Publications

Our users' publications in EMBO J, JACS, J Biol Chem, Mol Cell Biol, Nature and PNAS USA report the discoveries of new protein structures, signaling mechanisms and NMR methods.

Open all sections

2015 publications

Derek Woolfson and colleagues

- Baker EG, Bartlett GJ, Crump MP, Sessions RB, Linden N, Faul CFJ, Woolfson DN (2015). Local and macroscopic electrostatic interactions in single alpha-helices, Nature Chemical Biology, doi: 10.1038/nchembio.1739

2014 publications

Ulrich Günther and colleagues

- Günther UL, Chong MG, Volpari T, Koczula K, Atkins K, Bunce CM, FL Khanim (2014). Metabolic Fluxes in Cancer Metabolism. In Tumor Cell Metabolism. Pathways, Regulation, Biology (Eds.: S Mazurek, M Shoshan), 315-348. Springer. DOI 10.1007/978-3-7091-1824-5.
- JT Bjerrum, Y Wang, F Hao, M Coskun, C Ludwig, U Günther, OH Nielsen (2014). Metabonomics of human fecal extracts characterize ulcerative colitis, Crohn's disease and healthy individuals. Metabolomics, DOI 10.1007/s11306-014-0677-3.
- Khanim F, Davies N, Veliça P, Hayden R, Ride J, Pararasa C, Chong MG, Gunther U, Veerapen N, Winn P, Farmer R, Trivier E, Rigoreau L, Drayson M, Bunce C (2014). Selective AKR1C3 inhibitors do not recapitulate the anti-leukaemic activities of the pan-AKR1C inhibitor medroxyprogesterone acetate. Br J Cancer. 18;110(6):1506-16.

Arnout Kalverda and colleagues

- Kalverda AP, Gowdy J, Thompson GS, Homans SW, Henderson PJF & Patching SG (2014). Trosy NMR with a 52 KDa sugar transport protein and the binding of a small molecule inhibitor. Molecular Membrane Biology 31:131-140.

Mark Pfuhl and colleagues

- Rostkova E, Gautel M, Pfuhl M (2014). Solution NMR assignment of the heavy chain complex of the human cardiac myosin regulatory light chain. Biomol NMR Assign. doi: 10.1007/s12104-014-9543-5.

Michael Overduin and colleagues

- Kufareva I, M Lenoir, F Dancea, P Sridhar, E Rausch, C Bissig, J Gruenberg, R Abagyan, M Overduin (2014). Discovery of novel membrane binding structures and functions. Biochem Cell Biol, in press.
- Jamshad M, V Grimard, I Idini, TJ Knowles, MR Dowle, N Schofield, YP Lin, R Finka, RE Palmer, M Overduin, C Govaerts, JM Ruysschaert, KJ Edler, TR Dafforn Structural analysis of a nanoparticle containing a lipid bilayer used for detergent-free extraction of membrane proteins (2014). Nano Research, in press.
- RK Koppisetti, YG Fulcher, SH Prior, J Xu, M Lenoir, M Overduin, and SR Van Doren, Ambidextrous binding of cell and membrane bilayers by soluble matrix metalloproteinase-12 (2014). Nature Communications, in press.
- Lenoir, M, M Sugawara, J Kaur, LJ Ball, M Overduin, Structural Insights into the Activation of the RhoA GTPase by the Lbc Oncoprotein (2014). J Biol Chem, 289(34):23992-24004. PMCID: PMC4156082.
- Gulati, M Jamshad, T Knowles, R Downing, N Cant, JB Koenderink, RC Ford, M Overduin, ID Kerr, TR Dafforn & A Rothnie (2014). Detergent free purification of ABC transporters, Biochemical J, 461(2):269-278. PMID: 24758594.
- Butterworth, M Overduin and AJ Barr, Targeting Protein Tyrosine Phosphatase SHP2 for therapeutic intervention in cancer (2014). Future Med Chem, in press.

Mark Viant and colleagues

- RP Ellis, JI Spicer, JJ Byrne, U Sommer, MR Viant, DA White, S Widdicombe (2014). ^{1}H-NMR metabolomics reveals contrasting response by male and female mussels exposed to reduced seawater pH, increased temperature and a pathogen. Environ. Sci. Technol. (published on-line ahead of print).
- TD Williams, IM Davies, H Wu, AM Diab, L Webster, MR Viant, JK Chipman, MJ Leaver, SG George, CF Moffatt, CD Robinson (2014). Molecular responses of European flounder (*Platichthys flesus*) chronically exposed to contaminated estuarine sediments. Chemosphere108, 152-8.

2013 publications

Rudolf Allemann and colleagues

- Wysoczanski P, Mart RJ, Loveridge EJ, Williams C, Whittaker SB-M, Crump MP, Allemann RK (2013). 1H, 13C and 15N chemical shift assignments of unliganded Bcl-xL and its complex with a photoresponsive Bak-derived peptide. Biomol NMR Assign. 7(2):187-191.
- Loveridge EJ, Matthews SM, Williams C, Whittaker SB-M, Guenther UL, Evans RM, Dawson WM, Crump MP, Allemann RK (2013). Aliphatic (1)H, (13)C and (15)N chemical shift assignments of dihydrofolate reductase from the psychropiezophile *Moritellaprofunda*in complex with NADP(+) and folate. Biomol NMR Assign. 7(1):61-64.

Matt Crump and colleagues

- Haines AS, Dong X, Song Z, Farmer R, Williams C, Hothersall J, Ploskon E, Wattana-Amorn P, Stephens ER, Yamada E, Gurney R, Takebayashi R, Masschelein J, Cox RJ, Lavigne R, Willis CL, Simpson TJ, Crosby J, Winn PJ, Thomas CM, Crump MP (2013). A conserved motif flags acyl carrier proteins for beta-branching in polyketide synthesis. Nat Chem Biol, 9(11):685-692.

Ann Dixon and colleagues

- Probert F, Whittaker SB-M, Crispin M, Mitchell DA, Dixon AM (2013). Solution NMR analyses of the C-type carbohydrate recognition domain of DC-SIGNR protein reveal different binding modes for HIV-derived oligsaccharides and smaller glycan fragments. J Biol Chem. 288(31):22745-22757. PMCID: PMC3829359

Ulrich Günther and colleagues

- R Singhal, JB Carrigan, W Wei, P Taniere, RK Hejmadi, C Forde, C Ludwig, J Bunch, RL Griffiths, PJ Johnson, O Tucker, D Alderson, UL Günther, DG Ward (2013). MALDI profiles of proteins and lipids for the rapid characterisation of upper GI-tract cancers. J Proteomics 80C:207-215.

Christian Ludwig and colleagues

- J Adam, M Yang, C Bauerschmidt, M Kitagawa, L O'Flaherty, P Maheswaran, G Özkan, N Sahgal, D Baban, K Kato, K Saito, K Iino, K Igarashi, M Stratford, C Pugh, DA Tennant, C Ludwig, B Davies, PJ Ratcliffe, M El-Bahrawy, H Ashrafian, T Soga, PJ Pollard (2013). A Role for Cytosolic Fumarate Hydratase in Urea Cycle Metabolism and Renal Neoplasia. Cell Reports 3(5):1440-1448.

Geoff Moore and colleagues

- Figueiredo AM, Whittaker SB-M, Knowling SE, Radford SE, Moore GR (2013). Conformational dynamics is more important than helical propensity for the folding of the all alpha-helical protein Im7. Protein Science 22(12):1722-1738.

Michael Overduin and colleagues

- Browning DF, Matthews SA, Rossiter AE, Sevastsyanovich YR, Jeeves M, Mason JL, Wells TJ, Wardius CA, Knowles TJ, Cunningham AF, Bavro VN, Overduin M, Henderson IR (2013). Functional and Topological profiling of the Escherichia coli BamA protein, PLoS One. 8(12):e84512. PMID: 24376817. PMCID: PMC3871556
- Al-Jassar C, Bikker H, Overduin M*, Chidgey M (2013). Mechanistic basis of desmosome-targeted diseases, J Mol Biol, 425(21):4006-22, PMID: 23911551 (*corresponding author). PMCID: PMC3807649
- Al-Jassar C, Bernado, P, Chidgey M, Overduin M (2013). Hinged plakin domains provide specialized degrees of articulation in envoplakin, periplakin and desmoplakin, PLoS ONE 8(7): e69767. PMID: 23922795. PMCID: PMC3726778
- Bissig C, M Lenoir, MC Velluz, I Kufarena, R Abagyan, M Overduin*, J Gruenberg* (2013). Viral infection controlled by calcium dependent recognition of late endosome-specific lipid by the Alix Bro1 domain, Dev Cell 25:364-73, PMID: 23664863 (*joint corresponding authors). PMCID: PMC4129370
- Lenoir M & Overduin M (2013). PtdIns(4)P signalling and recognition sytems, Adv Exp Med Biol 991:59-83. PMID: 23775691.

Mark Pfuhl and colleagues

- Hood FE, Williams SJ, Burgess SG, Richards MW, Roth D, Straube A, Pfuhl M, Bayliss R, Royle SJ (2013). Coordination of adjacent domains mediates TACC3-ch-TOG-clathrin assembly and mitotic spindle binding. J Cell Biol 202(3):463-478. PMCID: PMC3734082

Mark Viant and colleagues

- WCEP Verberk, U Sommer, RL Davidson, MR Viant (2013). Anaerobic metabolism at thermal extremes: A metabolomic test of the oxygen limitation hypothesis in an aquatic insect. Integrative and Comparative Biology 53, 609-619. PMCID: PMC3776598
- A Lodi, S Tiziani, FL Khanim, UL Günther, MR Viant, GJ Morgan, CM Bunce, MT Drayson (2013). Proton NMR-based metabolite analyses of archived serial paired serum and urine samples from myeloma patients at different stages of disease activity identifies acetylcarnitine as a novel marker of active disease. PLoS ONE 8:e56422. PMCID: PMC3576408

Steve Young and colleagues

- SP Young, MR Viant, SR Kapoor, JJ Byrne, GR Wallace, A Filer, CD Buckley, GD Kitas, K Raza (2013). The impact of inflammation on metabolomic profiles in patients with arthritis. Arthritis and Rheumatism 65(8):2015-23. PMCID: PMC3840700
- Kapoor SR, Filer A, Fitzpatrick M, Fisher BA, Taylor PC, Buckley CD, McInnes IB, Raza K, Young SP (2013). Metabolic profiling predicts response to anti-TNFα therapy in patients with rheumatoid arthritis. Arthritis Rheum. 65(6):1448-56. PMCID: PMC3715109

Ana Zeri and colleagues

- Campos BM, Sforca ML, Ambrosio AL, Domingues MN, de Arruda Campos Brasil de Souza T, Barbosa JA, Paes Leme AF, Perez CA, Whittaker SB-M, Murakami MT, Zeri AC, Benedetti CE (2013). Plant Physiol 162(3):1311-1323. PMCID: PMC3707534

2012 publications

Christian Ludwig and colleagues

- C Ludwig, JM Easton, A Lodi, S Tiziani, SE Manzoor, AD Southam, JJ Byrne, LM Bishop, S He, TN Arvanitis, UL Günther, MR Viant (2012). Birmingham Metabolite Library: a publicly accessible database of 1-D 1H and 2-D 1H J-resolved NMR spectra of authentic metabolite standards (BML-NMR). Metabolomics 8(1):8-18.

Sara Whittaker and colleagues

- Figueiredo AM, Moore GR, Whittaker SB-M (2012). Understanding how small helical proteins fold: Conformational dynamics of Im proteins relevant to their folding landscapes. Biochem Soc Trans. 40(2):424-428.

Ulrich Günther and colleagues

- Rodriguez DA, Alcarraz-Vizan G, Diaz-Moralli S, Reed MA, Gomez FP, Falciani F, Günther UL, Roca J, Cascante M (2012). Plasma metabolic profile in COPD patients: Effects of exercise and endurance training. Metabolomics 8(3):508-516.

Michael Overduin and colleagues

- Rajesh S, Sridhar P, Tews AB, Feneant L, Cocquerel L, Ward DG, Berditchevski F, Overduin M (2012). Structural basis of ligand interactions of the large extracellular domain of tetraspanin CD81. J Virol. 86(18):9606-9616. PMCID: PMC3446547
- Markley JL, Akutsu H, Asakura T, Baldus M, Boelens R, Bonvin A, Kaptein R, Bax A, Bezsonova I, Gryk MR, Hoch JC, Korzhnev DM, Maciejewski MW, Case D, Chazin WJ, Cross TA, Dames S, Kessler H, Lange O, Madl T, Reif B, Sattler M, Eliezer D, Fersht A, Forman-Kay J, Kay LE, Fraser J, Gross J, Kortemme T, Sali A, Fujiwara T, Gardner K, Luo X, Rizo-Rey J, Rosen M, Gil RR, Ho C, Rule G, Gronenborn AM,
Ishima R, Klein-Seetharaman J, Tang P, van der Wel P, Xu Y, Grzesiek S, Hiller S, Seelig J, Laue ED, Mott H, Nietlispach D, Barsukov I, Lian LY, Middleton D, Blumenschein T, Moore G, Campbell I, Schnell J, Vakonakis IJ, Watts A, Conte MR, Mason J, Pfuhl M, Sanderson MR, Craven J, Williamson M, Dominguez C, Roberts G, Günther U, Overduin M, Werner J, Williamson P, Blindauer C, Crump M, Driscoll P, Frenkiel T, Golovanov A, Matthews S, Parkinson J, Uhrin D, Williams M, Neuhaus D, Oschkinat H, Ramos A, Shaw DE, Steinbeck C, Vendruscolo M, Vuister GW, Walters KJ, Weinstein H, Wüthrich K, Yokoyama S. (2012). In support of the BMRB. Nat Struct Mol Biol. 19(9):854-60, PMID: 22955930

Rudolf Allemann and colleagues

- Wysoczanski P, Mart RJ, Loveridge EJ, Williams C, Whittaker SB-M, Crump MP, Allemann RK (2012). NMR solution structure of a photoswitchable apoptosis activating Bak peptide bound to Bcl-x(L). J Amer Chem Soc. 134(18):7644-7647.

Matt Crump and colleagues

- Williams C, Hoppe H, Rezgui D, Strickland M, Forbes BE, Grutzner F, Frago S, Ellis RZ, Wattana-Amorn P, Prince SN, Zaccheo OJ, Nolan CM, Mungall AJ, Jones EY, Crump MP, Hassan AB (2012). An exon splice enhancer primes IGF2:IGFR binding site structure and function evolution. Science 338(6111):1209-1213.

Harald Schwalbe and colleagues

- Silvers R, Sziegat F, Tachibana H, Segawa SI, Whittaker SB-M, Günther UL, Gabel F, Huang JR, Blackledge M, Wirmer-Bartoschek J, Schwalbe H (2012). Modulation of structure and dynamics by disulphide bond formation in unfolded states. J Amer Chem Soc. 134(15):6846-6854.

Mark Viant and colleagues

- Hrydziuszko O, Viant MR (2012). Missing values in mass spectrometry based metabolomics: an undervalued step in the data processing pipeline. Metabolomics 8(1):S161-S174.
- H.Ashrafian, G. Czibik, M. Bellahcene, D. Aksentijević, A. C. Smith, S. J. Mitchell, M. S. Dodd, J. Kirwan, J. J. Byrne, C. Ludwig, H. Isackson, A. Yavari, N. B. Støttrup, H. Contractor, T. J. Cahill, N. Sahgal, D. R. Ball, R. I. D. Birkler, I. Hargreaves, D. A. Tennant, J. Land, C. A. Lygate, M. Johannsen, R. K. Kharbanda, S. Neubauer, C. Redwood, R. de Cabo, I. Ahmet, M. Talan, U. L. Günther, A. J. Robinson, M. R. Viant, P. J. Pollard, D. J. Tyler, H. Watkins (2012). Fumarate is cardioprotective via activation of the Nrf2 antioxidant pathway. *Cell Metabolism*15, 361-371. PMCID: PMC3314920

2011 publications

Michael Overduin and colleagues

- He, J, JL Scott, A Heroux, S Roy, M Lenoir, M Overduin, RV Stahelin and TG Kutateladze (2011) Molecular analysis of association of the FAPP1 PH domain with PI4P and Arf1, J Biol Chem, 286(21):18650-7.
- Jamshad M, Y-P Lin, T J Knowles, R Parslow, C Harris, M Wheatley, D R Poyner, R M Bill, O Thomas, M Overduin, T R Dafforn (2011) Detergent-free purification of membrane proteins with intact native membrane environment, Bioch. Soc. Trans. 39(3):813-8.
- Knowles, TJ, DF Browning, M Jeeves, R Maderbocus, S Rajesh, P Sridhar, E Manoli, D Emery, U Sommer, A Spencer, DL Leyton, D Squire, RR Chaudhuri, MR Viant, AF Cunningham, IR Henderson, M Overduin (2011) Structure and function of BamE within the outer membrane and the β-barrel assembly machine, EMBO Reports 12(2):123-8.
- Rajesh S, Knowles T, Overduin M (2011) Production of membrane proteins without cells or detergents, N Biotechnol. 28(3):250-4.
- Rossiter AE, Leyton DL, Tveen-Jensen K, Browning DF, SevastsyanovichY, Knowles TJ, Nicols K, CunninghamAF, Overduin M, Schembri MA and Henderson IR (2011) The essential BAM complex components BamD and BamA are required for autotransporter biogenesis, J Bacteriology 193(16):4250-3.
- Wolny MD, Grzybek M, Bok E, Chorzalska AD, Czogalla A, Lenoir M, Adamczyk K, Kolondra A, Diakowski W, Overduin M, Sikorski AF (2010) Key amino acid residues of ankyrin-sensitive phosphatidylethanolamine/ phosphatidylcholine-lipid binding site of βI–spectrin, PLoS One 6:21538.

Ulrich Günther and colleagues

- UL Günther (2011). Dynamic Nuclear Hyperpolarization in Liquids. Top Curr Chem, 335:23-69.
- Lizarraga D, Vinardell MP, van Delft JH, van Breda SG, Staal Y, Günther UL, Reed MA, Alcarraz-Vizan G, Torres JL, Cascante M (2011). A lyophilized red grape pomace containing proanthocyanidin-rich dietary fiber induces genetic and metabolic alterations in colon mucosa of female C57 BL/6J mice. J Nutr. 141(9):1597-1604.

Christian Ludwig and colleagues

- Jean-Louis H.A. Duprey, Dario M. Bassani, Eva I. Hyde, Christian Ludwig, Alison Rodger, Joseph S. Vyle, John Wilkie, Zheng-Yun Zhao and James H.R. Tucker (2011). Anthracene-modified oligonucleotides as fluorescent DNA mismatch sensors: discrimination between various base-pair mismatches. Supramolecular Chemistry 23(3-4):273–277.
- C Ludwig, UL Günther (2011). MetaboLab - advanced NMR data processing and analysis for metabolomics. BMC Bioinformatics 12:366.

Sara Whittaker and colleagues

- Whittaker SB-M, Clayden NJ, Moore GR (2011). NMR characterisation of the relationship between frustration and the excited state of Im7. J Mol Biol. 414:511-529.
- Lenoir M, Whittaker SB-M, Overduin M (2011). Secondary structure and (1)H, (13)C, (15)N resonance assignments of the Golgi-specific PH domain of FAPP1. Biomol NMR Assign. 5(2):185-7.

Rudolf Allemann and colleagues

- Loveridge EJ, Tey L-H, Behiry EM, Dawson WM, Evans RM, Whittaker SB-M, Günther UL, Williams C, Crump MP, Allemann RK (2011). The role of large-scale motions in catalysis by dihydrofolate reductase. J Amer Chem Soc. 133:20561-20570.

Andrew Almond and colleagues

- Sattelle BM, Almond A (2011). Is N-acetyl-D-glucosamine a rigid 4C1-chair? Glycobiology 21(12):1651-1662.

John Christodoulou and colleagues

- Nyon MP, Kirkpatrick J, Cabrita LD, Christodoulou J, Gooptu B (2011).^{1}H, ^{15}N and ^{13}C backbone resonance assignments of the archetypal serpin alpha1-antitrypsin. Biomol NMR Assign. 6(2):153-156.

Ann Dixon and colleagues

- Jenei ZA, Warren GZ, Hasan M, Zammit VA, Dixon AM (2011). Packing of transmembrane domain 2 of carnitine palmitoyltransferase-1A affects oligomerization and malonyl-CoA sensitivity of the mitochondrial outer membrane protein. FASEB J. 25:4522-4530.
- King G, Oates J, Patel D, van den Berg HA, Dixon AM (2011). Towards a structural understanding of the smallest known oncoprotein: investigation of the bovine papillomavirus E5 protein using solution-state NMR. Biochim Biophys Acta 1808(6):1493-1501.

Graham Jackson and colleagues

- Mugumbate G, Jackson GE, van der Spoel D (2011). Open conformation of adipokinetic hormone receptor from the malaria mosquito facilitates hormone binding. Peptides 32(3):553-559.

Colin Kenyon and colleagues

- Kenyon CP, Steyn A, Roth RL, Steenkamp PA, Nkosi TC, Oldfield LC (2011). The role of the C8 proton of ATP in the regulation of phosphoryl transfer within kinases and synthetases. BMC Biochemistry 12:36-53.

Andrew Peet and colleagues

- Davison JE, Davies NP, Wilson M, Sun Y, Chakrapani A, McKiernan PJ, Walter JH, Gissen P, Peet AC (2011) MR spectroscopy-based brain metabolite profiling in

propionic acidaemia: metabolic changes in the basal ganglia during acute decompensation and effect of liver transplantation. Orphanet J Rare Dis. 6(1):19.

- Davison JE, Davies NP, English MW, Philip S, MacPherson LK, Gissen P, Peet AC (2011) Magnetic resonance spectroscopy in the diagnostic evaluation of brainstem lesions in Alexander disease, J Child Neurol 26(3):356-60.
- Mirbahai L, Wilson M, Shaw CS, McConville C, Malcomson RDG, Griffin JL, Kauppinen RA, Peet AC (2011). (1)H magnetic resonance spectroscopy metabolites as biomarkers for cell cycle arrest and cell death in rat glioma cells. Int J Biochem & Cell Biol. 43(7):990-1001.
- Pan X, Wilson M, Mirbahai L, McConville C, Arvanitis TN, Griffin JL, Kauppinen RA, Peet AC (2011) In vitro metabolomic study detects increases in UDP-GlcNAc and UDP-GalNAc, as early phase markers of cisplatin treatment response in brain tumor cells. J Proteome Res. 10(8):3493-3500.
- Tortajada S, Fuster-Garcia E, Vicente J, Wesseling P, Howe FA, Julià-Sapé M, Candiota AP, Monleón D, Moreno-Torres A, Pujol J, Griffiths JR, Wright A, Peet AC, Martínez-Bisbal MC, Celda B, Arús C, Robles M, García-Gómez JM (2011) Incremental Gaussian Discriminant Analysis based on Graybill and Deal weighted combination of estimators for brain tumour diagnosis, J Biomed Inform. 44(4):677-687.
- Martin Wilson, Greg Reynolds, Risto A. Kauppinen, Theodoros N. Arvanitis and Andrew C. Peet (2011) A constrained least-squares approach to the automated quantitation of in-vivo 1H MRS data. Magnetic Resonance in Medicine 65(1): 1-12.

Teresa Pinheiro and colleagues

- Sanghera N, Correia BEFS, Correia JRS, Ludwig C, Agarwal S, Nakamura HK, Kuwata K, Samain E, Gill AC, Bonev B, Pinheiro TJT (2011). Deciphering the molecular details for the binding of the prion protein to main ganglioside GM1 of neuronal membranes. Chemistry & Biology 18(11):1422-1431.

Mark Searle and colleagues

- Garner TP, Long J, Layfield R, Searle MS (2011). Impact of p62/SQSTM1 UBA domain mutations linked to Paget's disease of bone on ubiquitin recognition. Biochemistry 50:4665-4674.
- Edwards J, Malaurie E, Knodrashov A, Long J, de Moor C, Searle MS, Emsley J (2011). Sequence determinants for the tandem recognition of UGU and CUG rich RNA elements by the two N-terminal RRMs of CELF1. Nucleic Acids Res 39(19):8638-8650.
- Garner TP, Strachan J, Shedden EC, Long JE, Cavey JR, Layfield R, Searle MS (2011). Independent interactions of ubiquitin-binding domains in a ubiquitin-mediated ternary complex. Biochemistry 50(42):9076-9087.

Mark Viant and colleagues

- Southam AD, Khanim F, Hayden RE, Gunther UL, Drayson MT, VIant MR, Bunce CM (2011) Mass spectrometry metabolomics analysis of acute myeloid leukemia cell responses to bezafibrate and medroxyprogesterone acetate. Experimental Hematology 39(8):S89-S90.
- Lodi A, Tiziani S, Khanim FL, Drayson MT, Günther UL, Bunce CM, Viant MR (2011) Hypoxia triggers major metabolic changes in AML cells without altering indomethacin-induced TCA cycle deregulation. ACS Chem Biol. 6(2):169-75.
- Poynton HC, Taylor NS, Hicks J, Colson K, Chan S, Clark C, Scanlan L, Loguinov AV, Vulpe C, Viant MR (2011) Metabolomics of microliter hemolymph samples enables an improved understanding of the combined metabolic and transcriptional responses of daphnia magna to cadmium. Environ Sci Technol. 45(8):3710-7.
- Römer I, White TA, Baalousha M, Chipman JK, Viant MR, Lead JR (2011). Aggregation and dispersion of silver nanoparticles in exposure media for aquatic toxicity tests. J Chromatogr. A 1218:4226-4233.
- Southam AD, Lange A, Hines A, Hill EM, Katsu Y, Iguchi T, Tyler CR, Viant MR (2011). Metabolomics reveals target and off-target toxicities of a model organophosphate pesticide to roach (*Rutilus rutilus*): Implications for biomonitoring. Environ Sci Technol. 45:3759-3767.
- Weber RJM, Southam AD, Sommer U, Viant MR (2011). Characterization of isotopic abundance measurements in high resolution FT-ICR and Orbitrap mass spectra for improved confidence of metabolite identification. Anal Chem. 83:3737-3743.
- Williams TD, Turan N, Diab AM, Wu H, Mackenzie C, Bartie KL, Hrydziuszko O, Lyons BP, Stentiford GD, Herbert MJ, Abraham KJ, Katsiadaki I, Leaver MJ, Taggart JB, George SG, Viant MR, Chipman JK, Faciani F (2011). Towards a system level understanding of non-model organisms sampled from the environment: A network biology approach. PLoS Comp Biol. 7:e1002126.

2010 publications

by **Andrew Almond** and colleagues:

- Sattelle BM, Shakeri J, Roberts IS, Almond A (2010). A 3D-structural model of unsulfated chondroitin from high-field NMR: 4-sulfation has little effect on backbone conformation. Carbohydr Res 345(2): 291-302.
- Sattelle BM, Hansen SU, Gardiner J, Almond A (2010). Free energy landscapes of iduronic acid and related monosaccharides. J Amer Chem Soc. 32:13132-13134.

by **Matt Crump** and colleagues:

- Ploskon E, Arthur CJ, Kanari A, Williams C, Wattana-Amorn P, Crosby J, Willis C, Crump MP (2010). Recognition of intermediate functionality by acyl carrier protein over a complete cycle of fatty acid biosynthesis. Chem & Biol. 17:776-785.

by **Ulrich Günther** and colleagues:

- Ludwig C, Marin-Montesinos I, Saunders MG, Günther UL (2010). Optimizing the polarization matrix for ex situ dynamic nuclear polarization. J Am Chem Soc 132(8): 2508-2509.
- Michiels P, Atkins K, Ludwig C, Whittaker S, van Dongen M, Günther U (2010). Assignment of the orphan nuclear receptor Nurr1 by NMR. Biomol NMR Assign 4(1):101-105.
- Ludwig C, Marin-Montesinos I, Saunders MG, Emwas AH, Pikramenou Z, Hammond SP, Günther UL (2010). Application of ex situ dynamic nuclear polarization in studying small molecules. Phys Chem Chem Phys, 12(22):5868-71.
- Clelia Cogliati, Laura Ragona, Mariapina D'Onofrio, Ulrich Günther, Sara Whittaker, Christian Ludwig, Simona Tomaselli, Michael Assfalg and Henriette Molinari (2010). Site-Specific Investigation of the Steady-State Kinetics and Dynamics of the Multistep Binding of Bile Acid Molecules to a Lipid Carrier Protein. Chem. Eur. J. 16:11300-11310.
- Ludwig C, Saunders M, Marin-Montesinos I, Günther U (2010). Quantum Rotor Induced Hyperpolarization. Proc Nat Acad Sci USA. 107(24):10799-10803.

by **Geoff Moore** and colleagues:

- Hecht O, Zhang Y, Li C, Penfold CN, James R, Moore GR (2010). Characterisation of the interaction of colicin A with its co-receptor TolA. FEBS Letters 584:2249-2252.

by **Michael Overduin** and colleagues:

- Lenoir M, Coskun U, Grzybek M, Cao X, Buschhorn SB, James J, Simons K, Overduin M (2010). Structural basis of wedging the Golgi membrane by FAPP pleckstrin homology domains. EMBO Rep 11(4): 279-284.

- Sugawara, M, S Whittaker, S Bishop, LJ Ball, M Overduin (2010) Resonance assignments of the human AKAP13 PH domain and stabilizing DH helix, Biomol NMR Assign 3 (2) 215-8.
- Knowles TJ, Sridhar P, Rajesh S, Manoli E, Overduin M, Henderson IR (2010) Secondary structure and 1H, 13C and 15N resonance assignments of BamE, a component of the outer membrane protein assembly machinery in Escherichia coli, Biomol NMR Assign 4(2):179-81
- Kolondra A, Lenoir M, Wolny M, Klauza I, Jezierski A, Overduin M, Sikorski AF and Grzybek M (2010) The role of hydrophobic interactions for ankyrin-spectrin complex formation. Biochimica et Biophysica Acta – Biomembranes, 1798(11):2084-9.

by **Andrew Peet** and colleagues:

- Davies NP, Wilson M, Natarajan K, Sun Y, Macpherson L, Brundler MA, Arvanitis TN, Grundy RG, Peet AC (2010). Non-invasive detection of glycine as a biomarker of malignancy in childhood brain tumours using in-vivo (1)H MRS at 1.5 Tesla confirmed by ex-vivo high-resolution magic-angle spinning NMR. NMR Biomed 23(1):80-87.
- Wilson M, Davies NP, Sun Y, Natarajan K, Arvanitis TN, Kauppinen RA, Peet AC (2010) A comparison between simulated and experimental basis sets for assessing short-TE in vivo ^{1}H MRS data at 1.5 T. NMR Biomed. 23(10):1117-26.
- Halliday NA, Peet AC, Britton MM. (2010) Detection of pH in microemulsions, without a probe molecule, using magnetic resonance. J Phys Chem B.;114(43):13745-51.
- Davison JE, Sun Y, Wilson M, Chakrapani A, Hendriksz CJ, Vijay S, Wassmer E, Davies NP, Peet AC, Gissen P (2010) Lactic acid and beyond: Quantitative in vivo metabolomic analysis of mitochondrial disease using magnetic resonance spectroscopy. J Inherit Metab Dis. 33:S87-S87.
- Wilson M, Reynolds G, Kauppinen RA, Arvanitis TN, Peet AC (2010) A constrained least-squares approach to the automated quantitation of in vivo ^{1}H magnetic resonance spectroscopy data. Magn Reson Med. 65(1):1-12.
- Easton JM, Harris LM, Viant MR, Peet AC, Arvanitis TN (2010) Linked metabolites: a tool for the construction of directed metabolic graphs. Comput Biol Med. 40(3):340-9.

by **Mark Sanderson** and colleagues:

- Bergeron J, Huthof H, Veselkov D, Simpson PJ, Matthews SJ, Malim MH, Sanderson MR (2010). HIV-1 Vif recruits the EloBC-Cul5 ubiquitin ligase via a novel coupled folding-and-binding mechanism. PLoS Pathogens 6(6):e1000925.

by **David Scott** and colleagues:

- Rajasekar KV, Tul Muntaha S, Tame JRH, Kommareddy S, Morris G, Wharton CW, Thomas CM, White SA, Hyde EI, Scott DJ (2010). Order and disorder in the domain organisation of the plasmid partition protein KorB. J Biol Chem. 285(20):15440-9.

by **Mark Viant** and colleagues:

- Ludwig C, Viant M (2010). Two-dimensional J-resolved NMR spectroscopy: review of a key methodology in the metabolomics toolbox. Phytochem Anal 21(1): 22-32.
- Van Scoy AR, Yu Lin C, Anderson BS, Philips BM, Martin MJ, McCall J, Todd CR, Crane D, Sowby ML, Viant MR, Tjeerdma RS (2010). Metabolic responses produced by crude versus dispersed oil in Chinook salmon pre-smolts via NMR-based metabolomics. Ecotoxicol Environ Saf. 73:710-7.
- Hines A, Staff FJ, Widdows J, Compton R, Falciani F, Viant MR (2010). Discovery and validation of metabolic signatures for predicting whole organism toxicology. Toxicol Sci. 115:369-378.
- Taylor NS, Weber RJM, White TA, Viant MR (2010). Discriminating between different acute chemical toxicities via changes in the daphnid metabolome. Toxicol Sci. 118:307-317.
- Katsiadaki I, Williams TD, Ball J, Bean TP, Wu H, Santos EM, Brown MM, Baker P, Ortega F, Falciani F, Craft JA, Tyler CR, Viant MR, Chipman JK (2010). Hepatic transcriptomic and metabolomic responses in the stickleback (Gasterosteus aculeatus) exposed to ethinyl-estradiol. Aquat Toxicol 97(3): 174-187.
- Hrydziuszko O, Silva MA, Perera MTPR, Richards DA, Murphy N, Mirza D, Viant MR (2010). Application of metabolomics to investigate the process of human orthotopic liver transplantation: A proof of principle study. OMICS - J Integrative Biol. 14:143-150.
- Lodi A, Tiziani S, Khanim FL, Drayson MT, Günther UL, Bunce CM, Viant MR (2010) Hypoxia triggers major metabolic changes in AML cells without altering indomethacin-induced TCA cycle deregulation. ACS Chem Biol. 18;6(2):169-75.

by **Steve Young** and colleagues:

- Sinclair AJ, Viant MR, Ball AK, Burdon MA, Walker EA, Stewart PM, Rauz S, Young SP (2010). NMR-based metabolomic analysis of cerebrospinal fluid and serum in neurological diseases - a diagnostic tool? NMR Biomed 23(2): 123-132.

2009 publications

by **Andrew Almond** and colleagues:

- Blundell CD, Roberts IS, Sheehan JK, Almond A (2009). Investigating the molecualr basis for the virulence of *Eschericiacoli*K5 by nuclear magnetic resonance (NMR) analysis of the K5 capsule polysaccharide. J Mol Biol & Microbiol. 17:71-82.

by**Matt Crump** and colleagues:

- Evans SE, Williams C, Arthur CJ, Ploskon E, Crosby J, Cox RJ, Willis CL, Simpson TJ, Crump MP (2009). Probing the interactions of early oplyketide intermediates with the actinorhodin ACP from *S. coelicolor*A3(2). J Mol Biol. 389:511-528.

by **Ulrich Günther** and colleagues:

- Knoblich K, Whittaker S, Ludwig C, Michiels P, Jiang T, Schaffhausen B, Guenther U (2009). Backbone assignment of the N-terminal polyomavirus large T antigen. Biomol NMR Assignments 3(1): 119-123.
- Ludwig C, Guenther UL (2009). Ligand based NMR methods for drug discovery. Front Biosci 14, 4565-4574.
- Ludwig C, Ward D, Martin A, Viant MR, Ismail T, Johnson PJ, Wakelam MJ, Günther UL (2009). Fast targeted multidimensional NMR metabolomics of colorectal cancer. Magn Reson Chem 47 Suppl 1: S68-73.
- Michiels PJ, Ludwig C, Stephan M, Fischer C, Möller G, Messinger J, van Dongen M, Thole H, Adamski J, Günther UL (2009). Ligand based NMR spectra demonstrate as additional phytoestrogen binding site for 17 ß-hydroxysteroid dehydrogenase type-1. J Steroid Biochem Mol Biol 117(4-5): 93-98.
- Romanska HM, Tiziani S, Howe R, Günther UL, Gulzar Z, Lalani E-N (2009). NMR detects PI3k/Akt-independent traits common to pluripotent murine embryonic stem cells and their malignant counterparts. Neoplasia 11(12): 1301-1308.
- Tiziani S, Lopes V, Günther UL (2009). Early stage diagnosis of oral cancer using H-1 NMR-based metabolomics. Neoplasia 11(3): 269-276.
- Tiziani S, Lodi A, Khanim FL, Viant MR, Bunce CM, Günther UL (2009). Metabolomic profiling of drug responses in acute myeloid leukaemia cell lines. PLoS One. 4(1):e4251.

by **Michael Overduin** and colleagues:

- Brombacher E, Urwyler S, Ragaz C, Weber SS, Kami K, Overduin M, Hilbi H (2009). The Rab1 guanine nucleotide exchange factor SidM is a major PtdIns(4)P-binding effector protein of Legionella pneumophila. J Biol Chem 284(8): 4846-4856.
- Kami K, Dafforn T, Chidgey M, Overduin M (2009). The desmoglein specific cytoplasmic region is intrinsically disordered in solution. J Mol Biol 386(2): 531-543.
- Kami K, Rajesh S, Overduin M (2009). Phospholipid interacting proteins by solution-state NMR spectroscopy. Methods Mol Biol. 462:291-306.
- Knowles TJ, Finka R, Smith C, Lin YP, Dafforn T, Overduin M (2009). Membrane proteins solubilized intact in lipid containing nanoparticles bounded by styrene maleic acid copolymer. J Amer Chem Soc 131(22):7484-7485.
- Knowles TJ, Scott-Tucker A, Overduin M, Henderson IR (2009). Membrane protein architects: the role of the BAM complex in outer membrane protein assembly. Nat Rev Microbiol. 7(3):206-214.
- Knowles TJ, McClelland DM, Rajesh S, Henderson IR, Overduin M (2009). Secondary structure and 1H, 13C and 15N backbone assignments of BamC, a component of the outer membrane protein assembly machinery in Eschericia coli. Biomol NMR Assignments 3(2): 203-206.
- Sugawara M, Whittaker S, Bishop S, Ball LJ, Overduin M (2009). Resonance assignments of the human AKAP13 PH domain and stabilizing DH helix. Biomol NMR Assignments 3(2): 215-218.

by **Andrew Peet** and colleagues:

- Hao J, Zou X, Wilson MP, Davies NP, Sun Y, Peet AC, Arvanitis TN (2009). A comparative study of feature extraction and blind source separation of independent component analysis (ICA) on childhood brain tumour (1)H magnetic resonance spectra. NMR Biomed 22(8): 809-818.
- Wilson M, Davies NP, Brundler MA, McConville C, Grundy RG, Peet AC (2009). High resolution magic angle spinning 1H NMR of childhood brain and nervous system tumours. Mol Cancer. 8:6.
- Wilson M, Davies NP, Grundy RG, Peet AC (2009). A quantitative comparison of metabolite signals as detected by in vivo MRS with ex vivo 1H HR-MAS for childhood brain tumours. NMR Biomed. 22(2):213-9.

by **Sheena Radford** and colleagues:

- Knowling SE, Figueiredo AM, Whittaker SB-M, Moore GR, Radford SE (2009). Amino acid insertion reveals a necessary three-helical intermediate in the folding pathway of the colicin E7 immunity protein Im7. J Mol Biol 392, 1074-1086.

by **Kai Simons** and colleagues:

- Cao X, Coskun Ü, Rössle M, Buschhorn S, Grzybek M, Dafforn T, Lenoir M, Overduin M, Simons K (2009). The Golgi protein FAPP2 tubulates membranes. PNAS 106(50):21121-21125.

by **Mark Viant** and colleagues:

- Parsons HM, Ludwig C, Viant MR (2009). Line-shape analysis of J-resolved NMR spectra: application to metabolomics and quantification of intensity errors from signal processing and high signal congestion. Magn Reson in Chem 47 Suppl 1: S86-95.
- Parsons HM, Ekman DR, Collette TW, Viant MR (2009). Spectral relative standard deviation: a practical benchmark in metabolomics. Analyst. 134(3):478-85.
- Viant MR, Bearden DW, Bundy JG, Burton IW, Collette TW, Ekman DR, Ezernieks V, Karakach TK, Lin CY, Rochfort S, de Ropp JS, Teng Q, Tjeerdema RS, Walter JA, Wu H (2009). International NMR-based environmental metabolomics intercomparison exercise. Environ Sci Technol. 43(1):219-225.
- Williams TD, Wu H, Santos EM, Ball J, Katsiadaki I, Brown MM, Baker P, Ortega F, Falciani F, Craft JA, Tyler CR, Chipman JK, Viant MR (2009). Hepatic transcriptomic and metabolomic responses in the stickleback (Gasterosteus aculeatus) exposed to environmentally relevant concentrations of dibenzanthracene. Environ Sci Technol. 43(16):6341-6348.

by **Steve Young** and colleagues:

- Young SP, Nessim M, Falciani F, Trevino V, Banerjee SP, Scott RAH, Murray PI, Wallace GR (2009). Metabolomic analysis of human vitreous humor differentiates ocular inflammatory disease. Molecular Vision 15: 1210-1217.

2008 publications

by **Ulrich Günther**and colleagues:

- Ludwig C, Michiels PJA, Wu X, Kavanagh KL, Pilka E, Jansson A, Oppermann U, Guenther UL (2008). SALMON: Solvent accessibility, ligand binding, and mapping of ligand orientation by NMR spectroscopy. J Med Chem. 51 1-3.
- Tiziani S, Emwas A-H, Lodi A, Ludwig C, Bunce CM, Viant MR, Guenther UL (2008). Optimised metabolite extraction from blood serum for 1H nuclear magnetic resonance spectroscopy. Analytical Biochem. 377: 16-23.
- Saunders MG, Ludwig C, Guenther UL (2008). Optimizing the signal enhancement in cryogenic ex situ DNP-NMR. J Am Chem Soc. 130(22): 6914-6915.
- Ludwig C, Michiels PJA, Lodi A, Ride J, Bunce CM, Guenther UL (2008). Evaluation of solvent accessibility epitopes for different dehydrogenase inhibitors. ChemMedChem. 3(9): 1371-1376.
- Emwas A-H, Saunders M, Ludwig C, Guenther UL (2008). Determinants for optimal enhancement in ex situ DNP experiments. Applied Magn Reson 34, 483-494.

by **Michael Overduin** and colleagues:

- Dancea, F, K Kami, M Overduin (2008). Lipid interaction networks of peripheral membrane proteins revealed by data-driven micelle docking, Biophys J, 57(2): 206-16.
- K Kami, S Rajesh, M Overduin, Phospholipid interacting protein domains by solution state NMR spectroscopy, Methods In Molecular Biology (Humana Press) 462:291-306.
- Jamshad M, Rajesh S, Stamatakic Z, McKeating JA, Dafforn T, Overduin M, Bill RM (2008). Structural characterization of recombinant human CD81 produced in Pichia pastoris. Protein Expr Purif. 57, 206-16.
- Jeeves M, McClelland D, Barr AJ, Overduin M (2008). Sequence-specific 1H, 13C and 15N backbone resonance assignments of the 35 kDa catalytic domain of human PTPN7. Biomol NMR Assignments 2, 101-103.
- Knowles TJ, Jeeves M, Bobat S, Dancea F, McClelland D, Palmer T, Overduin M, Henderson IR (2008). Fold and function of POTRA domains responsible for delivering unfolded proteins to membranes. Mol Microbiol. 68(5): 1216-1227.

by **Mark Viant** and colleagues:

- Tiziani S, Lodi A, Ludwig C, Parsons HM, Viant MR (2008). Effects of the application of different window functions and projection methods on processing of 1H J-resolved nuclear magnetic resonance spectra for metabolomics. Anal Chim Acta 610(1): 80-88.

- Xi Y, de Ropp JS, Viant MR, Woodruff DL, Yu P (2008). Improved identification of metabolites in complex mixtures using HSQC NMR spectroscopy. Anal Chim Acta 614(2): 127-133.
- Wu H, Southam AD, Hines A, Viant MR (2008). High throughput tissue extraction protocol for NMR and mass spectrometry based metabolomics. Anal. Biochem. 372, 204-212.

by **Eriks Kupce** and colleagues:

- Kupce E & Freeman R (2008). Hyperdimensional NMR spectroscopy. Progress in Nuclear Magnetic Resonance Spectroscopy 52(1): 22-30.

by **Andrew Peet** and colleagues:

- Davies NP, Wilson M, Harris LM, Natarajan K, Lateef S, Macpherson L, Sgouros S, Grundy RG, Arvanitis TN, Peet AC (2008). Identification and characterisation of childhood cerebellar tumours by in vivo proton MRS. NMR Biomed. 21(8): 908-918.

by **Claudia Blindauer** and colleagues:

- Blindauer CA (2008). Metallothioneins with unusual residues: Histidines as modulators of zinc affinity and reactivity. J Inorg Biochem 102(3): 507-521.

by **Alex Conner** and colleagues:

- Conner M, Hicks MR, Dafforn T, Knowles TJ, Ludwig C, Staddon S, Overduin M, Guenther UL, Thome J, Wheatley M, Poyner DR, Conner AC (2008). Functional and biophysical analysis of the C-terminus of the CGRP-receptor; a family B GPCR. Biochemistry 47, 8434-8444.

by **Ashley Martin**and colleagues:

- Ward DG, Nyangoma S, Joy H, Hamilton E, Wei W, Tselepis C, Steven N, Wakelam MJO, Johnson PJ, Ismail T, Martin A (2008). Proteomic profiling of urine for the detection of colon cancer. Proteome Science 6(19).

by **Christopher Thomas** and colleagues:

- Bingle LEH, Rajasekar KV, Muntaha S, Nadella V, Hyde EI, Thomas CM (2008). A single aromatic residue in transcriptional repressor protein KorA is critical for cooperativity with its co-regulator KorB. Mol. Microbiol. 70(6), 1502-1514.

2007 publications

by **Andrew Almond** and colleagues:

- Blundell,C.D., Mahoney,D.J., Cordell,M.R., Almond,A., Kahmann,J.D., Perczel,A., Taylor,J.D., Campbell,I.D., & Day,A.J. Determining the molecular basis for the pH-dependent interaction between the link module of human TSG-6 and hyaluronan. J. Biol. Chem. 282, 12976-12988 (2007)

by **Baz Jackson** and colleagues:

- Obiozo UM, Brondijk TH, White AJ, Boxel GV, Dafforn TR, White SA, Jackson JB. Substitution of tyrosine-146 in the dI component of proton-translocating transhydrogenase leads to reversible dissociation of the active dimer into inactive monomers. J Biol Chem. 282(50): 36434-36443 (2007)

by **Erics Kupce** and colleagues:

- Kupce,E. & Freeman,R. Compensated adiabatic inversion pulses: Broadband INEPT and HSQC. J. Magn Reson. 187, 258-265 (2007).
- Kupce,E. & Freeman,R. Fast multidimensional NMR by polarization sharing. Magn Reson. Chem. 45, 2-4 (2007).

by **Geoffrey Moore** and colleagues

- Whittaker,S.B.-M., Spence,G.R., Grossmann,J.G., Radford,S.E., & Moore,G.R. NMR analysis of the conformational properties of the trapped on-pathway folding intermediate of the bacterial immunity protein Im7. J. Mol. Biol. 366, 1001-1015 (2007).

by **Michael Overduin** and colleagues:

- Mahadev RK, Di Pietro SM, Olson JM, Payne GS, Overduin M (2007) Structure of Sla1p homology domain 1 and interaction with the NPFxD endocytic internalization motif. EMBO J, 26(7):1963-71.
- Knowles, T.J.; Bobat, S.; Jeeves, M.; Henderson I.R.; Overduin, M. (2007). Secondary structure and 1H, 13C and 15N resonance assignments of the Escherichia coli YaeT POTRA domain. Biomol NMR Assign. 1, 113-115.

by **Andrew Peet** and colleagues:

- Peet, Andrew C, Nigel P Davies, Lee Ridley, Marie-Anne Brundler, Dimitiris Kombogiorgas, Shaheen Lateef, Kal Natarajan, Spyros Sgouros, Lesley MacPherson, Richard G Grundy, Magnetic Resonance Spectroscopy suggests key differences in the metastatic behaviour of medulloblastoma. Eur J Cancer, 43, 1037-44, (2007).
- Kombogiorgas, D.; Sgouros, S.; Walsh, A.R.; Hockley, A. D.; Stevens, M.; Grundy, R.; Peet, A.; English, M.; Spooner, D. Outcome of children with posterior fossa medulloblastoma. A single institution experience over the decade 1994-2003. Diseases of the Childs Nervous System 23,: 399-405, (2007).
- Peet, A. C.; Lateef, S.; MacPherson, L.; Natarajan, K.; Sgouros, S.; Grundy, R.G.; Short Echo Time 1H Magnetic Resonance Spectroscopy of Childhood Brain Tumours. Diseases of the Childs Nervous System, 23, 163-169, (2007).
- Peet, Andrew C, Carmel McConville, Martin Wilson, Barry A Levine, Michelle Reed, Sara A Dyer, Emma C Edwards, Mary C Strachan, Dominic J McMullan, and Richard G Grundy, 1H Magnetic Resonance Spectroscopy identifies specific metabolite profiles associated with MYCN amplified and non-amplified tumour subtypes of neuroblastoma cell lines. NMR in Biomedicine,20, 692-700 (2007).

by **Mark Viant** and colleagues:

- Hines, G. S.; Oladiran, J. P.; Bignell, G. D.; Stentiford ; Viant, M. R. 2007. Direct Sampling of Organisms from the Field and Knowledge of their Phenotype: Key Recommendations for Environmental Metabolomics. Env. Sci. Technol. 41(9):3375-81.
- C.-Y. Lin, H. Wu, R. S. Tjeerdema and M. R. Viant, Evaluation of metabolite extraction strategies from tissue samples using NMR metabolomics. Metabolomics 3, 55-67 (2007).
- M. R. Viant, Metabolomics of aquatic organisms: the new omics on the block. Mar. Ecol. Prog. Series 332, 301-306 (2007).
- D. Southam, T. G. Payne, H. J. Cooper, T. N. Arvanitis, M. R. Viant. 2007. Dynamic range and mass accuracy of wide-scan direct infusion nano-electrospray fourier transform ion cyclotron resonance mass spectrometry-based metabolomics increased by the spectral stitching method. Anal. Chem. 79(12): 4595-4602.
- Rubtsov, D. V.; Jenkins, H.; Ludwig, C.; Easton, J.; Viant, M.R.; Guenther, U.L.; Griffin J.L.; Hardy, N. 2007. Proposed Reporting Requirements for the Description of NMR-based Metabolomics Experiments. Metabolomics 3(3): 223-229.

- Turner, M. A.; Viant, M.R.; Teh, S.J.; Johnson, M.L. 2007. Developmental rates, structural asymmetry and metabolic fingerprints of steelhead trout (Oncorhynchus mykiss) eggs incubated at two temperatures. Fish Physiol. Biochem. 33(1): 59-72.
- Parsons HM, Ludwig C, Gunther UL, Viant MR. 2007. Improved classification accuracy in 1- and 2-dimensional NMR metabolomics data using the variance stabilising generalised logarithm transformation. BMC Bioinformatics 8, Art. No. 234.
- Viant MR, Ludwig C, Rhodes SA, Gunther UL, Allaway D. 2007. Validation of a urine metabolome fingerprint in dog for phenotypic classification. Metabolomics 3(4): 453-463.

2006 publications

by **Andrew Almond** and colleagues:

- Blundell CD, Reed MA, Overduin M, Almond A. 2006. NMR spectra of oligosaccharides at ultra-high field (900 MHz) have better resolution than expected due to favourable molecular tumbling. Carbohydr Res. 341(12):1985-91.
- Blundell CD, Reed MA, & Almond A. Complete assignment of hyaluronan oligosaccharides up to hexasaccharides. Carbohydr. Res. 341, 2803-2815 (2006).
- Almond A, Deangelis PL & Blundell CD. Hyaluronan: the local solution conformation determined by NMR and computer modeling is close to a contracted left-handed 4-fold helix. J Mol Biol. 358, 1256-1269 (2006).
- Blundell CD, Deangelis PL & Almond A. Hyaluronan: the absence of amide-carboxylate hydrogen bonds and the chain conformation in aqueous solution are incompatible with stable secondary and tertiary structure models. Biochem. J. 396, 487-498 (2006).

by **Theo Arvanitis** and colleagues

- Reynolds, G M, M P Wilson, A C Peet, T N Arvanitis, “An algorithm for the automated quantitation of metabolites in in vitro NMR Signals”, Magnetic Resonance in Medicine, 56, 1211-1299, (2006). PMID171029227.

by **Ulrich Günther** and colleagues

- Mittag T, Franzoni L, Cavazzini D, Schaffhausen B, Rossi GL, Gunther UL. 2006 Retinol modulates site-specific mobility of apo-cellular retinol-binding protein to promote ligand binding. J Am Chem Soc. 128(30):9844-8.

by **Eva Hyde** and colleagues

- Rajasekar KV, Bingle LE, Thomas CM, Hyde EI. 2006. (1)H, (13)C and (15)N assignments of the KorA global transcriptional repressor protein from the low copy number IncP-1 plasmid, RK2. J Biomol NMR, 36:71.

by **Erics Kupce** and colleagues

- Kupce,E., Freeman,R., & John,B.K. Parallel acquisition of two-dimensional NMR spectra of several nuclear species. J. Am. Chem. Soc. 128, 9606-9607 (2006).

by **Geoffrey Moore** and colleagues

- Gsponer,J., Hopearuoho,H., Whittaker,S.B.-M., Spence,G.R., Moore,G.R., Paci,E., Radford,S.E., & Vendruscolo,M. Determination of an ensemble of structures representing the intermediate state of the bacterial immunity protein Im7. Proc. Natl. Acad. Sci. USA 103, 99-104 (2006).
- Le Duff,C.S., Whittaker,S.B.-M., Radford,S.E., & Moore,G.R. Characterisation of the conformational properties of urea-unfolded Im7: implications for the early stages of protein folding. J. Mol. Biol. 364, 824-835 (2006).

by **Michael Overduin** and colleagues:

- Cheever ML, Kutateladze TG, Overduin M. 2006. Increased mobility in the membrane targeting PX domain induced by phosphatidylinositol 3-phosphate. Protein Sci. 15(8):1873-82.
- Finkielstein CV, Overduin M, Capelluto DG. 2006 Cell migration and signaling specificity is determined by the phosphatidylserine recognition motif of rac1. J Biol Chem. 281(37):27317-26.
- Latysheva N, Muratov G, Rajesh S, Padgett M, Hotchin NA, Overduin M, Berditchevski F. Syntenin-1 is a new component of tetraspanin-enriched microdomains: mechanisms and consequences of the interaction of syntenin-1 with CD63. 2006 Mol Cell Biol, 26(20):7707-18.
- Lee, SA, J Kovacs, RV Stahelin, ML Cheever, M Overduin, TG Setty, C Burd, W Cho and TG Kutateladze (2006) Molecular Mechanism of membrane docking by the Vam7pPX domain, J Biol Chem 281(48):37091-101.
- Tokonzaba E, Capelluto DG, Kutateladze TG, Overduin M. 2006 Phosphoinositide, phosphopeptide and pyridone interactions of the Abl SH2 domain, Chem Biol Drug Design 67: 230-237.

by **Andrew Peet** and colleagues

- Arus, C.; Celda, B.; Dasmahaptra, S.; Dupplaw, D.; Gonzalez-Velez, H.; Van Huffel, S.; Lewis, P.; Lluch i Ariet, M.; Mier, M.; Peet, A.; Robles, M. On the Design of a web-based decision support system for brain tumour diagnosis using distributed agents, Proceedings of the 2006, IEEE/WIC/ACM International Conference on Web Intelligence and Intelligent Agent Technology, 0-7695-2749-3/06. (IF 0.82)

by **Mark Viant** and colleagues

- E. S. Rosenblum, R. S. Tjeerdema and M. R. Viant, Effects of Temperature on Host-Pathogen-Drug Interactions in Red Abalone, Haliotis rufescens, Determined by 1H NMR Metabolomics. Env. Sci. Technol. 40, 7077-7084 (2006).
- Viant, M.R.; Pincetich, C.A.; Hinton, D.E.; Tjeerdema, R.S. 2006. Toxic actions of dinoseb in medaka (Oryzias latipes) embryos as determined by in vivo 31P NMR, HPLC-UV and 1H NMR metabolomics. Aquat Toxicol. 76(3-4):329-42.
- Viant MR, Pincetich CA, Tjeerdema RS. 2006. Metabolic effects of dinoseb, diazinon and esfenvalerate in eyed eggs and alevins of Chinook salmon (Oncorhynchus tshawytscha) determined by (1)H NMR metabolomics.Aquat Toxicol. 77(4):359-71.
- Werner, I.; Viant, M. R. ; Rosenblum, E. S. ; Gantner, A. S. ; Tjeerdema R. S. ; Johnson, M. L. Cellular responses to temperature stress in steelhead trout (Onchorynchus mykiss) parr with different rearing histories. Fish Physiol. Biochem. 32, 261-273 (2006).
- Xi, Y. ; de Ropp, J. ; Viant, M. R. ; Woodruff, D. L. ; Yu, P. Automated Identification of Metabolites in Complex Mixtures by Pseudo-likelihood using 2D COSY NMR Spectroscopy. Metabolomics 2, 221-233 (2006).
- Lin, C.Y.; Viant, M. R.; Tjeerdema, R. S. Metabolomics: Methodologies and Applications in the Environmental Sciences. J. Pestic. Sci. 31, 245-251 (2006).

2005 publications

by **Ulrich Günther** and colleagues

- Dancea F, Günther U. 2005. Automated protein NMR structure determination using wavelet de-noised NOESY spectra. J Biomol NMR.33(3):139-52.
- Trbovic N, Dancea F, Langer T, Günther U. 2005. Using wavelet de-noised spectra in NMR screening. J Magn Reson.173(2):280-7.
- Nicoll AJ, Weston CJ, Cureton C, Ludwig C, Dancea F, Spencer N, Smart OS, Günther UL, Allemann RK. 2005. De novo design of a stable N-terminal helical foldamer. Org Biomol Chem. 3(24):4310-5.

by **Barry Levine** and colleagues

- Patchell VB, Gallon CE, Evans JS, Gao Y, Perry SV, Levine BA. 2005. The regulatory effects of tropomyosin and troponin-I on the interaction of myosin loop regions with F-actin. J Biol Chem. 280(15):14469-75.

by **Michael Overduin** and colleagues

- Brunecky R, Lee S, Rzepecki PW, Overduin M, Prestwich GD, Kutateladze AG, Kutateladze TG. 2005. Investigation of the binding geometry of a peripheral membrane protein. Biochemistry. 44(49):16064-71.
- Capelluto DG, Overduin M. 2005. Secondary structure, 1H, 13C and 15N resonance assignments and molecular interactions of the dishevelled DIX domain. J Biochem Mol Biol. 38(2):243-7.
- Lee SA, Eyeson R, Cheever ML, Geng J, Verkhusha VV, Burd C, Overduin M, Kutateladze TG. 2005. Targeting of the FYVE domain to endosomal membranes is regulated by a histidine switch. Proc Natl Acad Sci U S A. 102(37):13052-7.

by **Andrew Peet** and colleagues

- Peet, A.C.; Leach, M.O.; Pinkerton, C.R.; Price, P.; Williams, S.R.; Grundy, R.G. 2005. The development of functional imaging in the diagnosis, management and understanding of childhood brain tumours. Pediatr Blood Cancer. 44(2):103-13.

by **Mark Viant** and colleagues

- Rosenblum, E.S.; Viant, M.R.; Braid, B.M.; Moore, J.D.; Friedman, C.S.; Tjeerdema, R.S. 2005. Characterizing the Metabolic Actions of Natural Stresses in the California Red Abalone, Haliotis rufescens using 1H NMR Metabolomics. Metabolomics 1, 199-209
- Stentiford, G.D.; Viant, M.R.; Ward, D.G.; Johnson, P.J.; Martin, A.; Wenbin, W.; Cooper, H.J.; Lyons, B.P.; Feist SW. 2005. Liver tumors in wild flatfish: a histopathological, proteomic, and metabolomic study. OMICS.9(3):281-99.
- Viant, M.R.; Bundy, J.G.; Pincetich, C.A.; de Ropp, J.S.; Tjeerdema RS. 2005. NMR-Derived Developmental Metabolic Trajectories: An Approach for Visualizing the Toxic Actions of Trichloroethylene during Embryogenesis. Metabolomics. 1, 149-158
- Viant MR, Lyeth BG, Miller MG, Berman RF. 2005. An NMR metabolomic investigation of early metabolic disturbances following traumatic brain injury in a mammalian model. NMR Biomed.18(8):507-16.
- Harker HA, Viant MR, Keutsch FN, Michael EA, McLaughlin RP, Saykally RJ. 2005. Water Pentamer: Characterization of the Torsional-Puckering Manifold by Terahertz VRT Spectroscopy, J. Phys. Chem. A 109, 6483-6497.

© University of Birmingham 2015