

**Biology Department
Publications
2004**

Agarwal, R., **Eswaramoorthy, S., Kumaran, D.**, Binz, T., and **Swaminathan, S.** Structural analysis of Botulinum neurotoxin type E catalytic domain and its mutant Glu212→Gln reveals the pivotal role of the Glu212 carboxylate in the catalytic pathway. *Biochemistry* 43(21): 6637-6644 (June, 2004).

Agarwal, R., **Eswaramoorthy, S., Kumaran, D., Dunn, J. J.**, and **Swaminathan, S.** Cloning, high level expression, purification, and crystallization of the full length *Clostridium botulinum* neurotoxin type E light chain. *Protein Expression and Purification* 34(1): 95-102 (March, 2004).

Anderson, C. W., Inventor. DNA-PK assay. U.S. Patent No. 6,803,203 B1, Issued: October 12, 2004.

Awasthi, V. D., Meinken, G., Springer, K., Srivastava, S. C., and **Freimuth, P.** Biodistribution of radioiodinated adenovirus fiber protein knob domain after intravenous injection in mice. *Journal of Virology* 78(12): 6431-6438 (June, 2004).

Barac, T., **Tagahavi, S.**, Borremans, B., Provoost, A., Oeyen, L., Colpaert, J. V., Vangronsveld, J., and **van der Lelie, D.** Engineered endophytic bacteria improve phytoremediation of water-soluble, volatile, organic pollutants. *Nature Biotechnology* 22(5): 583-588 (May, 2004). Cover: A root of a poplar colonized by the green fluorescent protein-labeled endophytic bacterium *Pseudomonas putida* VM1453. (Photo courtesy of Kieran Germaine, David Ryan and David Dowling, Department of Applied Biology & Chemistry, Institute of Technology, Carlow, Ireland). On page 583, van der Lelie and colleagues describe a yellow lupin containing a modified endophytic symbiont capable of toluene degradation.

Scientific American, *Science News*, April 12, 2004, "Plants Dispatched to Decontaminate Soil" [<http://www.sciam.com/article.cfm?chanID=sa003&articleID=000CB4B3-C142-1075-814283414B7F0190>]

Batsford, S., **Dunn, J.**, and Mihatsch, M. Outer surface lipoproteins of *Borrelia burgdorferi* vary in their ability to induce experimental joint injury. *Arthritis & Rheumatism* 50(7): 2360-2369 (July, 2004).

Becker, M. and Weckert, E. On the possibility of determining structures of membrane proteins in two-dimensional crystals using X-ray free electron lasers. *Conformational Proteomics of Macromolecular Architecture: Approaching the Structure of Large Molecular Assemblies and Their Mechanisms of Action*, R. H. Cheng and L. Hammar, Editors, Chapter 6, pp. 133-147, World Scientific Publishing Co., Singapore (2004).

Bennett, P. V., Cintron, N. S., Gros, L., Laval, J., and **Sutherland, B. M.** Are endogenous clustered DNA damages induced in human cells? *Free Radical Biology and Medicine* 37(4): 488-499 (August, 2004).

Briggs, J. A. G., **Simon, M. N.**, Gross, I., Krausslich, H.-G., Fuller, S. D., Vogt, V. M., and Johnson, M. C. The stoichiometry of Gag protein in HIV-1. *Nature Structural & Molecular Biology* 11(7): 672-675 (July, 2004).

Brown, M. T. and **Mangel, W. F.** Interaction of actin and its 11-amino acid C-terminal peptide as cofactors with the adenovirus proteinase. *FEBS Letters* 563(1-3): 213-218 (April, 2004).

Bulavin, D. V., Phillips, C., Nannenga, B., Timofeev, O., Donehower, L. A., **Anderson, C. W.**, Appella, E., and Fornace, Jr., A. J. Inactivation of the Wip1 phosphatase inhibits mammary tumorigenesis through p38 MAPK-mediated activation of the p16^{Ink4a}-p19^{Arf} pathway. *Nature Genetics* 36(4): 343-350 (April, 2004).

Chao, Y. and **Fu, D.** Kinetic study of the antiport mechanism of an *Escherichia coli* zinc transporter, ZitB. *Journal of Biological Chemistry* 279(13): 12043-12050 (March, 2004).

Chao, Y. and **Fu, D.** Thermodynamic studies of the mechanism of metal binding to the *Escherichia coli* zinc transporter YiiP. *Journal of Biological Chemistry* 279(17): 17173-17180 (April, 2004).

Chen, Z., Green, T. J., Luo, M., and **Li, H.** Visualizing the RNA molecule in the bacterially expressed vesicular stomatitis virus nucleoprotein-RNA complex. *Structure* 12: 227-235 (February, 2004).

Daniels, B. V., **Jiang, J.-S.**, and **Fu, D.** Crystallization and preliminary crystallographic analysis of the *Escherichia coli* water channel AqpZ. *Acta Crystallographica Section D: Biological Crystallography* D60: 561-563 (March, 2004).

Ding, S.-Y., Rumbles, G., Jones, M., Tucker, M. P., Nedeljkovic, J., Simon, M. N., **Wall, J. S.**, and Himmel, M. E. Bioconjugation of (CdSe)ZnS quantum dots using a genetically engineered multiple polyhistidine tagged cohesion/dockerin protein polymer. *Macromolecular Materials and Engineering* 289(7): 622-628 (July, 2004).

Eswaramoorthy, S., Kumaran, D., Keller, J., and Swaminathan, S. Role of metals in the biological activity of *Clostridium botulinum* neurotoxins. *Biochemistry* 43(8): 2209-2216 (March, 2004).

Friedberg, E. C. The discovery that xeroderma pigmentosum (XP) results from defective nucleotide excision repair. *Mutation Research: DNA Repair* 3(2): 188-194 (February, 2004). [Included in this paper is the paper by **Setlow, R. B.**, Regan, J. D., German, J., and Carrier, W. L. Evidence that xeroderma pigmentosum cells do not perform the firststep in the repair of ultraviolet damage to their DNA (reprinted from *Proceedings of the National Academy of Sciences USA* 64: 1035-1041, 1969).]

Freimuth, P. I., Inventor. Structure of adenovirus bound to cellular receptor CAR. U.S. Patent No. 6,737,234 B1, Issued: May 18, 2004.

Gallagher, D. T., Monbouquette, H. G., Schroder, I., **Robinson, H.**, Holden, M. J., and Smith, N. N. Structure of alanine dehydrogenase from *Archaeoglobus*: Active site analysis and relation to bacterial cyclodeaminases and mammalian mu crystallin. *Journal of Molecular Biology* 342(1): 119-130 (September, 2004).

Georgakilas, A. G., Bennett, P. V., Wilson III, D. M., and **Sutherland, B. M.** Processing of bistranded abasic DNA clusterd in γ -irradiated human hematopoietic cells. *Nucleic Acids Research* 32(18): 5609-5620 (October, 2004).

Georgiev, G., Gilfoy, N., Cebe, P., and **Capel, M.** Phase transitions and structural parameters of HIQ-40 liquid crystalline co-polyester. *Polymer* 45: 3429-3440 (May, 2004).

Germaine, K., Keogh, E., Garcia-Cabellos, G., Borremans, B., **van der Lelie, D.**, Barac, T., Oeyen, L., Vangronsveld, J., Moore, F. P., Moore, E. R. B., Campbell, C. D., Ryan, D., and Dowling, D. N. Colonisation of poplar trees by *gfp* expressing bacterial endophytes. *FEMS Microbiology Ecology* 48: 109-118 (April, 2004).

Golan, G., Zharkov, D. O., Fernandes, A. S., Zaika, E., **Kycia, J. H.**, Wawrzak, Z., Grollman, A. P., and Shoham, G. Crystallization and preliminary crystallographic analysis of endonuclease VIII in its uncomplexed form. *Acta Crystallographica Section D: Biological Crystallography* D60(8): 1476-1480 (August, 2004).

Gopalan, G., He, Z., Balmer, Y., Romano, P., Gupta, R., **Heroux, A.**, Buchanan, B. B., Swaminathan, K., and Luan, S. Structural analysis uncovers a role for redox in regulating FKBP13, an immunophilin of the chloroplast thylakoid lumen. *Proceedings of the National Academy of Sciences USA* 101(38): 13945-13950 (September, 2004).

Gupta, S., **Mangel, W. F.**, McGrath, W. J., Perek, J. L., Lee, D. W., Takamoto, K., and Chance, M. R. DNA binding provides a molecular strap activating the adenovirus proteinase. *Molecular & Cellular Proteomics* 3(10): 950-959 (October, 2004).

Cover: On the cover, Synchrotron Protein Footprinting--the study of protein structure and dynamics in solution using synchrotron x-ray generated hydroxyl radicals. The x-ray beam is shown in *blue* exciting water molecules and forming hydroxyl radicals. The radicals diffuse through the solution and react with surface accessible side chains of the adenovirus protease seen in space filling mode on the *left*. Protease digestion followed by chromatography and mass spectrometry is used to identify the extent and sites of oxidation. DNA binding to the protease protects specific residues from attack. Using this data, a model of DNA (*red*) binding to the protease is developed that provides a molecular mechanism for DNA-dependent activation. For details, see the article by Gupta *et al.*, pages 950-959.

Hainfeld, J. F., Powell, R. D., and Hacker, G. W. Nanoparticle molecular labels. *Nanobiotechnology: Concepts, Applications and Perspectives*, C. M. Niemeyer and C. A. Mirkin, Editors, Chapter 23, pp. 353-386, Wiley-Vch, Weinheim, Germany (March, 2004).

Heilmann, I., Mekhedov, S., King, B., Browse, J., and **Shanklin, J.** Identification of the Arabidopsis palmitoyl-monogalactosyldiacylglycerol Δ^7 -desaturase gene, *FAD5*, and effects of plastidial retargeting of Arabidopsis desaturases on the *fad5* mutant phenotype. *Plant Physiology* 136: 4237-4245 (December, 2004).

Heilmann, I., Pidkowich, M., Girke, T., and **Shanklin, J.** Switching desaturase enzyme specificity by alternate subcellular targeting. *Proceedings of the National Academy of Science USA* 101(28): 10266-10271 (July, 2004).

Hou, M.-H., **Robinson, H.**, Gao, Y.-G., and Wang, A. H.-J. Crystal structure of the $[\text{Mg}^{2+}-(\text{chromomycin A}_3)_2]-\text{d}(\text{TTGGCCAA})_2$ complex reveals GGCC binding specificity of the drug dimer chelated by a metal ion. *Nucleic Acids Research* 32(7): 2214-2222 (April, 2004).

Huai, Q., Wang, H., Zhang, W., Colman, R. W., **Robinson, H.**, and Ke, H. Crystal structure of phosphodiesterase 9 shows orientation variation of inhibitor 3-isobutyl-1-methylxanthine binding. *Proceedings of the National Academy of Sciences USA* 101(26): 9624-9629 (June, 2004).

Impey, S., McCorkle, S. R., Cha-Molstad, H., Dwyer, J. M., Yochum, G. S., Boss, J. M., McWeeney, S., **Dunn, J. J.**, Mandel, G., and Goodman, R. H. Defining the CREB regulon: A genome-wide analysis of transcription factor regulatory regions. *Cell* 119: 1041-1054 (December, 2004).

Jiang, J. and **Sweet, R. M.** Protein Data Bank depositions from synchrotron sources. *Journal of Synchrotron Radiation* 11(Pt. 4): 319-327 (July, 2004).

Karthikeyan, S., Zhou, Q., Zhao, Z., Kao, C.-L., Tao, Z., **Robinson, H.**, Liu, H.-W., and Zhang, H. Structural analysis of *Pseudomonas* 1-aminocyclopropane-1-carboxylate deaminase complexes: Insight into the mechanism of a unique pyridoxal-5'-phosphate dependent cyclopropane ring-opening reaction. *Biochemistry* 43(42): 13328-13339 (October, 2004).

Lacks, S. A. Transformation. *The Pneumococcus*, E. I. Tuomanen, Editor, Chapter 7, pp. 89-115, ASM Press, Washington, DC (June, 2004).

Lashuel, H. A. and **Wall, J. S.** Molecular electron microscopy approaches to elucidating the mechanisms of protein fibrillogenesis. *Methods in Molecular Biology*, Vol. 299: Amyloid Proteins: Methods and Protocols, E. M. Sigurdsson, Editor, Chapter 7, pp. 81-102, Humana Press, Inc., Totowa, NJ (December, 2004).

Li, H., Qian, L., Chen, Z., Thibault, D., Liu, G., Liu, T., and Thanassi, D. G. The outer membrane usher forms a twin-pore secretion complex. *Journal of Molecular Biology* 344(5): 1397-1407 (December, 2004).

Lovelace, J. J., Soares, A. S., Bellamy, H. D., **Sweet, R. M.**, Snell, E. H., and Borgstahl, G. E. O. First results of digital topography applied to macromolecular crystals. *Journal of Applied Crystallography* 37(Pt. 3): 481-485 (June, 2004).

Mao, J., Gao, Y.-G., Odeh, S., **Robinson, H.**, Montalvetti, A., Docampo, R., and Oldfield, E. Crystallization and preliminary X-ray diffraction study of the farnesyl diphosphate synthase from *Trypanosoma brucei*. *Acta Crystallographica Section D: Biological Crystallography* D60: 1863-1866 (October, 2004).

Mosesson, M. W., DiOrio, J. P., Hernandez, I., **Hainfeld, J. F.**, **Wall, J. S.**, and Grieninger, G. The ultrastructure of fibrinogen-420 and the fibrin-420 clot. *Biophysical Chemistry* 112(2-3): 209-214 (December, 2004).

Nettles, J. H., **Li, H.**, Cornett, B., Krahn, J. M., Snyder, J. P., and Downing, K. H. The binding mode of epothilone A on α,β -tubulin by crystallography. *Science* 305: 866-869 (August, 2004).

Ni, S., **Robinson, H.**, Marsing, G. C., Bussiere, D. E., and Kennedy, M. A. Structure of 2C-methyl-D-erythritol-2,4-cyclodiphosphate synthase from *Shewanella oneidensis* at 1.6 Å: Identification of farnesyl pyrophosphate trapped in a hydrophobic cavity. *Acta Crystallographica Section D: Biological Crystallography* D60: 1949-1957 (November, 2004).

Phillips, J. D., Whitby, F. G., Warby, C. A., Labbe, P., Yang, C., Pflugrath, J. W., Ferrara, J. D., **Robinson, H.**, Kushner, J. P., and Hill, C. P. Crystal structure of the oxygen-dependant coproporphyrinogen oxidase (Hem13p) of *Saccharomyces cerevisiae*. *Journal of Biological Chemistry* 279(37): 38960-38968 (September, 2004).

Qiu, W.-G., Bruno, J. F., Attie, O., Casjens, S. R., Xu, Y., **Dunn, J. J.**, Schutzer, S. E., Fraser, C. M., and Luft, B. J. Genetic exchange and plasmid transfers in *Borrelia burgdorferi* sensu stricto revealed by three-way genome comparisons and multilocus sequence typing. Proceedings of the National Academy of Sciences USA 101(39): 14150-14155 (September, 2004).

Reipa, V., **Shanklin, J.**, and Vilker, V. Substrate binding and the presence of ferredoxin affect the redox properties of the soluble plant Δ^9 -18:0-acyl carrier protein desaturase. Chemical Communications 2004: 2406-2407 (November, 2004).

Renella, G., Mench, M., **van der Lelie, D.**, Pietramellara, G., Ascher, J., Ceccherini, M. T., Landi, L., and Nannipieri, P. Hydrolase activity, microbial biomass and community structure in long-term Cd-contaminated soils. Soil Biology & Biochemistry 36: 443-451 (March, 2004).

Saxena, S., Yuan, P., Dhar, S. K., Senga, T., Takeda, D., **Robinson, H.**, Kornbluth, S., Swaminathan, K., and Dutta, A. A dimerized coiled-coil domain and an adjoining part of geminin interact with two sites on Cdt1 for replication inhibition. Molecular Cell 15: 245-258 (July, 2004).

Schwarzenbacher, R., Stenner-Liewen, F., Liewen, H., **Robinson, H.**, Yuan, H., Bossy-Wetzel, E., Reed, J. C., and Liddington, R. C. Structure of the *Chlamydia* protein CADD reveals a redox-enzyme that modulates host cell apoptosis. Journal of Biological Chemistry 279(28): 29320-29324 (July, 2004).

Setlow, J. K., Editor, *Genetic Engineering: Principles and Methods*, Vol. 26, 316 p., Kluwer Academic/Plenum Publishers, NY (August, 2004).

Setlow, R. B. Historical Reflections: A second life in science -- working after the age of 65. Mutation Research: DNA Repair 3(4): 441-449 (April, 2004).

Shanklin, J. and Cahoon, E. B., Inventors. Mutant fatty acid desaturase. U.S. Patent No. 6,686,186 B2, issued February 3, 2004.

Smith, N., Mayhew, M., Holden, M. J., Kelly, H., **Robinson, H.**, **Heroux, A.**, Vilker, V. L., and Gallagher, D. T. Structure of C73G putidaredoxin from *Pseudomonas putida*. Acta Crystallographica Section D: Biological Crystallography D60: 816-822 (May, 2004).

Surana, N. K., Grass, S., Hardy, G. G., **Li, H.**, Thanassi, D. G., and St. Geme III, J. W. Evidence for conservation of architecture and physical properties of Omp85-like proteins throughout evolution. Proceedings of the National Academy of Sciences USA 101(40): 14497-14502 (October, 2004).

Sutherland, B. M., Inventor. Method for assaying clustered DNA damages. U.S. Patent No. 6,789,022 B2, issued September 7, 2004.

Swaminathan, S. Toward therapeutics for *Clostridium botulinum* neurotoxins. *Synchrotron Radiation News* 17(4): 16-24 (July/August, 2004). Cover: Structural studies leading to drug design for botulinum neurotoxins (pp. 16).

Swaminathan, S., Eswaramoorthy, S., and Kumaran, D. Structure and enzymatic activity of botulinum neurotoxins. *Movement Disorders* 19(S8): S17-S22 (March, 2004).

Van Ooteghem, S. A., Jones, A., **van der Lelie, D.**, Dong, B., and Mahajan, D. H₂ production and carbon utilization by *Thermotoga neapolitana* under anaerobic and microaerobic growth conditions. *Biotechnology Letters* 26: 1223-1232 (August, 2004).

Vassilev, A., Schwitzguebel, J.-P., Thewys, T., **van der Lelie, D.**, and Vangronsveld, J. The use of plants for remediation of metal-contaminated soils. *Scientific World Journal* 4: 9-34 (January, 2004).

Wei, Y., **Li, H.**, and **Fu, D.** Oligomeric state of the *Escherichia coli* metal transporter YjiP. *Journal of Biological Chemistry* 279(38): 39251-39259 (September, 2004).

Woo, E.-J., Kim, Y.-G., Kim, M.-S., Han, W.-D., Shin, S., **Robinson, H.**, Park, S.-Y., and Oh, B.-H. Structural mechanism for inactivation and activation of CAD/DFP40 in the apoptotic pathway. *Molecular Cell* 14(4): 531-539 (May, 2004). Cover: A biochemical hallmark of programmed cell death is the degradation of chromosomal DNA into nucleosomal units. Caspase-activated DNase, also known as DNA fragmentation Factor 40, is responsible for this process. In this issue, Woo et al. report the crystal structure of the enzyme (pp. 531-539), which reveals a deep active site crevice that appears ideal for distinguishing internucleosomal DNA from nucleosomal DNA.

Ye, R., Goodarzi, A. A., Kurz, E. U., Saito, S., Higashimoto, Y., Lavin, M. F., Appella, E., **Anderson, C. W.**, and Lees-Miller, S. P. The isoflavonoids genistein and quercetin activate different stress signaling pathways as shown by analysis of site-specific phosphorylation of ATM, p53 and histone H2AX. *Mutation Research: DNA Repair* 3: 235-244 (March, 2004).

Zaika, E. I., Perlow, R. A., **Matz, E.**, Broyde, S., Gilboa, R., Grollman, A. P., and Zharkov, D. O. Substrate discrimination by formamidopyrimidine-DNA glycosylase: A mutational analysis. *Journal of Biological Chemistry* 279(6): 4849-4861 (February, 2004).

Zhang, X. and **Studier, F. W.** Multiple roles of T7 RNA polymerase and T7 lysozyme during bacteriophage T7 infection. *Journal of Molecular Biology* 340(4): 707-730 (July, 2004).

Zhang, Y.-B., Howitt, J., McCorkle, S., Lawrence, P., Springer, K., and **Freimuth, P.** Protein aggregation during overexpression limited by peptide extensions with large net negative charge. *Protein Expression and Purification* 36(2): 207-216 (August, 2004).