopy. *European Journal of Oral Sciences* 114, 133-138.
- Crawford, C., Nelson, A. & Patel, I. (2006). Development of an approach to the synthesis of the ABC ring system of Hemibrevetoxin B. *Organic Letters* 8, 4231-4234.

- Das, C., Inkson, N. J., Read, D. J., Kelmanson, M. A. & McLeish, T. C. B. (2006). Computational linear rheology of general branch-on-branch polymers. *Journal of Rheology* 50, 207-235.
- Das, C., Read, D. J., Kelmanson, M. A. & McLeish, T. C. B. (2006). Dynamic scaling in entangled mean-field gelation polymers. *Phys. Rev. E* 74.
- Davies, R. P. W., Aggeli, A., Beevers, A. J., Boden, N., Carrick, L. M., Fishwick, C. W. G., McLeish, T. C. B., Nyrkova, I. & Semenov, A. N. (2006). Self-assembling beta-sheet tape forming peptides. *Supramolecular Chemistry* 18, 435-443.
- Dobrzynski, H., Tellez, J. O., Barnes, K., Chandler, N. J., Qureshi, M. A., Imrit, N., Greener, I. D., Baldwin, S. A., Billeter, R., Boyett, M. R. & Howarth, F. C. (2006). Effects of streptozotocin-induced diabetes on connexin43 mRNA and protein expression in ventricular muscle. *Journal of Molecular and Cellular Cardiology* 40, 1008-1008.
- Dove, B., Brooks, G., Bicknell, K., Wurm, T. & Hiscox, J. A. (2006). Cell cycle perturbations induced by infection with the coronavirus infectious bronchitis virus and their effect on virus replication. *J. Virol.* 80, 4147-4156.
- Dove, B. K., Bicknell, K., Brooks, G., Harrison, S. & Hiscox, J. A. (2006). Infectious bronchitis coronavirus induces cell-cycle perturbations. In *Nidoviruses: Toward Control of Sars and Other Nidovirus Diseases*, Vol. 581, pp. 357-362.
- Dove, B. K., You, J. H., Reed, M. L., Emmett, S. R., Brooks, G. & Hiscox, J. A. (2006). Changes in nucleolar morphology and proteins during infection with the coronavirus infectious bronchitis virus. *Cellular Microbiology* 8, 1147-1157.
- Dubuis, E., Rockliffe, N., Hussain, M., Boyett, M., Wray, D. & Gawler, D. (2006). Evidence for multiple Src binding sites on the alpha 1c L-type Ca^{2+} channel and their roles in activity regulation. *Cardiovascular Research* 69, 391-401.
- Edwards, T. A., Butterwick, J. A., Zeng, L., Gupta, Y. K., Wang, X., Wharton, R. P., Palmer, A. G. & Aggarwal, A. K. (2006). Solution structure of the Vts1 SAM domain in the presence of RNA. *J. Mol. Biol.* 356, 1065-1072.
- Ellingham, M., Bunka, D. H. J., Rowlands, D. J. & Stonehouse, N. J. (2006). Selection and characterization of RNA aptamers to the RNA-dependent RNA polymerase from foot-and-mouth disease virus. *RNA* 12, 1970-1979.
- Ewan, L. C., Jopling, H. M., Jia, H. Y., Mittar, S., Bagherzadeh, A., Howell, G. J., Walker, J. H., Zachary, I. C. & Ponnambalam, S. (2006). Intrinsic tyrosine kinase activity is required for vascular endothelial growth factor receptor 2 ubiquitination, sorting and degradation in endothelial cells. *Traffic* 7, 1270-1282.
- Geierhaas, C. D., Best, R. B., Paci, E., Vendruscolo, M. & Clarke, J. (2006). Structural comparison of the two alternative transition states for folding of TI I27. *Biophys. J.* 91, 263-275.
- Gillings, A. S., Yang, J., Marley, A. E., Holman, G. D., Peckham, M., Kilgour, E. & Baldwin, S. A. (2006). Investigation of the role of Kv1.3 as a potential regulator of peripheral insulin sensitivity. *Diabetologia* 49, 366-366.

- Gold, N. D. & Jackson, R. M. (2006). Fold independent structural comparisons of protein-ligand binding sites for exploring functional relationships. *J. Mol. Biol.* 355, 1112-1124.
- Gold, N. D. & Jackson, R. M. (2006). A searchable database for comparing protein-ligand binding sites for the analysis of structure-function relationships. *Journal of Chemical Information and Modeling* 46, 736-742.
- Gold, N. D. & Jackson, R. M. (2006). SitesBase: a database for structure-based protein-ligand binding site comparisons. *Nucleic Acids Res.* 34, D231-D234.
- Gosal, W. S., Myers, S. L., Radford, S. E. & Thomson, N. H. (2006). Amyloid under the atomic force microscope. *Protein Pept. Lett.* 13, 261-270.
- Graham, R. S., Bent, J., Hutchings, L. R., Richards, R. W., Groves, D. J., Embrey, J., Nicholson, T. M., McLeish, T. C. B., Likhtman, A. E., Harlen, O. G., Read, D. J., Gough, T., Spares, R., Coates, P. D. & Grillo, I. (2006). Measuring and predicting the dynamics of linear monodisperse entangled polymers in rapid flow through an abrupt contraction. A small angle neutron scattering study. *Macromolecules* 39, 2700-2709.
- Griffiths, R. A., Boyne, J. A. & Whitehouse, A. (2006). Herpesvirus saimiri-based gene delivery vectors. *Current Gene Therapy* 6, 1-15.
- Gsponer, J., Hopearuoho, H., Whittaker, S. B. M., Spence, G. R., Moore, G. R., Paci, E., Radford, S. E. & Vendruscolo, M. (2006). Determination of an ensemble of structures representing the intermediate state of the bacterial immunity protein Im7. *Proc. Natl. Acad. Sci. U. S. A.* 103, 99-104.
- Hawkins, R. J. & McLeish, T. C. B. (2006). Coupling of global and local vibrational modes in dynamic allosteric proteins. *Biophys. J.* 91, 2055-2062.
- Hawkins, R. J. & McLeish, T. C. B. (2006). Dynamic allosteric of protein alpha helical coiled-coils. *Journal of the Royal Society Interface* 3, 125-138.
- Heeley, E. L., Fernyhough, C. M., Graham, R. S., Olmsted, P. D., Inkson, N. J., Embrey, J., Groves, D. J., McLeish, T. C. B., Morgovan, A. C., Meneau, F., Bras, W. & Ryan, A. J. (2006). Shear-induced crystallization in blends of model linear and long-chain branched hydrogenated polybutadienes. *Macromolecules* 39, 5058-5071.
- Heikkila, T., Thirumalairajan, S., Davies, M., Parsons, M. R., McConkey, A. G., Fishwick, C. W. G. & Johnson, A. P. (2006). The first *de novo* designed inhibitors of *Plasmodium falciparum* dihydroorotate dehydrogenase. *Bioorg. Med. Chem. Lett.* 16, 88-92.
- Holyoake, J., Caulfeild, V., Baldwin, S. A. & Sansom, M. S. P. (2006). Modeling, docking, and simulation of the major facilitator superfamily. *Biophys. J.* 91, L84-L86.
- Hooper, N. M. (2006). Foreword: lipid rafts/biophysics, cell signalling, trafficking and processing. *Mol. Membr. Biol.* 23, 1-3.
- Horn, W. T., Tars, K., Grahn, E., Heigstrand, C., Baron, A. J., Lago, H., Adams, C. J., Peabody, D. S., Phillips, S. E. V., Stonehouse, N. J., Liljas, L. & Stockley, P. G.

(2006). Structural basis of RNA binding discrimination between bacteriophages Q beta and MS2. *Structure* 14, 487-495.

Hyland, C., Pinney, J. W., McConkey, G. A. & Westhead, D. R. (2006). metaSHARK: a WWW

platform for interactive exploration of metabolic networks. *Nucleic Acids Res.* 34, W725-W728.

Inkson, N. J., Graham, R. S., McLeish, T. C. B., Groves, D. J. & Fernyhough, C. M. (2006). Viscoelasticity of monodisperse comb polymer melts. *Macromolecules* 39, 4217-4227.

Jack, E., Newsome, M., Stockley, P. G., Radford, S. E. & Middleton, D. A. (2006). The organization of aromatic side groups in an amyloid fibril probed by solid-state H-2 and F-19 NMR spectroscopy. *J. Am. Chem. Soc.* 128, 8098-8099.

Jahn, T. R., Parker, M. J., Homans, S. W. & Radford, S. E. (2006). Amyloid formation under physiological conditions proceeds via a native-like folding intermediate. *Nat. Struct. Mol. Biol.* 13, 195-201.

Jen, C. H., Manfield, I. W., Michalopoulos, I., Pinney, J. W., Willats, W. G. T., Gilmartin, P. M. & Westhead, D. R. (2006). The Arabidopsis co-expression tool ((ACT)): a WWW-based tool and database for microarray-based gene expression analysis. *Plant Journal* 46, 336-348.

Jeuken, L. J. C., Connell, S. D., Henderson, P. J. F., Gennis, R. B., Evans, S. D. & Bushby, R. J. (2006). Redox enzymes in tethered membranes. *J. Am. Chem. Soc.* 128, 1711-1716.

Johnson, A. P., Boda, K., Weaver, S., Valko, A. & Valko, V. (2006). *De novo* design tools for the generation of synthetically accessible ligands. *Abstr. Pap. Am. Chem. Soc.* 231.

Johnson, R., Gamblin, R. J., Ooi, L., Bruce, A. W., Donaldson, I. J., Westhead, D. R., Wood, I. C., Jackson, R. M. & Buckley, N. J. (2006). Identification of the REST regulon reveals extensive transposable element-mediated binding site duplication. *Nucleic Acids Res.* 34, 3862-3877.

Ju, M. & Wray, D. (2006). Molecular regions responsible for differences in activation between heag channels. *Biochem. Biophys. Res. Commun.* 342, 1088-1097.

Kawakami, M., Byrne, K., Brockwell, D. J., Radford, S. E. & Smith, D. A. (2006). Viscoelastic study of the mechanical unfolding of a protein by AFM. *Biophys. J.* 91, L16-L18.

Kawakami, M., Byrne, K., Khatri, B. S., McLeish, T. C. B. & Smith, D. A. (2006). Viscoelastic properties of single poly(ethylene glycol) molecules. *Chemphyschem* 7, 1710-1716.

- King, A. E., Ackley, M. A., Cass, C. E., Young, J. D. & Baldwin, S. A. (2006). Nucleoside transporters: from scavengers to novel therapeutic targets. *Trends Pharmacol. Sci.* 27, 416-425.
- Kirkham, J., Andreev, I., Robinson, C., Brookes, S. J., Shore, R. C. & Smith, D. A. (2006). Evidence for direct amelogenin-target cell interactions using dynamic force spectroscopy. *European Journal of Oral Sciences* 114, 219-224.
- Kobrinsky, E., Stevens, L., Kazmi, Y., Wray, D. & Soldatov, N. M. (2006). Molecular rearrangements of the K(v)2.1 potassium channel termini associated with voltage gating. *J. Biol. Chem.* 281, 19233-19240.
- Laguri, C., Stenzel, R. A., Donohue, T. J., Phillips-Jones, M. K. & Williamson, M. P. (2006). Activation of the global gene regulator PrrA (RegA) from *Rhodobacter sphaeroides*. *Biochemistry* 45, 7872-7881.
- Laurie, A. T. R. & Jackson, R. M. (2006). Methods for the prediction of protein-ligand binding sites for Structure-Based Drug Design and virtual ligand screening. *Current Protein & Peptide Science* 7, 395-406.
- Le Duff, C. S., Whittaker, S. B. M., Radford, S. E. & Moore, G. R. (2006). Characterisation of the conformational properties of urea-unfolded Im7: Implications for the early stages of protein folding. *J. Mol. Biol.* 364, 824-835.
- Leach, R. N., Gell, C., Wigneshweraraj, S., Buck, M., Smith, A. & Stockley, P. G. (2006). Mapping ATP-dependent activation at sigma(54) promoter. *J. Biol. Chem.* 281, 33717-33726.
- Mankouri, J., Taneja, T. K., Smith, A. J., Ponnambalam, S. & Sivaprasadarao, A. (2006). Kir6.2 mutations causing neonatal diabetes prevent endocytosis of ATP-sensitive potassium channels. *Embo J.* 25, 4142-4151.
- Marincs, F., Manfield, I. W., Stead, J. A., McDowall, K. J. & Stockley, P. G. (2006). Transcript analysis reveals an extended regulon and the importance of protein-protein co-operativity for the *Escherichia coli* methionine repressor. *Biochem. J.* 396, 227-234.
- Masca, S. I., Rodriguez-Mendieta, I. R., Friel, C. T., Radford, S. E. & Smith, D. A. (2006). Detailed evaluation of the performance of microfluidic T mixers using fluorescence and ultraviolet resonance Raman spectroscopy. *Review of Scientific Instruments* 77.
- McCormick, C. J., Brown, D., Griffin, S., Challinor, L., Rowlands, D. J. & Harris, M. (2006). A link between translation of the hepatitis C virus polyprotein and polymerase function; possible consequences for hyperphosphorylation of NS5A. *J. Gen. Virol.* 87, 93-102.
- McCormick, C. J., Maucourant, S., Griffin, S., Rowlands, D. J. & Harris, M. (2006). Tagging of NS5A expressed from a functional hepatitis C virus replicon. *J. Gen. Virol.* 87, 635-640.
- McLeish, T. C. B. (2006). Diffusive searches in high-dimensional spaces and apparent 'two-state' behaviour in protein folding. *J. Phys.-Condes. Matter* 18, 1861-1868.

- Murphy, J. E., Tacon, D., Tedbury, P. R., Hadden, J. M., Knowling, S., Sawamura, T., Peckham, M., Phillips, S. E. V., Walker, J. H. & Ponnambalam, S. (2006). LOX-1 scavenger receptor mediates calcium-dependent recognition of phosphatidylserine and apoptotic cells. *Biochem. J.* 393, 107-115.
- Myers, S. L., Jones, S., Jahn, T. R., Morten, I. J., Tennent, G. A., Hewitt, E. W. & Radford, S. E. (2006). A systematic study of the effect of physiological factors on beta 2-microglobulin amyloid formation at neutral pH. *Biochemistry* 45, 2311-2321.
- Myers, S. L., Thomson, N. H., Radford, S. E. & Ashcroft, A. E. (2006). Investigating the structural properties of amyloid-like fibrils formed *in vitro* from beta 2-microglobulin using limited proteolysis and electrospray ionisation mass spectrometry. *Rapid Commun. Mass Spectrom.* 20, 1628-1636.
- Needham, C. J., Bradford, J. R., Bulpitt, A. J., Care, M. A. & Westhead, D. R. (2006). Predicting the effect of missense mutations on protein function: analysis with Bayesian networks. *BMC Bioinformatics* 7.
- Needham, C. J., Bradford, J. R., Bulpitt, A. J. & Westhead, D. R. (2006). Inference in Bayesian networks. *Nature Biotechnology* 24, 51-53.
- Neelov, I. M., Adolf, D. B., McLeish, T. C. B. & Paci, E. (2006). Molecular dynamics simulation of dextran extension by constant force in single molecule AFM. *Biophys. J.* 91, 3579-3588.
- Netherton, C. L., McCrossan, M. C., Denyer, M., Ponnambalam, S., Armstrong, J., Takamatsu, H. H. & Wileman, T. E. (2006). African swine fever virus causes microtubule-dependent dispersal of the trans-golgi network and slows delivery of membrane protein to the plasma membrane. *J. Virol.* 80, 11385-11392.
- Omaetxebarria, M. J., Hagglund, P., Elortza, F., Hooper, N. M., Arizmendi, J. M. & Jensen, O. N. (2006). Isolation and characterization of glycosylphosphatidylinositol-anchored peptides by hydrophilic interaction chromatography and MALDI tandem mass spectrometry. *Analytical Chemistry* 78, 3335-3341.
- Phillips, S. E. V. (2006). Turning up the HEAT on translation. *Structure* 14, 806-807.
- Potter, C. A., Jeong, E. L., Williamson, M. P., Henderson, P. J. F. & Phillips-Jones, M. K. (2006). Redox-responsive *in vitro* modulation of the signalling state of the isolated PrrB sensor kinase of *Rhodobacter sphaeroides* NCIB 8253. *FEBS Lett.* 580, 3206-3210.
- Protopapa, E., Aggeli, A., Boden, N., Knowles, P. F., Salay, L. C. & Nelson, A. (2006). Electrochemical screening of self-assembling beta-sheet peptides using supported phospholipid monolayers. *Medical Engineering & Physics* 28, 944-955.
- Radford, S. E. (2006). GroEL: More than just a folding cage. *Cell* 125, 831-833.
- Ranson, N., Stromer, T., Bousset, L., Melki, R. & Serpell, L. C. (2006). Insights into the architecture of the Ure2p yeast protein assemblies from helical twisted fibrils. *Protein Sci.* 15, 2481-2487.

- Ranson, N. A., Clare, D. K., Farr, G. W., Houldershaw, D., Horwich, A. L. & Saibil, H. R. (2006). Allosteric signaling of ATP hydrolysis in GroEL-GroES complexes. *Nat. Struct. Mol. Biol.* 13, 147-152.
- Redondo, C., Burke, B. J. & Findlay, J. B. C. (2006). The retinol-binding protein system: A potential paradigm for steroid-binding globulins? *Hormone and Metabolic Research* 38, 269-278.
- Reed, M. L., Dove, B. K., Jackson, R. M., Collins, R., Brooks, G. & Hiscox, J. A. (2006). Delineation and modelling of a nucleolar retention signal in the coronavirus nucleocapsid protein. *Traffic* 7, 833-848.
- Rella, M. & Jackson, R. M. (2006). Identification of novel ACE2 inhibitors by structure-based pharmacophore modeling and virtual screening. *Abstr. Pap. Am. Chem. Soc.* 231.
- Rella, M., Rushworth, C. A., Guy, J. L., Turner, A. J., Langer, T. & Jackson, R. M. (2006). Structure-based pharmacophore design and virtual screening for novel angiotensin converting enzyme 2 inhibitors. *Journal of Chemical Information and Modeling* 46, 708-716.
- Remaut, H., Rose, R. J., Hannan, T. J., Hultgren, S. J., Radford, S. E., Ashcroft, A. E. & Waksman, G. (2006). Donor-strand exchange in chaperone-assisted pilus assembly proceeds through a concerted beta strand displacement mechanism. *Mol. Cell* 22, 831-842.
- Robinson, M. A., Wood, J. P. A., Capaldi, S. A., Baron, A. J., Gell, C., Smith, D. A. & Stonehouse, N. J. (2006). Affinity of molecular interactions in the bacteriophage phi 29 DNA packaging motor. *Nucleic Acids Res.* 34, 2698-2709.
- Saidijam, M., Benedetti, G., Ren, Q. H., Xu, Z. Q., Hoyle, C. J., Palmer, S. L., Ward, A., Bettaney, K. E., Szakonyi, G., Meuller, J., Morrison, S., Pos, M. K., Butaye, P., Walravens, K., Langton, K., Herbert, R. B., Skurray, R. A., Paulsen, I. T., O'Reilly, J., Rutherford, N. G., Brown, M. H., Bill, R. M. & Henderson, P. J. F. (2006). Microbial drug efflux proteins of the major facilitator superfamily. *Current Drug Targets* 7, 793-811.
- Seeber, M., Fanelli, F., Paci, E. & Caflisch, A. (2006). Sequential unfolding of individual helices of bacterioopsin observed in molecular dynamics simulations of extraction from the purple membrane. *Biophys. J.* 91, 3276-3284.
- Shimokhina, N., Bronowska, A. & Homans, S. W. (2006). Contribution of ligand desolvation to binding thermodynamics in a ligand-protein interaction. *Angew. Chem.-Int. Edit.* 45, 6374-6376.
- Smith, A. M., Jahn, T. R., Ashcroft, A. E. & Radford, S. E. (2006). Direct observation of oligomeric species formed in the early stages of amyloid fibril formation using electrospray ionisation mass spectrometry. *J. Mol. Biol.* 364, 9-19.
- Spencer, K. A. & Hiscox, J. A. (2006). Characterisation of the RNA binding properties of the coronavirus infectious bronchitis virus nucleocapsid protein amino-terminal region. *FEBS Lett.* 580, 5993-5998.

- Spencer, K. A. & Hiscox, J. A. (2006). Expression and structural analysis of infectious bronchitis virus nucleoprotein. In *Nidoviruses: Toward Control of Sars and Other Nidovirus Diseases*, Vol. 581, pp. 133-138.
- Stead, J. A., Keen, J. N. & McDowall, K. J. (2006). The identification of nucleic acid-interacting proteins using a simple proteomics-based approach that directly incorporates the electrophoretic mobility shift assay. *Molecular & Cellular Proteomics* 5, 1697-1702.
- Suzuki, S. & Henderson, P. J. F. (2006). The hydantoin transport protein from *Microbacterium liquefaciens*. *J. Bacteriol.* 188, 3329-3336.
- Taylor, D. R. & Hooper, N. M. (2006). The prion protein and lipid rafts. *Mol. Membr. Biol.* 23, 89-99.
- Tezuka-Kawakami, T., Gell, C., Brockwell, D. J., Radford, S. E. & Smith, D. A. (2006). Urea-induced unfolding of the immunity protein Im9 monitored by spFRET. *Biophys. J.* 91, L42-L44.
- Thirumurugan, K., Sakamoto, T., Hammer, J. A., Sellers, J. R. & Knight, P. (2006). The cargo-binding domain regulates structure and activity of myosin 5. *Nature* 442, 212-215.
- Thomas, D. A., Francis, P., Smith, C., Ratcliffe, S., Ede, N. J., Kay, C., Wayne, G., Martin, S. L., Moore, K., Amour, A. & Hooper, N. M. (2006). A broad-spectrum fluorescence-based peptide library for the rapid identification of protease substrates. *Proteomics* 6, 2112-2120.
- Tuthill, T. J., Bubeck, D., Rowlands, D. J. & Hogle, J. M. (2006). Characterization of early steps in the poliovirus infection process: Receptor-decorated liposomes induce conversion of the virus to membrane-anchored entry-intermediate particles. *J. Virol.* 80, 172-180.
- Unwin, R. D., Smith, D. L., Blinco, D., Wilson, C. L., Miller, C. J., Evans, C. A., Jaworska, E., Baldwin, S. A., Barnes, K., Pierce, A., Spooncer, E. & Whetton, A. D. (2006). Quantitative proteomics reveals posttranslational control as a regulatory factor in primary hematopoietic stem cells. *Blood* 107, 4687-4694.
- Vohra, R. S., Murphy, J. E., Walker, J. H., Ponnambalam, S. & Homer-Vanniasinkam, S. (2006). Atherosclerosis and the lectin-like oxidized low-density lipoprotein scavenger receptor. *Trends in Cardiovascular Medicine* 16, 60-64.
- Wallace, E. J., Hooper, N. M. & Olmstedz, P. D. (2006). Effect of hydrophobic mismatch on phase behavior of lipid membranes. *Biophys. J.* 90, 4104-4118.
- West, D. K., Brockwell, D. J., Olmsted, P. D., Radford, S. E. & Paci, E. (2006). Mechanical resistance of proteins explained using simple molecular models. *Biophys. J.* 90, 287-297.
- West, D. K., Brockwell, D. J. & Paci, E. (2006). Prediction of the translocation kinetics of a protein from its mechanical properties. *Biophys. J.* 91, L51-L53.

- West, D. K., Olmsted, P. D. & Paci, E. (2006). Free energy for protein folding from nonequilibrium simulations using the Jarzynski equality. *Journal of Chemical Physics* 125.
- West, D. K., Olmsted, P. D. & Paci, E. (2006). Mechanical unfolding revisited through a simple but realistic model. *Journal of Chemical Physics* 124.
- West, D. K., Paci, E. & Olmsted, P. D. (2006). Internal protein dynamics shifts the distance to the mechanical transition state. *Phys. Rev. E* 74.
- Wijma, H. J., Jeuken, L. J. C., Verbeet, M. P., Armstrong, F. A. & Canters, G. W. (2006). A random-sequential mechanism for nitrite binding and active site reduction in copper-containing nitrite reductase. *J. Biol. Chem.* 281, 16340-16346.
- Williams, G. J., Woodhall, T., Farnsworth, L. M., Nelson, A. & Berry, A. (2006). Creation of a pair of stereochemically complementary biocatalysts. *J. Am. Chem. Soc.* 128, 16238-16247.
- Wilson, A. J., van Gestel, J., Sijbesma, R. P. & Meijer, E. W. (2006). Amplification of chirality in benzene tricarboxamide helical supramolecular polymers. *Chem. Commun.*, 4404-4406.
- You, J. H., Reed, M. L., Dove, B. K. & Hiscox, J. A. (2006). Three-dimensional reconstruction of the nucleolus using meta-confocal microscopy in cells expressing the coronavirus nucleoprotein. In *Nidoviruses: Toward Control of Sars and Other Nidovirus Diseases*, Vol. 581, pp. 313-318.
- Zhang, J., Smith, K. M., Tackaberry, T., Sun, X. J., Carpenter, P., Slugoski, M. D., Robins, M. J., Nielsen, L. P. C., Nowak, I., Baldwin, S. A., Young, J. D. & Cass, C. E. (2006). Characterization of the transport mechanism and permeant binding profile of the uridine permease Fui1p of *Saccharomyces cerevisiae*. *J. Biol. Chem.* 281, 28210-28221.
- Zhang, J., Sun, X. J., Smith, K. M., Visser, F., Carpenter, P., Barron, G., Peng, Y. S., Robins, M. J., Baldwin, S. A., Young, J. D. & Cass, C. E. (2006). Studies of nucleoside transporters using novel autofluorescent nucleoside probes. *Biochemistry* 45, 1087-1098.
- Zhang, J., Tackaberry, T., Ritzel, M. W. L., Raborn, T., Barron, G., Baldwin, S. A., Young, J. D. & Cass, C. E. (2006). Cysteine-accessibility analysis of transmembrane domains 11-13 of human concentrative nucleoside transporter 3. *Biochem. J.* 394, 389-398.
- Zsoldos, Z., Reid, D., Simon, A., Sadjad, B. S. & Johnson, A. P. (2006). eHITS: An innovative approach to the docking and scoring function problems. *Current Protein & Peptide Science* 7, 421-435.