University of Birmingham

Dr Peter Winn

Lecturer

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About

Dr Winn specialises in molecular modelling of biomolecules, including structural bioinformatics and anlysis of protein amino-acid sequences. His interest is at the interface of protein evolution and function, and how these are related to biological organisation. As well as trying to gain general insight into the rules that govern bio-molecules, of particular interest at this time are the polyketide synthases, extremely large proteins that synthesise biomolecules by the carefully co-ordinated interactions of their many domains. Polyketide synthases are a family of proteins that are responsible for the synthesis of naturally occuring polyketides, which are the basis of most of the key antibiotics in current use, as well as many other "blockbuster" pharmaceuticals such as the statins.

Qualifications

PhD University of Essex.

BSc University of Bristol.

Biography

Dr Winn studied Chemical Physics at the University of Bristol and completed a PhD on “Polarisation Effects in Molecular Simulations” at the University of Essex. He has since worked in various aspects of molecular interaction including developing techniques for drug discovery at the University of Oxford, the study of protein interactions at the EMBL Heidelberg and EML-research Heidelberg (since renamed HITS). He has been an independent researcher at the University of Birmingham since 2007. He is currently interested in how molecular interactions lead to biological organisation and function.

Teaching

Undergraduate tutorials.

Protein Structure (BIO261)

First year Maths Skills for Biosciences (BIO132)

First year chemical kinetics for biochemists (BIO143)

Second year literature searching skills (BIO240)

Co-ordinater of the MRes Molecular and Cellular Biology Programme

Organiser of the Master Research Techniques Module (BIOM13)

Plagiarism Prevention Contact at Undergraduate and Postgraduate levels.

Second Year Exams Committee

Postgraduate supervision

For a list of possible PhD projects offered by Dr Winn **www.findaphd.com/search/customlink.asp?inst=birm-Biol&supersurname=Winn (http://www.findaphd.com/search/customlink.asp?inst=birm-Biol&supersurname=Winn)**

Research

Research Theme within School of Biosciences: **Molecular Microbiology (/research/activity/microbiology/index-old.aspx)** and **Molecular and Cell Biology (/research/activity/cellbiology/index.aspx)**

Understanding Cellular Organisation at the Atomic Level

The group is interested in the physical and chemical processes important for biological organization. In particular, how does this influence **protein (http://en.wikipedia.org/wiki/Protein)** evolution? Cellular function comes from organized processes of events, often in response to external stimuli. The aim of the group is to use mathematical models of the processes involved better to understand these biological process. Organisational events result from physical interactions between different biological components, most commonly including one or more proteins. The complexity of the biological systems challenges the application of modelling techniques. It is necessary to develop models that are simple enough to be understood (calculable), but are complex enough to give a biologically meaningful result. Beyond the immediate intellectual curiosity that these systems arouse, better understanding of the elements of biological function and organisation will give a better insight into human disease

and will advance bio- and nano- technology.

Current biological systems being investigated include the protein interactions involved in the biosynthesis of the antibiotics thiomarinol and mupirocin (with the group of Prof Thomas, University of Birmingham), the structure and function of the signalling protein EvgS, which is part of a **two component regulatory system (http://en.wikipedia.org/wiki/Two-component_regulatory_system)** (with Dr Lund, University of Birmingham), and plant signalling proteins (with Dr Coates, University of Birmingham). Recent work has investigated **ubiquitin (http://en.wikipedia.org/wiki/Ubiquitin)** and the molecular machinery of ubiquitination and similar pathways including co-developing the ubiquitin resource (**www.ubiquitin-resource.org (http://www.ubiquitin-resource.org/)**). Controlled **ubiquitination (http://en.wikipedia.org/wiki/Ubiquitin)** is critical for the correct functioning of eukaryotic cells.We have also been involved in modelling the structure of the beta globin gene locus **(Wong,et al, 2009). (http://www3.interscience.wiley.com/journal/122666958/abstract)** and how it might regulate the changes in the type of hemoglobin produced during mammalian development (from embryo to adult) and in studying the function of **cytochromes P450 (http://en.wikipedia.org/wiki/P450)** , which are important proteins for many biosynthetic pathways and for the disposal of foreign compounds, including poisons and medicines.

Other areas of ongoing research include: Protein conformation, protonation states and function; Prediction of protein interactions; Understanding how higher protein organization leads to specific functionality; Discovery of small molecule inhibitors; Structural interpretation of bio-physical data, notably mass spectrometry data and FRET.

Publications

1. F. Khanim, N. Davies, P Veliça, R Hayden, J. Ride, C. Pararasa, G. Chong, U. Gunther, N. Veerapen, **P. Winn**, R. Farmer, P. Davies, E. Trivier, L. Rigoreau, M. Drayson and C. Bunce. Selective AKR1C3 inhibitors do not recapitulate the anti-leukaemic activities of the pan-AKR1C family inhibitor medroxyprogesterone acetate., British Journal of Cancer, 2014 Mar 18;110(6):1506-

2. A. S. Haines, X. Dong, Z Song, R. Farmer, C. Williams, J. Hothersall, E. Płoskoń, P. Wattana-amorn, E. R. Stephens, E Yamada, R. Gurney, Y Takebayashi, J. Masschelein, R. J. Cox, R Lavigne, C. L. Willis, T. J. Simpson, J. Crosby, **P. J. Winn**, C. M. Thomas, M. P. Crump, A conserved motif flags Acyl Carrier Proteins for β-branch insertion during type-I polyketide synthesis *Nature Chemical Biology*

3. A. W. Jones, P. J. Winn, H. J., Cooper, The Radical Ion Chemistry of *S*-Nitrosylated Peptides, *JASMS*, 2012, 23 (12), 2063-2074

4. L. A. Moody, Y. Saidi, E. J. Smiles, S. J. Bradshaw, M. Meddings, **P. J. Winn**, J. C. Coates ARABIDILLO gene homologues in basal land plants: species-specific gene duplication and likely functional redundancy *Planta*. 2012, 236 (6), 1927-1941

5. V. Cojocaru**, P J. Winn**, R. C. Wade**.** Multiple, ligand-dependent routes from the active site of cytochrome P450 2C9. *Curr. Drug. Metab.,* 2012, 2012, 13(2),143-54.

6. D. B. Kokh, S. Corni, **P. J. Winn**, M. Höfling, R. R. Gabdoulline, K. E. Gottschalk, R. C. Wade.ProMetCS:An Atomistic Force Field for Modeling Protein-Metal Surface Interactions in a Continuum Aqueous Solvent. *J. Chem. Theory and Comp*., 2010, 1753-1768.

7. H. Wong† , **P. J. Winn†** ; J. Mozziconacci. A molecular model of chromatin organisation and transcription: how a multi-RNA polymerase II machine transcribes and remodels the beta-globin locus during development. *Bioessays*, 2009, 31(12), 1357-66.

8. C. J. R, Illingworth, **P. J. Winn**, G. G. Ferenczy, C. A. Reynolds. Progress in Modelling Electrostatics and Polarization Through Effective Multipoles and Induced Charges. *Studia Univeristatis Babes-Bolyai Chemia,* 2008, 53(2), 21-27.

9. D. Motiejunas, R. R. Gabdoulline, T. Wang, A. Feldman-Salit, T Johann, **P. J. Winn** and R. C. Wade. Protein-protein docking by simulating the process of association subject to biochemical constraints. *Proteins*, 2008, 71(4), 1955-1969.

10. **P. J. Winn,** M. Zahran, J. N. Battey, Y. Zhou, R. C. Wade. A. Banerjee. Structural and electrostatic Properties of Ubiquitination and Related Pathways. *Frontiers in Bioscience*, 2007, 12, 3419-3430.

11. V. Cojocaru † , **P. J. Winn†** , R. C. Wade. The Ins and Outs of Cytochrome P450s, *Biochim. Biophys. Acta*, 2007, 1770(3), 390-401.

12. C. J. R. Illingworth, S. S. Gooding, **P. J. Winn**, G. A. Jones, G. G. Ferenczy, C. A. Reynolds. Classical Polarization in Hydrid QM/MM methods. *J. Phys. Chem. A.*, 2006, 110(20), 6487-6497.

13. R. C. Wade, D Motiejunas, K Schleinkofer, Sudarko, **P. J. Winn**, A. Banerjee, A. Kariakin, C. Jung. Multiple molecular recognition mechanisms. Cytochrome P450-A case study. *Biochim. Biophys. Acta*, 2005, 1754(1-2), 239-244.

14. K. Schleinkofer, Sudarko, **P. J. Winn**, S. K. Luedemann, R. C. Wade Do mammalian cytochrome P450s exhibit multiple ligand access pathways and ligand channelling? *EMBO Reports*, 2005, 6(6), 584-589.

15. **P. J. Winn**, K. Schleinkofer, A. Banerjee, R. C. Wade. Issues in high-throughput comparative modelling: A case study using the ubiquitin E2 conjugating enzymes, *Proteins*, 2005, 58(2), 367-75.

16. **P. J. Winn**, T. L. Religa, J. N. D. Battey, A. Banerjee, R. C. Wade. Determinants of functionality in the ubiquitin conjugating enzyme family. *Structure*, 2004, 12(9), 1563-74

17. R. C. Wade, I. Schlichting, **P. J. Winn**, Sudarko. A survey of ligand pathways to and from the active site of cytochromes P450. *J. Inorg. Biochem.,* 2004, 98(7), 1175-82.

18. **P. J. Winn†** , S. K. Luedemann† , R. Gauges, V. Lounnas and R. C. Wade. Comparison of the dynamics of substrate access channels in three cytochrome P450s reveals different opening mechanisms and a new functional role for a buried arginine. *PNAS (USA)*, 2002, 99(8), 5361-5366.

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