

MARK R. VIANT
PhD CChem MRSC CPhys MInstP CBiol MSB

School of Biosciences
University of Birmingham
B15 2TT, U.K.

Phone: +44-(0)121-414-2219
Fax: +44-(0)121-414-5925
E-mail: M.Viant@bham.ac.uk

CURRENT RESEARCH INTERESTS

- Pioneering the application of metabolomics to the environmental sciences, in particular to discover molecular markers that are predictive of organism health and reproductive fitness, with relevance to biological-effects environmental monitoring and chemical risk assessment.
- Developing novel analytical methods in metabolomics, with a particular focus on high resolution Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry and 2-dimensional NMR spectroscopy, as well as developing bioinformatic strategies for the optimal processing of high dimensionality metabolomics datasets and automated metabolite identification.
- Leading the development of mass spectrometry based clinical metabolomics at the University of Birmingham, with particular emphasis on liver and heart surgery, inflammation biology and cancer, and with the goals to better understand the mechanistic basis of disease and to discover diagnostic markers.

ACADEMIC APPOINTMENTS

- **Professor of Metabolomics**, School of Biosciences, University of Birmingham, UK, 2010-present.
- **Director of NERC Biomolecular Analysis Facility - Metabolomics Node**, University of Birmingham, UK, 2009-present.
- **Adjunct Scientist, Mote Marine Laboratory**, Sarasota, Florida, USA, 2009-present.
- Reader in Metabolomics, School of Biosciences, University of Birmingham, UK, 2008-2010.
- NERC Advanced Fellow, School of Biosciences, University of Birmingham, UK, 2003-2008.
- Lecturer, University of California, Davis, USA, Fall Quarter 2002.
- Assistant Research Toxicologist (Research Faculty), University of California, Davis, USA, 2001-2003.
- Postdoctoral Researcher, Department of Environmental Toxicology, University of California, Davis, USA, 1999-2001.
- Postdoctoral Researcher, Department of Chemistry, University of California, Berkeley, USA, 1994-97.

EDUCATION

- Ph.D., Chemical Physics, University of Southampton, UK, October 1994. Dissertation: The investigation of long-range atom-ion interactions by microwave and millimeter wave spectroscopy. Advisor: Prof. Alan Carrington FRS CBE
- M.S., Avian Sciences (emphasis in Environmental Toxicology), University of California, Davis, USA, September 1999. Thesis: Analysis of the regulation of brain-derived neurotrophic factor mRNA expression in the developing avian hypothalamus. GPA: 4.0/4.0. Advisor: Dr. D. Michael Fry.
- B.Sc., Chemistry, 1st Class (Hons.), University of Southampton, UK, July 1991.

HONORS, AWARDS AND PROFESSIONAL QUALIFICATIONS

- NERC Advanced Fellowship (2003-08).
- Chartered Biologist, Institute of Biology (2002).
- Chartered Physicist, Institute of Physics (2001).
- Royal Commission for the Exhibition of 1851 Postdoctoral Research Fellowship (1994-96).
- Chartered Chemist, Royal Society of Chemistry (1994).
- British Petroleum Research Studentship (1991-94).
- David Runciman Boyd prize: awarded for outstanding performance to a student graduating in the honours school of Chemistry, University of Southampton, U.K. (1991).
- N. K. Adam prize: awarded to the best student in Chemistry in the second year exams for the degree of Bachelor of Science, University of Southampton, U.K. (1990).

- John Scott-Montagu prize: awarded for the best academic performance in Chemistry at the end of the first year of undergraduate study, University of Southampton, U.K. (1989).

PROFESSIONAL SERVICE

International service, related to expertise in metabolomics

- Director of national NERC Biomolecular Analysis Facility - Metabolomics Node (2009-present).
- Chair of Environmental Metabolomics Special Interest Group of the international Metabolomics Society (2009-present).
- Board of Directors of the international Metabolomics Society (2008-present).
- Co-chair of Environmental Context Working Group of the international Metabolomics Standards Initiative (2006-present).
- Invited expert in Metabolomics: Joint SETAC-SOT Pellston Workshop on Molecular Biology and Risk Assessment: Evaluation of the Potential Roles of Genomics in Regulatory Ecotoxicology, Pellston, Michigan, USA, 18th-22nd September 2005.
- Invited expert in Metabolomics: OECD/IPCS Workshop on Toxicogenomics, Kyoto, Japan, 13th-15th October 2004.
- Invited expert in Metabolomics: Joint SETAC-SOT Pellston Workshop on Emerging Molecular and Computational Approaches for Cross-Species Extrapolations, Portland, Oregon, USA, 18th-22nd July 2004.

Scientific leadership at the University of Birmingham

- Academic Lead of Organisms and Environment Research Theme, School of Biosciences (2010-present).
- Executive Management Board member for HWB-NMR Spectroscopy Facility (2010-present).
- Chair of Steering Group of Systems Science for Health initiative (2009-present).
- Executive Management Board member for AWM Science City Translational Medicine Program (2008-present).
- Scientific lead for metabolomics research service in the Functional Genomics Facility, School of Biosciences (2008-present).
- Member of the Advanced Mass Spectrometry Facility management committee (2005-present).

Related to publishing and reviewing

- Guest Editor for special issue of *Metabolomics* journal on 'Environmental Metabolomics' (2009).
- Member of NERC Peer Review College (2008-present).
- Editorial board of international journal *Environmental Toxicology and Chemistry* (3 yr term, 2007-09).
- Editorial board of international journal *Metabolomics* (2004-present).
- NIEHS reviewer: Chairperson of Special Emphasis Panel on Metabolomics (2003).
- Reviewed grant applications for multiple agencies including the NERC, BBSRC, EPSRC, Wellcome Trust, NIH, and the Danish Agency for Science, Technology and Innovation.
- Reviewed manuscripts for multiple journals including *Analytical Chemistry*, *Environmental Science and Technology*, *Molecular Systems Biology*, *Nature Biotechnology*, *Nature Protocols* and *Toxicological Sciences*.

Related to conferences

- Chair of Environmental Metabolomics Workshop at Metabolomics2010, the Annual International Conference of the Metabolomics Society, Amsterdam, The Netherlands, June 2010.
- Chair of Microbial and Environmental Metabolomics Session at the Fifth Annual International Conference of the Metabolomics Society, Edmonton, Canada, September 2009.
- Chair of Environmental Metabolomics Session at MetaboMeeting 2008, Lyon, France, April 2008.
- Co-chair of Environmental Metabolomics Session at the Third Annual International Conference of the Metabolomics Society, Manchester, UK, June 2007.
- Co-chair of NERC International Opportunity Workshop on Fish Toxicogenomics: Advancing Practical Implementation, Averoio, Portugal, May 2007.
- Organizing committee member: 5th UC Davis Conference for Environmental Health Science (2003).
- Organizing committee member: Metabolomics Workshop, UC Davis (2003).

PROFESSIONAL AFFILIATIONS

- Member of the Metabolomics Society (2005-present).
- Member of the Society of Biology (2002-present).
- Member of the Institute of Physics (2001-present).
- Member of the Society of Environmental Toxicology and Chemistry (2000-present).
- Member of the Royal Society of Chemistry (1994-present).

RESEARCH GRANTS IN UK

As Principal Investigator

- 2010-13 Is oxidative stress the principal mode of toxicity for metal oxide nanoparticles?, NERC (NE/H008764/1). **£616,275.**
- 2009-12 NERC Biomolecular Analysis Facility – Metabolomics Node, NERC (R8-H10-61). **£473,573.**
- 2009-12 Lipidomics: A novel approach for characterising environmental stress, NERC CASE Award from the Centre for Environment, Fisheries and Aquaculture Science. **£9,000.**
- 2009-09 Joint NIST/NERC environmental metabolomics intercomparison study, National Institute of Standards and Technology, US. **£1,600.**
- 2008-09 Automated metabolite identification and quantification using J-resolved NMR spectroscopy, BBSRC (BB/F016298/1). **£92,700.**
- 2007-07 Cellular Metabolism in Human Liver Transplants: An Assessment by FT-ICR Mass Spectrometry-based Metabolomics and in vivo Microdialysis, Pilot project funding from MRC/EPSRC Institutional Discipline Bridging Award to Birmingham. **£2,304.**
- 2007-07 Conjugated bilirubin study, Children's Liver Fund. **£500.**
- 2006-10 Diagnosing toxicant specific disruption of sexual development in wild fish using metabolomics, Environment Agency. **£10,000.**
- 2006-10 Diagnosing toxicant specific disruption of sexual development in wild fish using metabolomics (with C. Tyler et al., Exeter), NERC (NE/D002508/1). **£404,609** (of which £189,960 to Birmingham).
- 2005-08 Integrated metabolomic and transcriptomic studies of stress response mechanisms in flatfish liver, BBSRC CASE Award from the Centre for Environment, Fisheries and Aquaculture Science. **£11,700.**
- 2004-07 Application of metabolomics to the development of a predictive biomarker model for *Mytilus edulis*, NERC CASE Award from the Centre for Environment, Fisheries and Aquaculture Science. **£3,000.**
- 2003-08 Development of a predictive biomarker model for the marine and estuarine environments using state-of-the-art NMR-based metabolomics and bioinformatic techniques, NERC Advanced Fellowship (NER/J/S/2002/00618). **£296,740.**

As Co-Investigator

- 2011-15 INFLAME: Indoor contamination with flame retardant chemicals: Causes and impacts (with S. Harrad et al.), Marie Curie Initial Training Networks. **£3,150,000** (of which £555,081 to Birmingham).
- 2011-14 From Airborne Exposures to Biological Effects (FABLE): the impact of nanoparticles on health (with J. Ayres et al.), NERC-MRC (NE/I008314/1). **£1,514,271.**
- 2011-14 Lipid, sugar and protein biomarkers for ancient tuberculosis and leprosy (with G. Besra et al.), The Leverhulme Trust (F/00094/BL). **£172,984.**
- 2010-14 Manufactured nanomaterial bioavailability and environmental exposure (with J. R. Lead et al.), NERC-EPSRC (NE/H013148/1). **£1,252,224** (of which £704,485 to Birmingham).
- 2010-15 NUTRITOX: Challenges towards sustainable aquafeeds – Plant nutrient and contaminant interactions (with M.H.G. Berntssen et al., NIFES), Norwegian Research Council. 25.7M NOK (of which 300,000 NOK, ca. **£33,500** to Birmingham).
- 2010-12 The effects of metabolic manipulation on metabolomic profiling and adenosine triphosphate kinetics in left ventricular hypertrophy secondary to aortic stenosis (with D. Pagano et al.), British Heart Foundation (PG/10/036/28341). **£92,055.**

- 2010-10 Case for the development of a 5-10 year NERC Omics Strategy (NEOMICS) through community consultation (with D. Field, CEH, et al.), NERC, **£99,898** (of which £4,664 to Birmingham).
- 2009-10 Shared mechanisms of pathogenesis in Dystonia: Plasma biochemical profile in Dyt 1 dystonia using Fourier transform ion cyclotron resonance mass spectrometry in a metabolomics based study (with H. S. Pall), Dystonia Society's 25th Anniversary Competition. **£25,000**.
- 2008-18 Experimental medicine network of excellence - Science City Translational Medicine (with P. Stewart et al.), Advantage West Midlands, **£2,452,845**.
- 2008-12 Clinical research infrastructure and trials platforms - Science City Translational Medicine (with P. Stewart et al.), Advantage West Midlands, **£3,115,000**.
- 2008-12 HWB-NMR: a national resource for biomolecular research (with M. Overduin et al.), Wellcome Trust (083796), **£497,000**.
- 2008-08 New spectrometers for centres of excellence in biomedical research (with H. Cooper, U. Günther and M. Overduin et al.), The Wolfson Foundation, **£500,000**.
- 2008-09 Distinguishing toxic from adaptive responses in fish using "omics" – a key need for integration of toxicogenomics into environmental risk assessment (with J. K. Chipman et al.), NERC (NE/F008465/1). **£48,716**.
- 2008-09 Data mining and integration strategies for ecotoxicogenomics (with T. Ebbels et al., Imperial College), NERC (NE/F001398/1). **£164,642** (of which £6,301 to Birmingham).
- 2007-08 Purchase of a 600 MHz ACAS magnet and cryogenic probe for high throughput metabolomics and ligand discovery (with M. Overduin et al.), BBSRC REI (BB/E013198/1). **£255,686**.
- 2006-07 High throughput systems biology analysis, modelling and simulation of large biological data sets (with F. Falciani et al.), BBSRC REI (BB/D524624/1). **£108,488**.
- 2005-08 International Consortium on Fish Toxicogenomics (with J. K. Chipman et al.), NERC (NE/D000793/1). **£147,907**.
- 2005-08 Molecular and genomic ecotoxicology knowledge transfer for environmental chemical risk assessment (with J. K. Chipman et al.), NERC (NE/D000807/1). **£59,674**.
- 2005-06 Cryogenic probe for the Henry Wellcome Building for Biomolecular NMR Spectroscopy (with M. Overduin et al.), Wellcome Trust (077311). **£180,112**.
- 2005-08 Metabolic and transcriptional pathway inference using State Space models: An application to understanding acid response (with F. Falciani et al.), BBSRC (BB/C515104/1). **£257,512**.
- 2005-09 MOTET: Metabolomics and Oncology, Transfer of European Technology (with U Günther and C Bunce), EU 6th Framework Marie Curie Host Fellowships for the Transfer of Knowledge (MTKD-CT-2004-014434). **€10,534**.
- 2005-08 Identifying and defining the bases of individual and population susceptibility and adaptation to environmental pollutants in fish: An integrated 'omic' approach (with J. K. Chipman et al.), NERC (NE/C507661/1). **£1,582,008** (of which £492,761 to Birmingham).
- 2004-05 Establishment of a European High Throughput NMR Centre for Metabolomics and Ligand Discovery (with M. Overduin et al.), BBSRC REI (BB/C511513/1). **£200,000**.

RESEARCH GRANTS IN USA

As Principal Investigator

- 2003-05 Of Mice and Metabolomics: Quantifying Susceptibility to Endocrine Disruption (with M. G. Miller and J. L. Spearow, UC Davis), NIEHS Center for Environmental Health Sciences Pilot Projects Program. **\$29,443**.
- 2003-04 NMR-based Metabolomic Approach for Investigating Developmental Toxicity in Fish Embryos, UC Davis NMR Facility Award. **\$2,000**.
- 2002-03 The Identification of Novel Biomarkers for Early-Stage Withering Syndrome in Red Abalone using NMR-Based Metabonomics, UC Davis NMR Facility Award. **\$1,900**.

As Co-Investigator

- 2004-06 Acute and Chronic Effects of Crude Oil and Dispersed Oil on Chinook Salmon Smolts (with R. S. Tjeerdema, UC Davis), National Oceanic and Atmospheric Administration - University of New Hampshire Cooperative Institute for Coastal and Estuarine Environmental Technology. **\$150,000**.

- 2004-06 Influence of Temperature on the Pharmacokinetics and Efficacy of Oxytetracycline in RLP-Infected Abalone (with R. S. Tjeerdema, UC Davis, C. S. Friedman, University of Washington, and J. D. Moore, UC Davis Bodega Marine Laboratory), National Oceanic and Atmospheric Administration, U.S. Department of Commerce, National and California Sea Grant College Programs. **\$102,282.**
- 2003-05 Acute and Chronic Effects of Crude Oil and Dispersed Oil on Chinook Salmon Smolts (with R. S. Tjeerdema, UC Davis), UC Wildlife Health Center, Oiled Wildlife Care Network. **\$106,111.**
- 2001-03 Characterizing the Role of Environmental Stressors in the Development of Withering Syndrome in Red Abalone (with R. S. Tjeerdema and C. S. Friedman, UC Davis), National Oceanic and Atmospheric Administration, U.S. Department of Commerce, National and California Sea Grant College Programs. **\$166,395.**
- 2001-02 The Microbial Degradation of Pesticides Important to Rice Culture (with R. S. Tjeerdema and D. G. Crosby, UC Davis), UC Rice Research Board. **\$35,968.**
- 2001-02 Occurrence and Fate of the New Algal Toxin Azaspiracid in California Coastal Waters (with R. S. Tjeerdema and S. J. Gee, UC Davis), UC Toxic Substances Research & Teaching Program. **\$24,415.**
- 2000-01 The Microbial Degradation of Pesticides Important to Rice Culture (with R. S. Tjeerdema and D. G. Crosby, UC Davis), UC Rice Research Board. **\$27,010.**

PUBLICATIONS – PEER REVIEWED ARTICLES

In press

94. T. D. Williams, N. Turan, A. M. Diab, H. Wu, C. Mackenzie, K. L. Bartie, O. Hrydziusko, B. P. Lyons, G. D. Stentiford, M. J. Herbert, K. J. Abraham, I. Katsiadaki, M. J. Leaver, J. B. Taggart, S. G. George, **M. R. Viant**, J. K. Chipman, F. Falciani, A network biology approach to ecotoxicology reveals novel pathways linked to environmental chemical exposure. *PLoS Comp. Biol.* (in press).
93. I. Römer, T. A. White, M. Baalousha, J. K. Chipman, **M. R. Viant**, J. R. Lead, Aggregation and dispersion of silver nanoparticles in exposure media for aquatic toxicity tests. *J. Chromatogr. A* (in press).

Published

92. R. J. M. Weber, A. D. Southam, U. Sommer, **M. R. Viant**, 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 (2011).
91. A. D. Southam, A. Lange, A. Hines, E. M. Hill, Y. Katsu, T. Iguchi, C. R. Tyler, **M. R. Viant**, 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 (2011).
90. H. C. Poynton, N. S. Taylor, J. Hicks, K. Colson, S. Chan, C. Clark, L. Scanlan, A. V. Loguinov, C. Vulpe, **M. R. Viant**, Integration of metabolomic and transcriptomic signatures offers a coordinated model of cadmium toxicity in *Daphnia magna*. *Environ. Sci. Technol.* **45**, 3710-3717 (2011).
89. T. Knowles, D. Browning, M. Jeeves, R. Maderbocus, S. Rajesh, P. Sridhar, E. Manoli, D. Emery, U. Sommer, A. Spencer, D. Leyton, D. Squire, R. Chaudhuri, **M. R. Viant**, A. Cunningham, I. Henderson, M. Overduin, Structure and function of BamE within the outer membrane and the β -barrel assembly machine. *EMBO Reports* **12**, 123-128 (2011).
88. A. Lodi, S. Tiziani, F. L. Khanim, M. T. Drayson, U. L. Günther, C. M. Bunce, **M. R. Viant**, Treatment of acute myeloid leukemia cell lines with indomethacin in both hypoxic and non-hypoxic conditions results in generation of reactive oxygen species and deregulation of TCA cycle. *ACS Chem. Biol.* **6**, 169-175 (2011).
87. N. S. Taylor, R. J. M. Weber, T. A. White, **M. R. Viant**, Discriminating between different acute chemical toxicities via changes in the daphnid metabolome. *Toxicol. Sci.* **118**, 307–317 (2010).
86. R. J. M. Weber, **M. R. Viant**, MI-Pack: Increased confidence of metabolite identification in mass spectra by integrating accurate masses and metabolic pathways. *Chemometrics and Intelligent Laboratory Systems* **104**, 75-82 (2010).
85. A. R. Van Scoy, C. Y. Lin, B. S. Anderson, B. M. Philips, M. J. Martin, J. McCall, C. R. Todd, D. Crane, M. L. Sowby, **M. R. Viant**, R. S. Tjeerdema, Metabolic responses produced by crude versus

- dispersed oil in Chinook salmon pre-smolts via NMR-based metabolomics. *Ecotoxicol. Environ. Saf.* **73**, 710-717 (2010).
84. A. Hines, F. J. Staff, J. Widdows, R. Compton, F. Falciani, **M. R. Viant**, Discovery and validation of metabolic signatures for predicting whole organism toxicology. *Toxicol. Sci.* **115**, 369-378 (2010) – selected as **Highlight Article** for Issue 2 and in **Top 5 Papers** for 2010.
 83. I. Katsiadaki, T. D. Williams, J. Ball, T. P. Bean, H. Wu, E. M. Santos, M. M. Brown, P. Baker, F. Ortega, F. Falciani, J. A. Craft, C. R. Tyler, **M. R. Viant**, J. K. Chipman, Hepatic transcriptomic and metabolomic responses in the stickleback (*Gasterosteus aculeatus*) exposed to ethinyl-estradiol. *Aquat. Toxicol.* **97**, 174-187 (2010).
 82. O. Hrydziusko, M. A. Silva, M. T. P. R. Perera, D. A. Richards, N. Murphy, D. Mirza, **M. R. Viant**, Application of metabolomics to investigate the process of human orthotopic liver transplantation: A proof of principle study. *OMICS - Journal of Integrative Biology* **14**, 143-150 (2010).
 81. A. J. Sinclair, **M. R. Viant**, A. K. Ball, M. A. Burdon, E. A. Walker, P. M. Stewart, S. Rauz, S. P. Young, NMR-based metabolomic analysis of cerebrospinal fluid and serum in neurological diseases - A diagnostic tool? *NMR in Biomedicine* **23**, 123-132 (2010).
 80. J. M. Easton, L. M. Harris, **M. R. Viant**, A. C. Peet, T. N. Arvanitis, Linked Metabolites: A tool for the construction of directed metabolic graphs. *Comput. Biol. Med.* **40**, 340-349 (2010).
 79. E. M. Santos, J. S. Ball, T. D. Williams, H. Wu, F. Ortega, R. van Aerle, I. Katsiadaki, F. Falciani, **M. R. Viant**, J. K. Chipman, C. R. Tyler, Identifying health impacts of exposure to copper using transcriptomics and metabolomics in a fish model. *Environ. Sci. Technol.* **44**, 820-826 (2010).
 78. G. van Aggelen, G. T. Ankley, W. S. Baldwin, D. W. Bearden, W. H. Benson, J. K. Chipman, T. W. Collette, J. A. Craft, N. D. Denslow, M. R. Embry, F. Falciani, S. G. George, C. C. Helbing, P. F. Hoekstra, T. Iguchi, Y. Kagami, I. Katsiadaki, P. Kille, L. Liu, P. G. Lord, T. McIntyre, A. O'Neill, H. Osachoff, E. J. Perkins, E. M. Santos, R. C. Skirrow, J. R. Snape, C. R. Tyler, D. Versteeg, **M. R. Viant**, D. C. Volz, T. D. Williams, L. Yu, Integrating omic technologies into aquatic ecological risk assessment and environmental monitoring: Hurdles, achievements and future outlook. *Environmental Health Perspectives* **118**, 1-5 (2010).
 77. C. Ludwig, **M. R. Viant**, Two-dimensional *J*-resolved NMR spectroscopy: Review of a key methodology in the metabolomics toolbox. *Phytochemical Analysis* **21**, 22-32 (2010).
 76. F. L. Khanim, R. E. Hayden, J. Birtwistle, A. Lodi, S. Tiziani, N. J. Davies, J. P. Ride, **M. R. Viant**, U. L. Günther, J. C. Mountford, H. Schrewe, R. M. Green, J. A. Murray, M. T. Drayson and C. M. Bunce, Combined bezafibrate and medroxyprogesterone acetate: Potential novel therapy for acute myeloid leukaemia. *PLoS ONE* **4**, e8147 (2009).
 75. C. Y. Lin, B. S. Anderson, B. M. Phillips, A. C. Peng, S. Clark, J. Voorhees, H.-D. I. Wu, M. J. Martin, J. McCall, C. R. Todd, F. Hsieh, D. Crane, **M. R. Viant**, M. L. Sowby, R. S. Tjeerdema, Characterization of the metabolic actions of crude versus dispersed oil in salmon smolts via NMR-based metabolomics. *Aquat. Toxicol.* **95**, 230-238 (2009).
 74. T. K. Karakach, R. Knight, E. M. Lenz, **M. R. Viant**, J. A. Walter, Analysis of time course ¹H NMR metabolomics data by multivariate curve resolution. *Magn. Reson. Chem.* **47**, S105-S117 (2009).
 73. H. M. Parsons, C. Ludwig, **M. R. Viant**, 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. Chem.* **47**, S86-S95 (2009).
 72. C. Ludwig, D. G. Ward, A. Martin, **M. R. Viant**, T. Ismail, P. J. Johnson, M. J. O. Wakelam, U. L. Günther, Fast targeted multidimensional NMR metabolomics of colorectal cancer. *Magn. Reson. Chem.* **47**, S68-S73 (2009).
 71. S. He, X. Li, **M. R. Viant**, X. Yao, Profiling mass spectrometry proteomics data using Smoothed Nonlinear Energy Operator and Bayesian Additive Regression Trees. *Proteomics* **9**, 4176-4191 (2009).
 70. T. D. Williams, H. Wu, E. M. Santos, J. Ball, I. Katsiadaki, M. M. Brown, P. Baker, F. Ortega, F. Falciani, J. A. Craft, C. R. Tyler, J. K. Chipman and **M. R. Viant**, Hepatic transcriptomic and metabolomic responses in the stickleback (*Gasterosteus aculeatus*) exposed to environmentally relevant concentrations of dibenzanthracene. *Environ. Sci. Technol.* **43**, 6341-6348 (2009).
 69. T. G. Payne, A. D. Southam, T. N. Arvanitis, **M. R. Viant**, A signal filtering method for improved quantification and noise discrimination in Fourier transform ion cyclotron resonance mass spectrometry-based metabolomics data. *J. Amer. Soc. Mass Spectrom.* **20**, 1087-1095 (2009).

68. N. S. Taylor, R. J. M. Weber, A. D. Southam, T. G. Payne, O. Hrydziusko, T. N. Arvanitis, **M. R. Viant**, A new approach to toxicity testing in *Daphnia magna*: Application of high throughput FT-ICR mass spectrometry metabolomics. *Metabolomics* **5**, 44-58 (2009).
67. J. G. Bundy, M. P. Davey, **M. R. Viant**, Environmental metabolomics: A critical review and future perspectives. *Metabolomics* **5**, 3-21 (2009).
66. S. Tiziani, A. Lodi, F. L. Khanim, **M. R. Viant**, C. M. Bunce, U. L. Günther, Metabolomic profiling of drug responses in acute myeloid leukaemia cell lines. *PLoS ONE* **4**, e4251 (2009).
65. H. M. Parsons, D. R. Ekman, T. W. Collette, **M. R. Viant**, Spectral relative standard deviation: A practical benchmark in metabolomics. *The Analyst* **134**, 478-485 (2009).
64. **M. R. Viant**, D. W. Bearden, J. G. Bundy, I. W. Burton, T. W. Collette, D. R. Ekman, V. Ezernieks, T. K. Karakach, C. Y. Lin, S. Rochfort, J. S. de Ropp, Q. Teng, R. S. Tjeerdema, J. A. Walter, H. Wu, International NMR-based Environmental Metabolomics Intercomparison Exercise. *Environ. Sci. Technol.* **43**, 219-225 (2009).
63. A. D. Southam, J. M. Easton, G. D. Stentiford, C. Ludwig, T. N. Arvanitis, **M. R. Viant**, Metabolic changes in flatfish hepatic tumours revealed by NMR-based metabolomics and metabolic correlation networks. *J. Proteome Res.* **7**, 5277-5285 (2008).
62. T. C. Hawes, A. Hines, **M. R. Viant**, J. S. Bale, M. R. Worland, P. Convey, Metabolomic fingerprint of cryo-stress in a freeze-tolerant insect. *Cryoletters* **29**, 505-515 (2008).
61. **M. R. Viant**, Recent developments in environmental metabolomics. *Molecular Biosystems* **4**, 980-986 (2008).
60. S. Tiziani, A.-H. Emwas, A. Lodi, C. Ludwig, C. M. Bunce, **M. R. Viant** and U. L. Günther, Optimised Metabolite Extraction from Blood Serum for ¹H Nuclear Magnetic Resonance Spectroscopy. *Anal. Biochem.* **377**, 16-23 (2008).
59. Y. Xi, J. S. de Ropp, **M. R. Viant**, D. L. Woodruff and P. Yu, Improved Screening for Metabolites in Complex Mixtures using HSQC NMR Spectroscopy. *Anal. Chim. Acta* **614**, 127-133 (2008).
58. S. Tiziani, A. Lodi, C. Ludwig, H. M. Parsons and **M. R. Viant**, Effects of the application of different window functions to processing of ¹H J-resolved NMR spectra for metabolomics. *Anal. Chim. Acta* **610**, 80-88 (2008).
57. H. Wu, A. D. Southam, A. Hines and **M. R. Viant**, High throughput tissue extraction protocol for NMR and mass spectrometry based metabolomics. *Anal. Biochem.* **372**, 204-212 (2008).
56. **M. R. Viant**, C. Ludwig, S. Rhodes, U. L. Günther and D. Allaway, Validation of a urine metabolome fingerprint in dog for phenotypic classification. *Metabolomics* **3**, 453-463 (2007).
55. G.-C. Lee, J. de Ropp, **M. R. Viant**, D. L. Woodruff and P. Yu, Heuristic Search for 2D NMR Alignment to Support Metabolite Identification, *Lecture Notes In Computer Science* **4614**, 447-458 (2007).
54. A. Hines, W. H. Yeung, J. Craft, M. Brown, J. Kennedy, J. Bignell, G. D. Stentiford and **M. R. Viant**, Comparison of Histological, Genetic, Metabolomic and Lipid-based Methods for Sex Determination in Marine Mussels. *Anal. Biochem.* **369**, 175-186 (2007).
53. S.-A. Sansone, D. Schober, H. J. Atherton, O. Fiehn, H. Jenkins, P. Rocca-Serra, D. V. Rubtsov, I. Spasic, L. Soldatova, C. Taylor, A. Tseng and **M. R. Viant**, Metabolomics Standards Initiative: Ontology Working Group work in progress. *Metabolomics* **3**, 249-256 (2007).
52. D. V. Rubtsov, H. Jenkins, C. Ludwig, J. Easton, **M. R. Viant**, U. Guenther, J. L. Griffin and N. Hardy, Proposed Reporting Requirements for the Description of NMR-based Metabolomics Experiments. *Metabolomics* **3**, 223-229 (2007).
51. L. W. Sumner, A. Amberg, D. Barrett, M. H. Beale, R. Beger, C. A. Daykin, T. W.-M. Fan, O. Fiehn, R. Goodacre, J. L. Griffin, T. Hankemeier, N. Hardy, J. Harnly, R. Higashi, J. Kopka, A. N. Lane, J. C. Lindon, P. Marriott, A. W. Nicholls, M. D. Reily, J. J. Thaden and **M. R. Viant**, Proposed Minimum Reporting Standards for Chemical Analysis. *Metabolomics* **3**, 211-221 (2007).
50. N. Morrison, D. Bearden, J. G. Bundy, T. Collette, F. Currie, M. P. Davey, N. S. Haigh, D. Hancock, O. A. H. Jones, S. Rochfort, S.-A. Sansone, D. Štys, Q. Teng, D. Field and **M. R. Viant**, Standard Reporting Requirements for Biological Samples in Metabolomics Experiments: Environmental Context. *Metabolomics* **3**, 203-210 (2007).

49. H. M. Parsons, C. Ludwig, U. L. Günther and **M. R. Viant**, Improved classification accuracy in 1- and 2-dimensional NMR metabolomics data using the variance stabilising generalised logarithm transformation. *BMC Bioinformatics* **8**, 234 (2007).
48. R. E. Blunt, K. A. Walsh, D. K. Ashton, **M. R. Viant** and J. K. Chipman, Knowledge Transfer Initiative between Molecular Biologists and Environmental Researchers and Regulators. *Environ. Sci. Pollut. Res.* **14**, 293-296 (2007).
47. A. D. Southam, T. G. Payne, H. J. Cooper, T. N. Arvanitis, **M. R. Viant**, Dynamic range and mass accuracy of wide-scan direct infusion nanoelectrospray Fourier transform ion cyclotron resonance mass spectrometry-based metabolomics increased by the spectral stitching method. *Anal. Chem.* **79**, 4595-4602 (2007).
46. A. Hines, G. S. Oladiran, J. P. Bignell, G. D. Stentiford and **M. R. Viant**, Direct Sampling of Organisms from the Field and Knowledge of their Phenotype: Key Recommendations for Environmental Metabolomics. *Env. Sci. Technol.* **41**, 3375-3381 (2007).
45. M. A. Turner, **M. R. Viant**, S. J. Teh and M. L. Johnson, Developmental rates, structural asymmetry and metabolic fingerprints of steelhead trout (*Oncorhynchus mykiss*) eggs incubated at two temperatures. *Fish Physiol. Biochem.* **33**, 59-72 (2007).
44. 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).
43. **M. R. Viant**, Metabolomics of aquatic organisms: the new omics on the block. *Mar. Ecol. Prog. Series* **332**, 301-306 (2007).
42. Y. Xi, J. de Ropp, **M. R. Viant**, D. L. Woodruff and Ping Yu, Automated Identification of Metabolites in Complex Mixtures by Pseudo-likelihood using 2D COSY NMR Spectroscopy. *Metabolomics* **2**, 221-233 (2006).
41. 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).
40. I. Werner, **M. R. Viant**, E. S. Rosenblum, A. S. Gantner, R. S. Tjeerdema and M. L. Johnson, Cellular responses to temperature stress in steelhead trout (*Oncorhynchus mykiss*) parr with different rearing histories. *Fish Physiol. Biochem.* **32**, 261-273 (2006).
39. C.-Y. Lin, **M. R. Viant** and R. S. Tjeerdema, Metabolomics: Methodologies and Applications in the Environmental Sciences. *J. Pestic. Sci.* **31**, 245-251 (2006).
38. **M. R. Viant**, C. A. Pincetich and R. S. Tjeerdema, Metabolic effects of dinoseb, diazinon and esfenvalerate in eyed eggs and alevins of Chinook salmon (*Oncorhynchus tshawytscha*) determined by ¹H NMR metabolomics. *Aquat. Toxicol.* **77**, 359-371 (2006).
37. **M. R. Viant**, C. A. Pincetich, D. E. Hinton and R. S. Tjeerdema, 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**, 329-342 (2006).
36. **M. R. Viant**, B. G. Lyeth, M. G. Miller and R. F. Berman, An NMR Metabolomic Investigation of Early Metabolic Disturbances Following Traumatic Brain Injury in a Mammalian Model, *NMR in Biomedicine* **18**, 507-516 (2005).
35. G. D. Stentiford, **M. R. Viant**, D. G. Ward, P. J. Johnson, A. Martin, W. Wei, H. J. Cooper, B. P. Lyons and S. W. Feist, Liver Tumours in Wild Flatfish: A Histopathological, Proteomic and Metabolomic Study, *OMICS - Journal of Integrative Biology* **9**, 281-299 (2005).
34. H. A. Harker, **M. R. Viant**, F. N. Keutsch, E. A. Michael, R. P. McLaughlin and R. J. Saykally, Water Pentamer: Characterization of the Torsional-Puckering Manifold by Terahertz VRT Spectroscopy, *J. Phys. Chem. A* **109**, 6483-6497 (2005).
33. E.S. Rosenblum, **M. R. Viant**, B. M. Braid, J. D. Moore, C. S. Friedman and R. S. Tjeerdema, Characterizing the Metabolic Actions of Natural Stresses in the California Red Abalone, *Haliotis rufescens* using ¹H NMR Metabolomics, *Metabolomics* **1**, 199-209 (2005).
32. **M. R. Viant**, J. G. Bundy, C. A. Pincetich, J. S. de Ropp and R. S. Tjeerdema, NMR-Derived Developmental Metabolic Trajectories: An Approach for Visualizing the Toxic Actions of Trichloroethylene during Embryogenesis, *Metabolomics* **1**, 149-158 (2005).

31. C. A. Pincetich, **M. R. Viant**, D. E. Hinton and R. S. Tjeerdema, Metabolic Changes in Japanese Medaka (*Oryzias latipes*) during Embryogenesis and Hypoxia as determined by *in vivo* ³¹P NMR, *Comp. Biochem. Physiol. C* **140**, 103-113 (2005).
30. K. R. Schmelzer, C. S. Johnson, **M. R. Viant**, J. F. Williams and R. S. Tjeerdema, Influence of Organic Carbon on Reductive Dechlorination of Thiobencarb in California Rice Field Soils, *Pest Manag. Sci.* **61**, 68-74 (2005).
29. P. L. TenBrook, **M. R. Viant**, D. M. Holstege, J. F. Williams and R. S. Tjeerdema, Characterization of California Rice Field Soils Susceptible to Delayed Phytotoxicity Syndrome, *Bull. Environ. Contam. Toxicol.* **73**, 448-456 (2004).
28. P. V. Purohit, D. M. Rocke, **M. R. Viant** and D. L. Woodruff, Discrimination Models using Variance Stabilizing Transformation of Metabolomic NMR Data, *OMICS - Journal of Integrative Biology* **8**, 118-130 (2004).
27. **M. R. Viant**, I. Werner, E. S. Rosenblum, A. S. Gantner, R. S. Tjeerdema and M. L. Johnson, Correlation Between Heat-Shock Protein Induction and Reduced Metabolic Condition in Juvenile Steelhead Trout (*Oncorhynchus mykiss*) Chronically Exposed to Elevated Temperature, *Fish Physiol. Biochem.* **29**, 159-171 (2003).
26. **M. R. Viant**, E. S. Rosenblum and R. S. Tjeerdema, NMR-Based Metabolomics: A Powerful Approach for Characterizing the Effects of Environmental Stressors on Organism Health, *Env. Sci. Technol.* **37**, 4982-4989 (2003).
25. **M. R. Viant**, Improved Methods for the Acquisition and Interpretation of NMR Metabolomic Data, *Biochem. Biophys. Res. Comm.* **310**, 943-948 (2003).
24. P. L. TenBrook, S. M. Kendall, **M. R. Viant** and R. S. Tjeerdema, Toxicokinetics and Biotransformation of *p*-Nitrophenol in Red Abalone (*Haliotis rufescens*), *Aquat. Toxicol.* **62**, 329-336 (2003).
23. J. R. Millam, C. B. Craig-Veit, M. E. Batchelder, **M. R. Viant**, T. M. Herbeck and L. W. Woods, An Avian Bioassay for Environmental Estrogens: The Growth Response of Zebra Finch (*Taeniopygia guttata*) Chick Oviduct to Oral Estrogens, *Environ. Toxicol. Chem.* **21**, 2663-2668 (2002).
22. **M. R. Viant**, C. A. Pincetich, J. H. Walton, R. S. Tjeerdema and D. E. Hinton, Utilizing *in vivo* Nuclear Magnetic Resonance Spectroscopy to Study Sublethal Stress in Aquatic Organisms, *Mar. Environ. Res.* **54**, 553-557 (2002).
21. **M. R. Viant**, J. H. Walton, P. L. TenBrook and R. S. Tjeerdema, Sublethal Actions of Copper in Abalone (*Haliotis rufescens*) as Characterized by *in vivo* ³¹P NMR, *Aquat. Toxicol.* **57**, 139-151 (2002).
20. A. E. Quaglino, C. B. Craig-Veit, **M. R. Viant**, A. L. Erichsen, D. M. Fry and J. R. Millam, Oral Estrogen Masculinizes Female Zebra Finch Song System, *Horm. Behav.* **41**, 236-241 (2002).
19. **M. R. Viant**, E. S. Rosenblum and R. S. Tjeerdema, Optimized Method for the Determination of Phosphoarginine in Abalone Tissue by High-performance Liquid Chromatography, *J. Chromatogr. B* **765**, 107-111 (2001).
18. **M. R. Viant**, J. H. Walton and R. S. Tjeerdema, Comparative Sublethal Actions of 3-Trifluoromethyl-4-nitrophenol in Marine Molluscs as Measured by *in vivo* ³¹P NMR, *Pestic. Biochem. Physiol.* **71**, 40-47 (2001).
17. F. N. Keutsch, R. S. Fellers, M. G. Brown, **M. R. Viant**, P. B. Petersen and R. J. Saykally, Hydrogen Bond Breaking Dynamics of the Water Trimer in the Translational and Librational Band Region of Liquid Water, *J. Am. Chem. Soc.* **123**, 5938-5941 (2001).
16. F. N. Keutsch, R. S. Fellers, **M. R. Viant** and R. J. Saykally, Far-infrared laser VRT Spectroscopy of Water Clusters in the Librational Band Region of Liquid Water, *J. Chem. Phys.* **114**, 4005-4015 (2001).
15. **M. R. Viant**, J. R. Millam, M. E. Delany and D. M. Fry, Regulation of Brain-derived Neurotrophic Factor mRNA Levels in Avian Hypothalamic Slice Cultures, *Neuroscience* **99**, 373-380 (2000).
14. M. G. Brown, **M. R. Viant** and R. J. Saykally, Far Infrared Laser VRT Spectroscopy of Water Clusters, Proceedings of the 1997 NATO Advanced Study Institute Conference on *Recent Theoretical and Experimental Advances in Hydrogen Bonded Clusters*, Heraklion, Crete, Greece, S. S. Xantheas (Ed.), pp. 101-108 (2000).
13. M. G. Brown, **M. R. Viant**, R. P. McLaughlin, C. J. Keoshian, J. D. Cruzan, R. J. Saykally and A. van der Avoird, Quantitative Characterization of the Water Trimer Torsional Manifold by Terahertz Laser Spectroscopy and Theoretical Analysis: (H₂O)₃, *J. Chem. Phys.* **111**, 7789-7800 (1999).

12. **M. R. Viant**, M. G. Brown, J. D. Cruzan, R. J. Saykally, M. Geleijns and A. van der Avoird, Quantitative Characterization of the (D₂O)₃ Torsional Manifold by Terahertz Laser Spectroscopy and Theoretical Analysis, *J. Chem. Phys.* **110**, 4369-4381 (1999).
11. J. D. Cruzan, **M. R. Viant**, M. G. Brown, D. D. Lucas, K. Liu and R. J. Saykally, Terahertz Laser Vibration-rotation-tunneling Spectrum of the Water Pentamer-d10: Constraints on the Bifurcation Tunneling Dynamics, *Chem. Phys. Lett.* **292**, 667-676 (1998).
10. **M. R. Viant**, J. D. Cruzan, D. D. Lucas, M. G. Brown, K. Liu and R. J. Saykally, Pseudorotation in Water Trimer Isotopomers using Terahertz Laser Spectroscopy, *J. Phys. Chem. A* **101**, 9032-9041 (1997).
9. J. D. Cruzan, **M. R. Viant**, M. G. Brown and R. J. Saykally, Terahertz Laser Vibration-rotation-tunneling Spectroscopy of the Water Tetramer, *J. Phys. Chem. A* **101**, 9022-9031 (1997).
8. K. Liu, M. G. Brown, **M. R. Viant**, J. D. Cruzan and R. J. Saykally, Far-infrared VRT Spectroscopy of two Water Trimer Isotopomers: Vibrationally Averaged Structures and Rearrangement Dynamics, *Mol. Phys.* **89**, 1373-1396 (1996).
7. K. Liu, R. S. Fellers, **M. R. Viant**, R. P. McLaughlin, M. G. Brown and R. J. Saykally, A Long Path Length Pulsed Slit Valve Appropriate for High Temperature Operation: Infrared Spectroscopy of Jet-cooled Large Water Clusters and Nucleotide Bases, *Rev. Sci. Instrum.* **67**, 410-416 (1996).
6. **M. R. Viant**, R. S. Fellers, R. P. McLaughlin and R. J. Saykally, Infrared Laser Spectroscopy of Uracil in a Pulsed Slit Jet, *J. Chem. Phys.* **103**, 9502-9505 (1995).
5. A. Carrington, J. M. Hutson, M. M. Law, C. A. Leach, A. J. Marr, A. M. Shaw and **M. R. Viant**, Microwave Spectroscopy and Interaction Potential of the Long-range He...Ar⁺ Ion, *J. Chem. Phys.* **102**, 2379-2403 (1995).
4. A. Carrington, C. A. Leach, A. J. Marr, C. H. Pyne, A. M. Shaw, **M. R. Viant** and Y. D. West, Near-dissociation Microwave Spectra of Rare-gas Diatomic Ions, *Chem. Phys. Lett.* **212**, 473-479 (1993).
3. A. Carrington, C. A. Leach and **M. R. Viant**, Nuclear Hyperfine Structure in the Electronic Millimeter Wave Spectrum of H₂⁺, *Chem. Phys. Lett.* **206**, 77-82 (1993).
2. A. Carrington, C. A. Leach, R. E. Moss, T. C. Steimle, **M. R. Viant** and Y. D. West, Microwave Electronic Spectroscopy, Electric Field Dissociation and Photofragmentation of the H₂⁺ Ion, *J. Chem. Soc. Faraday Trans.* **89**, 603-614 (1993).
1. A. Carrington, R. A. Kennedy, C. A. Leach, A. J. Marr, I. R. McNab, R. E. Moss, C. H. Pyne, **M. R. Viant** and Y. D. West, Spectroscopy of HD⁺ in High Angular Momentum States, *Chem. Phys.* **166**, 145-166 (1992).

PUBLICATIONS – BOOK CHAPTERS

6. **M. R. Viant**, Environmental metabolomics using ¹H NMR spectroscopy, In: *Environmental Genomics. Methods in Molecular Biology*, Volume 410, (Ed. C. C. Martin), Chapter 9, Humana Press Inc., Totowa, NJ (2008).
5. C. R. Tyler, A. L. Filby, T. Iguchi, V. J. Kramer, J. Larsson, G. van Aggelen, K. van Leeuwen, **M. R. Viant**, D. E. Tillitt, Application of Genomics to Tiered Testing, In: *Genomics in Regulatory Ecotoxicology: Applications and Challenges* (Eds. G. T. Ankley, A. L. Miracle, E. J. Perkins, G. P. Daston), Chapter 3, CRC Press (2008).
4. **M. R. Viant**, C. Ludwig and U. L. Günther, 1D and 2D NMR Spectroscopy: from Metabolic Fingerprinting to Profiling, In: *Metabolomics, Metabonomics and Metabolic Profiling* (Ed. W. J. Griffiths), Chapter 2, RSC Publishing, Cambridge, UK (2008).
3. S. A. Sansone, M. D. Waters and **M. R. Viant**, Databases and standardisation of reporting methods for metabolic studies, In: *The Handbook of Metabonomics and Metabolomics* (Eds. John C. Lindon, Jeremy K. Nicholson and Elaine Holmes), Chapter 8, Elsevier, Amsterdam (2007).
2. **M. R. Viant**, Revealing the Metabolome of Animal Tissues Using ¹H Nuclear Magnetic Resonance Spectroscopy, In: *Metabolomics: Methods and Protocols. Methods in Molecular Biology*, Volume 358, (Ed. W. Weckwerth), Chapter 13, Humana Press Inc., Totowa, NJ (2007).
1. J. C. Cook, N. D. Denslow, T. Iguchi, E. A. Linney, A. Miracle, J. R. Shaw, **M. R. Viant** and T. R. Zacharewski, "Omics" Approaches in the Context of Environmental Toxicology, In: *Genomic Approaches for Cross-Species Extrapolation in Toxicology* (Eds. W. H. Benson and R. T. Di Giulio), Chapter 1, CRC Press (2007).

INVITED TALKS

International level

- ‘Predicting the reproductive fitness of *Daphnia magna* from metabolic signatures’, SETAC Europe Annual Meeting, Milan, Italy, 16th May 2011.
- **Keynote speaker** - ‘Integrating metabolomics with physiology: Towards ‘Systems Toxicology’’, 3rd Norwegian National Environmental Toxicology Symposium, Bergen, Norway, 14th-16th April 2010.
- ‘Toxicity screening in *Daphnia magna* for ecological risk assessment: Application of FT-ICR mass spectrometry based metabolomics’, Fifth Annual International Conference of The Metabolomics Society, Edmonton, Canada, 30th Aug-2nd Sept 2009.
- ‘High mass accuracy and resolution: Key specifications in mass spectrometry based metabolomics’, Fifth Annual International Conference of The Metabolomics Society, Edmonton, Canada, 30th Aug-2nd Sept 2009.
- ‘FT-ICR mass spectrometry based metabolomics provides insight into the liver cancer metabolome’, The Second Maga Circe Conference on “Metabolomics and Cancer”, Anzio, Italy, May 14th 2009.
- ‘Novel methods for assessing toxicity in *Daphnia magna*: Application of mass spectrometry-based metabolomics’, Research seminar, University of California, Berkeley, USA, 8th September 2008.
- ‘Environmental metabolomics: Is it living up to expectations?’, Research seminar, University of California, Davis, USA, 3rd September 2008.
- ‘Background variability in the mussel metabolome’, NERC International Workshop On Fish Toxicogenomics “Moving into monitoring and regulation”, Vancouver, Canada, 21st-23rd April 2008.
- ‘International NMR-based environmental metabolomics intercomparison exercise’, NERC International Workshop On Fish Toxicogenomics “Moving into monitoring and regulation”, Vancouver, Canada, 21st-23rd April 2008.
- ‘What can metabolic profiling offer environmental toxicology?’, 11th International Congress of Toxicology, Montreal, Canada, July 16th 2007.
- ‘From peaks to knowledge: Interpreting multivariate metabolic models’, Third Annual International Conference of The Metabolomics Society, Manchester, UK, 11th-14th June 2007.
- ‘Environmental Metabolomics: Applications of NMR and mass spectrometry’, European Commission Workshop on Omics and the Environment, JRC, Ispra, Italy, 8th March 2007.
- ‘Development of FT-ICR mass spectrometry based metabolomics’, Advances in Metabolic Profiling, London, UK, 19th October 2006.
- ‘Characterising the stress responses of aquatic organisms using metabolomics’, 24th Annual Meeting of the European Society of Comparative Physiology and Biochemistry, Antwerp, Belgium, 17th September 2006.
- ‘Applications of NMR spectroscopy and advanced mass spectrometry in environmental metabolomics’, Princeton ACS 2006 Seminar Series, Princeton University, New Jersey, USA, 22nd June 2006.
- ‘Applications of metabolomics to aquatic toxicology’, Invited Seminar, NRC Institute of Marine Biosciences, Halifax, Nova Scotia, Canada, 30th May 2006.
- ‘Applications of NMR spectroscopy and advanced mass spectrometry in environmental metabolomics’, 89th Canadian Chemistry Conference, Halifax, Nova Scotia, Canada, 29th May 2006.
- ‘Comparison of experimental strategies in NMR metabolomics: Limitations and solutions’, 26th Annual Meeting of the Society of Environmental Toxicology and Chemistry, Baltimore, Maryland, USA, 13th-17th November 2005.
- ‘What can metabolomics offer chemical risk assessment?’, Joint SETAC-SOT Pellston Workshop on Molecular Biology and Risk Assessment: Evaluation of the Potential Roles of Genomics in Regulatory Ecotoxicology, Pellston, Michigan, USA, 18th-22nd September 2005.
- ‘The Nuts & Bolts of NMR Metabolomics: from Sample Preparation to Spectral Processing’, Training Workshop on Metabolomics & Nutrition, Trinity Centre for Health Sciences, St. James’s Hospital, Dublin, Ireland, 11th January 2005.
- ‘Environmental Metabolomics’, OECD/IPCS Workshop on Toxicogenomics, Kyoto, Japan, 14th October 2004.

National level

- ‘Using metabolite signatures to predict whole organism traits of ecological importance’, Towards a Systems Biology Approach to Ecotoxicology workshop, University of Birmingham, UK, 19th January 2011.
- ‘Integrating metabolomics with physiology: Towards "Systems Ecotoxicology"', Joint BES/SEB/BS Stress Responses conference, London, UK, 7th January 2011.
- ‘Can metabolomic signatures predict molecular and whole animal toxicity? A fundamental challenge in environmental biomarker research’, International Seminar Series, University of Manchester, UK, 4th March 2010.
- ‘The new NERC metabolomics facility: Enabling the study of toxic effects on the metabolome’, NERC SOFI Marine Environment and Human Health workshop, Cefas, Weymouth, UK, 8-9th February 2010.
- ‘NERC facility for environmental metabolomics research’, British Ecological Society Annual Meeting, University of Hertfordshire, UK, 9th September 2009.
- ‘Metabolomics: A useful tool for measuring environmental stress in marine invertebrates?’, Invited seminar, Plymouth Marine Laboratory, Plymouth, UK, 5th June 2009.
- ‘Environmental and genetic influences on the mussel metabolome: a field study’, Ecological Genetics Group Annual Meeting, University of Warwick, UK, 2nd April 2009.
- ‘Novel methods for assessing toxicity in *Daphnia magna*: Application of FT-ICR mass spectrometry-based metabolomics’, Invited seminar, University of Exeter, UK, 19th March 2009.
- ‘Metabolomics: A useful tool for measuring environmental stress?’, Invited seminar, University of Hull, UK, 15th October 2008.
- ‘An optimised SIM-stitching approach for FT-ICR mass spectrometry based metabolomics’, Thermo User Meeting, London, UK, 19th June 2007.
- ‘Optimised analytical and bioinformatic methods for FT-ICR mass spectrometry based metabolomics: a SIM-stitching approach’, RSC/BMSS Meeting - Emerging Mass Spectrometry Technologies for the Biosciences, Jealott’s Hill International Research Centre, UK, 13th February 2007.
- ‘Metabolomics of aquatic wildlife: Trials, tribulations and the need for optimised data processing’, MetaboMeeting 3, Imperial College, London, UK, 18th December 2006.
- ‘Using metabolomics to assess organism health: Successes, technical advances and remaining challenges’, Invited Seminar, School of Pharmacy, University of London, London, 29th March 2006.
- ‘Application of fast 2-dimensional NMR methods for classification of cancer’, MetaboMeeting 1.0, Cambridge, UK, 18th-19th July 2005.
- ‘Applications of metabolomics to aquatic toxicology and disease’, Invited Seminar, Plymouth Marine Laboratory, Plymouth, 25th January 2005.
- ‘Metabolomics: what, how and why, and its application to aquatic toxicology and disease’, Invited Seminar, Brunel University, UK, 9th December 2004.
- ‘Applications of Metabolic Fingerprinting for the Diagnosis of Environmental Diseases’, The Consortium for Post-Genome Science, 2nd Conference on ‘Genomes to Systems’, Manchester, UK, 2nd September 2004.
- ‘Environmental Metabolomics’, Invited Seminar, Exeter University, UK, 2nd June 2004.
- ‘Metabolomics: A Powerful Technique for Phenotyping the Biochemical Changes Associated with Disease and Toxic Insult’, Invited Seminar, Centre for Environment, Fisheries and Aquaculture Science, Weymouth Laboratory, UK, 5th January 2004.
- ‘The Nuts and Bolts of NMR-Based Metabolomics’, 5th Annual UC Davis Conference for Environmental Health Scientists, The Embassy Suites, Napa, California, USA, August 25th 2003 (based in US at the time).
- ‘Metabolomics: A Novel Method for Rapidly Assessing an Organism’s Response to a Toxic Insult’, Friends of Environmental Toxicology Day, University of California, Davis, USA, May 30th 2003 (based in US at the time).
- ‘Effects of Sublethal Copper Exposure on Red Abalone Measured by *In Vivo* ³¹P NMR Spectroscopy’, Friends of Environmental Toxicology Day, University of California, Davis, USA, May 13th 2000 (based in US at the time).
- ‘Far-infrared Laser Vibration-rotation-tunneling Spectroscopy of Water Clusters’, Department of Chemistry and Biochemistry, Arizona State University, USA, April 15th 1996 (based in US at the time).

RESEARCH STUDENT AND POSTDOCTORAL RESEARCHER SUPERVISION

Postdoctoral research fellow supervision

- 2011-12 Dr. Ralf Weber (BHF)
2011-13 Dr. Nadine Taylor (NERC)
2010-13 Dr. Eva Zelena (University supported)
2010-13 Dr. Jennifer Kirwan (University supported)
2009-12 Dr. Jonathan Byrne (NERC)
2009-12 Dr. Ulf Sommer (NERC)
2009-13 Dr. Andrew Southam (NERC & LLR)
2009-10 Dr. Anja Woiciechowsky (EU)
2008-10 Dr. John Carrigan (EU)
2008-09 Dr. Adam Hines (NERC)
2008-09 Dr. Huanhuan Chen (BBSRC)
2006-09 Dr. Alessia Lodi (EU)
2006-09 Dr. Stefano Tiziani (EU)
2006-07 Dr. Louisa Alfazema (NERC)
2005-07 Dr. Abdul-Hamid Emwas (EU)
2005-08 Dr. Huifeng Wu (NERC)

PhD student supervision

- 2011-14 Jinkang Zhang, EU (co-supervisor).
2010-13 Kate Duffy, University supported (co-supervisor).
2010-13 Alex Gavin, NERC (co-supervisor).
2009-12 Tom White, NERC (primary supervisor).
2008-11 Stefania Clemente, NERC (primary supervisor).
2007-11 Olga Hrydziuszko, University of Birmingham (primary supervisor).
2007-10 Dr. Ralf Weber, Darwin Trust (primary supervisor). Thesis title - *Increased confidence of metabolite identification in high-resolution mass spectra using prior biological and chemical knowledge-based approaches.*
2006-10 Dr. Nadine Taylor, NERC (primary supervisor). Thesis title - *Novel approaches to toxicity testing in Daphnia magna.*
2006-10 Dr. Tristan Payne, EPSRC (co-supervisor). Thesis title - *Prolonging the metabolome using Fourier transform ion cyclotron resonance mass spectrometry, optimised signal processing, noise filtering and constraint satisfaction methods.*
2005-09 Dr. Helen Parsons, NERC/EPSRC (primary supervisor). Thesis title - *Optimised spectral processing and lineshape analysis in 2-dimensional J-resolved NMR spectroscopy based metabolomics.*
2005-09 Dr. Paul Eccles, NERC (co-supervisor). Thesis title - *Examining the suitability of molecular and metabolomic-based techniques as tools for assessing the effects of pharmaceuticals in the aquatic environment.*
2005-09 Dr. Andrew Southam, BBSRC CASE (primary supervisor). Thesis title - *The molecular characterisation of flatfish hepatic tumours by metabolomics and transcriptomics.*
2004-09 Dr. John Easton, EPSRC (co-supervisor). Thesis title - *Optimised analysis and visualisation of metabolic data using graph theoretical approaches.*
2004-08 Dr. Adam Hines, NERC CASE (primary supervisor). Thesis title - *The development and evaluation of NMR based metabolomics as a tool for environmental monitoring using the common mussel.*

PhD examining (internal and external)

- 2011 Dr. Felicity Currie, University of Manchester (Prof. Roy Goodacre's group)
2011 Dr. Alex Da Silva Couto Alves, Imperial College London (Dr. Tim Ebbel's group)
2010 Dr. Huw Jones, University of Birmingham (Prof. Kevin Chipman's group)
2010 Dr. Emma Wharfe, University of Manchester (Prof. Roy Goodacre's group)

- 2010 Dr. Ladan Mirbahai, University of Birmingham (Dr. Andrew Peet's group)
- 2009 Dr. Julia Fabrega-Climent, University of Birmingham (Prof. Jamie Lead's group)
- 2009 Mr. Russell Compton, University of Birmingham (Dr. Francesco Falciani's group)
- 2009 Mr. Will Tuffnail, University of Portsmouth (Dr. Richard Greenwood's group)
- 2009 Dr. Andrew Creese, University of Birmingham (Dr. Helen Cooper's group)
- 2008 Dr. Anel Flores, University of Sussex (Dr. Elizabeth Hill's group)
- 2007 Dr. Michael Silva, University of Birmingham (Prof. David Adam's group)
- 2006 Dr. Marie Brown, University of Manchester (Prof. Douglas Kell's group)
- 2006 Dr. Edward Clayson, University of Cambridge (Prof. Kevin Brindle's group)

TEACHING EXPERIENCE

Course development (University of Birmingham)

- MSc Analytical Genomics – Developed substantial component of module on 'omics analysis' (2008).
- MSc Toxicology – Member of Exam Board, contributing to annual course review (2003-present).

Lecturing (University of Birmingham)

- PhD, School of Biosciences – Core concepts course on metabolomics, 2005-present.
- PhD, School of Medicine – Lecture on metabolomics, 2005.
- PhD, School of Engineering – Lecture on metabolomics, 2005.
- MSc Analytical Genomics – Lectures and lab practicals on metabolomics, 2008-present.
- MSc Molecular Biotechnology – Lectures and laboratory practicals on metabolomics, 2010-present.
- MSc Clinical Oncology – Metabolomics, 2007-present.
- MSc Toxicology – Lectures on metabolomics; lectures and laboratory practicals on statistics; NMR/MS laboratory demonstration, 2003-present.
- BSc BIO107 Enzymes and Metabolism – Metabolomics, 2010.
- BSc BIO331 Omics – Metabolomics, 2004-present.

Tutor groups (University of Birmingham)

- MSc Toxicology (2003-present).
- BSc Biochemistry (2009-present).

Complete courses taught at University of California, Davis, USA

- ETX 220 - Analysis of Toxicants (Graduate class).
Co-instructed with Prof. Judi Charles. Fall Quarter 2002.

Guest lectures presented at University of California, Davis, USA

Presented series of lectures on metabolomics, NMR spectroscopy and environmental toxicology:

- PTX 203 – Principles of Pharmacology and Toxicology (Graduate class), May 2003.
- EAD 289D - Statistical Bioinformatics (Graduate class), February 2003.
- MGT 281 - Systems Analysis and Design (Professional class), October 2002.
- ETX 10 - Introduction to Environmental Toxicology (Undergraduate class), May 2000-2003.

PUBLIC SERVICE AND OUTREACH

- 'Metabolomics – A New Tool for Environmental Toxicologists'. Talk presented at the 30-year anniversary of the MSc Toxicology course, University of Birmingham, April 2010.
- 'The fat of the land'. Article published in NERC Planet Earth, Spring 2009.
<http://planetearth.nerc.ac.uk/features/story.aspx?id=331>
- BBC Radio 4 science programme 'Material World' on subject of metabolomics, 10th July 2008.
http://www.bbc.co.uk/radio4/science/thematerialworld_20080710.shtml
- BBC World Service science programme 'Changing World - Mapping Pollution', July 2006.
<http://www.thechangingworld.org/archives/wk45.php>

- ‘Environmental Metabolomics: The Study of Disease and Toxicity in Wildlife’. Article published on www.ActionBioscience.org, an educational resource of the American Institute of Biological Sciences, January 2006. <http://www.actionbioscience.org/genomic/viant.html>
- BBC Television and Radio 4 Interview concerning chemical contamination of Volvic mineral water, October 2005. http://news.bbc.co.uk/2/hi/programmes/working_lunch/4371780.stm
- ‘Metabolomics: Is it just another omics?’. Article published in Biotechnology News (Issue 48), distributed by the University of Birmingham to promote and stimulate interest in Biotechnology and the Life Sciences, Autumn 2004. <http://www.biotech.bham.ac.uk/BTNews48/Metabolomics.htm>

PERSONAL DEVELOPMENT COURSES

- ‘Communicating science to the public’, 2-day course provided by NERC, June 2009.
- ‘Business Mind Mapping’, 1-day course provided by Illumine Training, October 2008. Including training on improving creativity, planning more effectively, improving memory, and raising workplace effectiveness.
- ‘Research Team Leadership’, 2-day course provided by the Leadership Foundation for Higher Education, September 2007. Included training on vision, listening, teams, leadership, meetings and motivation.
- ‘Supervising students’, Staff Development Unit, Birmingham, October 2004.
- ‘Academic, academic related and research staff development review training’, Staff Development Unit, Birmingham, September 2004.
- ‘Managing your time’, Staff Development Unit, Birmingham, April 2004.