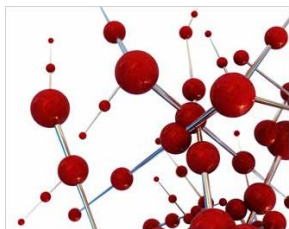


MANCHESTER
1824



MIB Newsletter

April/May 2011

Research News
Funding News
Congratulations
Seminars
Events / Symposia
Publications



More news and information about the MIB can be found on our website:

<http://www.mib.ac.uk/>

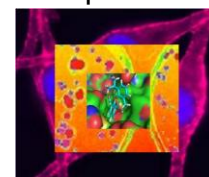
and in the [MIB brochure](#) available online



Research News

The Manchester Chemical Biology Network is launched

The new Manchester Chemical Biology Network was launched on 19th May in the Manchester Interdisciplinary Biocentre. Funded by the Research Councils (EPSRC, BBSRC and MRC) and with commitments from its 10 industrial partners, the network aims to provide a cross-disciplinary forum to unite researchers from across the chemical, biological and medical sciences with end users. This collaboration between research groups will provide a more effective platform to tackle the major challenges associated with discovery of new drugs and other products, of importance to human health and well being, using expertise ranging from synthetic chemistry through to cell biology. Over the initial 2 years of funding the network will host a number of meetings, researcher exchanges and pump prime funding for novel collaborations.



For more information please see the [MCBN website](#)

The launch event, led by Jason Micklefield, showcased work from across the network with talks from across the University (FEPS, FLS and FMHS) and from AstraZeneca, GSK, Pfizer, Syngenta and Imagen Biotech. More than 100 scientists and industry leaders attended the launch at the Manchester Interdisciplinary Biocentre – which has become a focal point for collaborative research across the physical and biological sciences. Talks from the event will shortly be available on the website.

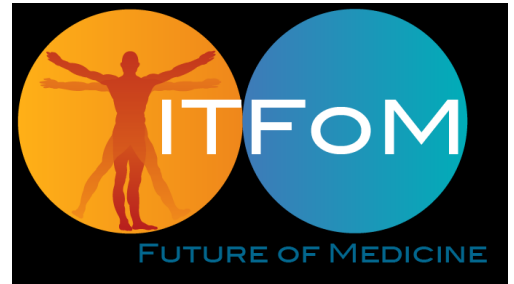


IT Future of Medicine (ITFoM)

The European Future Technologies (FET) Conference and Exhibition 2011 held in Budapest on 4 May 2011 will mark the official launch of the futuristic FET Flagship Initiatives by Neelie Kroes, European Commissioner for the European Digital Agenda. FET Flagships are large-scale, science driven and mission oriented initiatives that aim to achieve visionary technological goals. The scale of ambition will be over 10 years of coordinated effort, with a budget of up to one billion Euros for each of two Flagships. To prepare the

launch of the FET Flagships, six Pilot Actions will be funded with 1.5 million Euros each for a 12-month period starting in May 2011; in the second half of 2012, two of the Pilots will be selected and launched as full FET Flagship Initiatives in 2013.

As one of the six Pilot Actions, the **Information Technology Future of Medicine (ITFoM)** project brings together 26 partners and 20 associated members including academic institutes and private companies from 15 different countries. “They are like The Human Genome projects in which we participated”, says Hans Lehrach, Director at the Max Planck Institute for Molecular Genetics and The



Dahlem Centre for Genome Research and Medical Systems Biology in Berlin, Germany. Professor Lehrach is coordinator of the shortlisted ITFoM project, which aims to revolutionise our health care system. ITFoM In the past, innovation in Information and Communications Technology (ICT) and computing has been primarily driven by the requirements of “large” physics and a broad spectrum of commercial applications such as entertainment; medicine has played a relatively minor role. This, however, is set to change as the growing demands of data-rich, individualised medicine are likely to surpass those of all other ICT development fields. As data-intensive analysis and computer intensive modeling become common clinical practice, ICT capacity and organisation will become key limiting factors in medicine; this will result in a shift of resources from personnel-intensive to ICT-intensive applications. Clinical needs will be the driving force behind future ICT innovation. Data-rich, individualised medicine poses unprecedented challenges for ICT - in terms of hardware, storage and communication. Making personalised medicine a reality will thus require fundamental advances in the computational sciences. It is with this in mind that ITFoM brings together world leading research groups from across Europe and beyond. ITFoM proposes a medicine based on computer models (‘virtual patients’) derived from molecular, physiological, anatomical and environmental data generated on every individual patients. These ‘virtual patients’ will then be used to identify individually optimised prevention/therapy schedules, minimising potential side effects of treatment regimes.

To develop this ICT-driven medicine of the future, ITFoM will prepare for the amalgamation of four major areas:

- The first is medicine itself - from specimen analysis and diagnosis provision to clinical practice and patient consent;
- The second concerns analytical techniques, covering functional genomics and imaging technology analyses on a routine basis;
- The third focuses on integration, developing tools required to incorporate the gathered clinical data, and generated analytical data into models that will inform relevant health providers;
- The fourth area involves the ICT developments required to tackle the immense computational challenges.

Professor **Hans Westerhoff** and members of the [Manchester Centre for Integrative Systems Biology](#) at The University of Manchester are leading the integration work package. This is the first time that the ICT implications of worldwide-individualised patient care will be addressed in combination with genomics and medical requirements. Academic groups from a range of research backgrounds will join forces with their industry-based colleagues in making this proposal a reality. These research backgrounds include: exploring the potential of novel computing architectures; probabilistic programming languages; information processing paradigms; mathematical methods to model the complexity of biological systems; statistical machine learning methods to predict probable patient responses to

combinations of drugs; and algorithms to search for optimal combinations of complex interacting therapies.

The ultimate goals of ITFoM are twofold:

- The first goal is to give each patient's doctor the power to analyse a person's human genome at every stage of disease management – through diagnosis, treatment and follow-up. This will require a revolution in ICT technologies so that relevant computing, storage, networking and modeling technologies are developed;
- The second goal is to enable the connection of high throughput biomolecular characterization and clinical imaging technologies. Beneficiaries of this linkage will include: the patient and their doctor; drug researchers in both the discovery and development phases; epidemiologists attempting to analyse health trends; and policy- and decision-makers developing effective national and EU-wide health policy options and legislation. Enabling this connection will require a revolution in integrated information management and decision-making. This constitutes a fundamental transformation of biomedical science – from probability-based and empirical to evidence-based and knowledge-driven. The project outcomes will enable the prediction of health, disease, therapy and its effects for individual patients and through application in the clinic will change the future of medicine.

Web : www.ITFoM.eu

Royal Society of Chemistry's Ronald Belcher Award

Congratulations to **Paul Bassan** (Gardner research group) who has been awarded the very prestigious Royal Society of Chemistry's Ronald Belcher Award for his work on "*The scattering of IR radiation from biological cells and the development of a correction algorithm to remove the effects of resonant Mie scattering from IR spectra*".

This work has transformed the field of biomedical IR spectroscopy. In addition to the medal and £500, Paul has been invited to deliver a lecture at the Analytical Research Forum meeting to be held at the University of Manchester on 25-27th July 2011.

This is a fantastic achievement for a student who has not yet obtained his PhD! For further information see RSC [website](#)

Intellectual Property Awareness Resource

UMIP – the University's intellectual property (IP) commercialisation company would like to make you aware of its IP Awareness Resource, co-developed with Eversheds LLP. The resource is targeted at academics and research staff and its aim is to increase the awareness of IP and demonstrate the benefits of its commercialisation to the University and the IP generator.

You will find a series of video clips by professionals and academic colleagues on various aspects of IP and its commercialisation. We hope that this resource gives you a valuable insight into the types of IP which can be used to protect novel ideas/inventions and how, for example, IP can be commercialised via spin-out or licence with the help of UMIP. Also featured is information on IP and Academic Materials and IP within a research contract and consulting environment with links to various forms, process guides and booklets which you may find useful.

www.manchester.ac.uk/ipresource

Funding News

BBSRC and MRC Industrial CASE Studentships 2011/12

BBSRC's call for proposals for Industrial CASE Studentships is now open. Potential

applicants should check the BBSRC website at <http://www.bbsrc.ac.uk/business/training/industrial-case.aspx> for the latest information.

MRC Industrial CASE Scheme

<http://www.mrc.ac.uk/Fundingopportunities/Studentships/IndustrialCASE/MRC004608>

The closing date for both submissions is Thursday **28 July 2011**.

BBSRC Fellowship Schemes 2011/12

BBSRC's call for proposals for the following fellowship schemes will open shortly:

- David Phillips Fellowships
- Industrial Impact Fellowships

Potential applicants should keep an eye on the BBSRC website at <http://www.bbsrc.ac.uk> for full details when they become available. BBSRC is also intending to launch a new flexible award scheme to replace its other fellowships, further information will be available later this year.

The closing date for fellowship proposals in the above schemes is scheduled to be Tuesday 6 September 2011.

If you are interested in applying for a fellowship hosted in the MIB – please see our [website](#) for more details of the new **MIB research Career track fellowship** opportunities

BBSRC Industry Interchange Programme:

Short term exchange of researchers between the science base and industry

Industry Interchange Programme supports the short-term exchange, in either direction, of researchers between the science base and industry. The objective of the programme is to support interchanges that provide strategic advantage to the UK science base and industry arising from reciprocal access to facilities, expertise and/or knowledge, and an increased understanding of scientific issues of common concern. Individual awards are unlikely to exceed around £50,000.

The closing date for applications is 19 July 2011. Please note this will be the last round in this programme's current form. BBSRC will be developing a new flexible people movement scheme for launch later in the year. Application forms and further details can be found at: <http://www.bbsrc.ac.uk/business/people-information/industry-interchange.aspx> or by contacting Anuj Bhatt, Email: anuj.bhatt@bbsrc.ac.uk , Tel: 01793 413390

BBSRC Doctoral Training Partnerships

BBSRC has launched its call for 'Doctoral Training Partnerships' - a revision and development of its Quota Doctoral Training Grant scheme. The revised approach will retain many elements of the previous Quota PhD funding programme, but feature increased engagement between BBSRC and host institutions. The scheme will invest more than £60M in world class PhD training for student intakes in 2012, 2013 and 2014.

IMPORTANT: As highlighted on the BBSRC website (see link below) there will be a briefing meeting in central London on Thursday 23 June 2011. All potential applicants are strongly advised to register their attendance at this one day event. Numbers may become restricted so please sign up as soon as possible. To register your interest in attending, please email: darren.pirt@bbsrc.ac.uk

As with the Quota scheme, funding for BBSRC Doctoral Training Partnerships (DTPs) will

still be awarded competitively, with training excellence in strategically-important areas of bioscience the fundamental basis of any award. BBSRC will continue to fund all studentships at a full four-year duration and will expect its Doctoral Training Partners to further promote interdisciplinary and interdepartmental training.

The Doctoral Training Partnership (DTP) programme will, however, fund a smaller number of larger, institutional or multi-institutional partnerships, compared to the previous Quota scheme, which primarily awarded training grants at departmental or faculty level. These larger partnerships will enable greater coordination in the provision of specialist training and will benefit from closer working with BBSRC and its Training Awards Committee. The total number of studentships funded through the DTP scheme (220-30 p.a.) will be reduced compared to the existing Quota scheme, but funding for each student's experimental costs will increase to £5,000 p.a. to better support the research training costs of each studentship. Students funded under the DTP programme will also be required to participate in a three month professional internship during their PhD in order to widen their experience of different careers in which their research training can have an impact

Full details are available on the BBSRC website at: <http://www.bbsrc.ac.uk/dtp> Closing date for proposals: mid-September 2011 (date tbc)

Euroscience Young Researchers Award

The call for applications for the European Young Researchers' Award (EYRA) is currently open

The European Young Researchers' Award (EYRA) is granted to researchers demonstrating outstanding research performance as well as deep insight of the European Research Area. The award aims to inspire early stage researchers and experienced researchers to think 'European' by incorporating the European level into their research.

The Award is granted each year but the prize-giving-ceremony is held every two years at the Euroscience Open Forum (ESOF) where the two recipients will present their work. The Award consists of a Medal and a Certificate. A part of the award will be monetary in the form of a travel and accommodation grant for the stay in the ESOF city.

Full information can be found at <http://www.euroscience.org/eyra-2011,38531,en.html>

Enquires should be addressed to Dr Gail Cardew, Vice President, Euroscience: telephone 0207 670 2978; email gail@ri.ac.uk

Policy Framework on Research Data

EPSRC have set out their expectations concerning the management and provision of access to EPSRC-funded research data. The framework was implemented 1st May. Expectations to note include:

- Published research papers should include a short statement describing how and what terms any supporting research data may be accessed.
- Data that is not generated in digital format will be stored in a manner to facilitate it being shared in the event of valid request for access
- Appropriately structures metadata is published (normally within 12 months of the data being generated) and made freely accessible on the internet.
- Where access to data is restricted the published metadata should give the reason and summarise conditions which would satisfy access (for example commercially confidential data and a non-disclosure agreement).
- Data is preserved for a minimum of 10 years.

For further info: <http://www.epsrc.ac.uk/about/standards/researchdata/Pages/default.aspx>

Research Councils – Changes to requests for equipment

Following the RCUK report Efficiency 2011-15: Ensuring Excellence with Impact, additional guidance has been issued relating to requests for equipment included on proposals submitted to the Research Councils.

All proposals submitted to BBSRC, NERC, MRC and EPSRC must now follow the revised guidance. The necessary changes to the Je-S system have not yet been made, and so the provides information on how to apply in the interim. Similar measures may also be applied to any grants awarded after 1 May 2011.

NERC - <http://www.nerc.ac.uk/funding/news/researchgrants.asp>

BBSRC - <http://www.bbsrc.ac.uk/funding/apply/grants-guide.aspx>

EPSRC - <http://www.epsrc.ac.uk/newsevents/news/2011/Pages/equipmentfunding.aspx>

MRC – information to be updated

BBSRC – Bioinformatics and biological resources fund

Bioscience researchers have a continuing and growing need for access to state-of-the-art bioinformatics and biological resources:

- For bioinformatic resources (e.g. databases, software suites), there is a need to enable the management, analysis and sharing of large and/or complex datasets.
- For biological resources, access to materials that underpin cutting edge bioscience research is required e.g. culture and germplasm collections, mutant lines, DNA samples, clones, genetic libraries etc.

Yet issues remain around the provision of these infrastructures:

- Resources may already exist but are not readily available (e.g. funded by our project grants)
- Resources may have been established as a community resource for a fixed term and require more sustainable funding
- Researchers may need a resource that does not currently exist
- Existing resources may require development if they are to meet the needs of the UK bioscience community

Grants are available for up to 5 years to provide high quality, accessible, community resources that meet key UK needs.

Applications for biological resources may have a bioinformatics element included (e.g. to facilitate accessibility). Deadline: end of June (TBC)

Further info: [Website](#)

Funding Deadlines & Links

NERC <http://www.nerc.ac.uk/>

EPSRC <http://www.epsrc.ac.uk/default.htm>

BBSRC <http://www.bbsrc.ac.uk/funding/index.html> - next deadline 25th October 2011

MRC <http://www.mrc.ac.uk/index.htm>

Wellcome Trust <http://www.wellcome.ac.uk/Funding/Biomedical-science/index.htm>

ESRC <http://www.esrc.ac.uk/ESRCInfoCentre/index.aspx>

Core Facilities

TRANSCRIPTOMICS FACILITY

The transcriptomic Facility houses an Affymetrix Gene Suite, a CombiMatrix DNA synthesizer, a Roche LightCycler® 480 real-time qPCR instrument and quality control facilities to enable screening and accurate measurement of genes, transcripts and miRNAs.

Affymetrix Microarray Platform The Affymetrix™ GeneChip Expression Arrays are amongst the most widely used arrays for expression profiling, providing robust data with outstanding reproducibility. There is a large list of 3' arrays available covering model organisms. In addition to the 3' arrays the Gene and Exon Arrays enable researchers to analyze gene expression and gene regulation in high detail. Applications include case/control comparison studies, time course experiments, investigation of molecular mechanisms regulated by alternative splicing, discovery of new splice variants and discovery of disease-related deregulation of splicing.

CombiMatrix CustomArray® For a fully customisable approach the CombiMatrix B3 CustomArray® Synthesizer allows manufacture of high quality slide arrays for low (4x2K), medium (12K) or high (90K) density microarrays. Arrays are manufactured through in-situ synthesis, no spotting or printing is involved avoiding the inherent problems associated with these methods. Arrays can be re-used multiple times making them a cost effective choice. Easy to use software provides complete freedom to design the array of your choice. Applications include genome-wide and focused gene expression, SNP genotyping, comparative genomic hybridization (CGH), Tiling, ChIP-on-chip, miRNA, and resequencing. It can also be used to interrogate molecular interactions.

Real-Time PCR The LightCycler® 480 Real-Time PCR System is used for highly accurate qualitative and quantitative detection of nucleic acids and genotyping. The Universal Probe Library (UPL) contains 165 (90 routinely held in house) pre-validated, dual labelled fluorescent probes that can be used to quantify virtually any transcript (95-99%) from a multitude of organisms. Specificity is determined through the combination of sequence specific primers and one probe. Applications include targeted gene expression profiling and endpoint genotyping

For further information please contact: [Philip Day](#) on 2751621; or [Fiona Marriage](#) on 3065189;

Congratulations

[TOP](#)

Recent Grant Awards

Hans Westerhoff, Pedro Mendes, and Daniel Jameson. European Commission **IT Future of Medicine** one year award worth approx £126K

John Keane, Stavros Stivaros and Alan Jackson have been awarded approx £964K by the Department of Health for their project *“Improving the Diagnosis, Assessment and Outcome in Patients with Hydrocephalus and Raise Intracranial Pressure”*

MIB Football Tournament

Hi everyone - The time of year has come round again to dig out those football boots, get together a team and take part in the MIB 5 aside football tournament!

The tournament will take place on Friday 15th July from 2pm til 5pm at Powerleague central and is £10 per team to enter (subsidized by the MIB). This year we will also be hiring out the bar afterwards so we can all have a few drinks and get a little merry! Let's hope this year it won't rain!!!



Places are limited so it'll be first come first served, teams can consist of as many MIB people as you like, but you must have at least one girl on the pitch at all times. Also spectators are more than welcome. There is a balcony area to watch the football whilst having a drink or two. So come to support your lab in the event of the year! So if you want to take part email Hayley Bennett at hayley.bennett@manchester.ac.uk or ring Hayley on x65816

MIB and the Manchester 10K

Congratulations to all those from MIB who ran in the Manchester 10K!



Here's a photo of the post-run celebrations from a team from MCISB raising cash for the Bobby Moore Fund (over £500 so far!), showing Kieran Smallbone; Neil Swainston; Natalie Stanford; Daniel Jameson - not necessarily in that order !

From the top floor we also had: Simon Willies, Jennifer Hopwood, Dominique Richardson , Bas Groenendaal Martin Weissenborn, Anthony Green, Paul Kelly, Sabine Flitsch. Congratulations to Simon, on what I think is the fastest MIB time this year of 38'35" – a time to beat...

Seminars**MIB mini Research Conference**

2nd June in MIB LT 13.00-17.00

This afternoon event will see a mixture of talks from postgrads and postdocs (Ming Cheng Wu, Simon Willies, Linus Johannissen, C.J.Rupp, Marc Goodfellow, and Farhatullah Syed) together with general discussion on MIB research strategy and developments.

Everyone in the MIB is expected to attend!

Seminars in MIB

9th June 12.00 MIB LT

Jonathan Claydon (UoM, School of Chemistry)

Giovanna Zinzalla (RCUK senior research fellow, Univ. of London)

30th June 12.00 MIB LT

Christopher Ward (UoM, School of Dentistry)

Seminars throughout the University

NC3Rs will be holding a regional roadshow at the University on Wednesday 6th July. They will be showcasing their diverse range of funding opportunities, collaborative research programmes and CRACK-IT, a new (Innocentive/Dragon's Den style) initiative to connect academic and industry scientists. For program and registration (by 29th June) see: <http://www.nc3rs.org.uk/event.asp?id=1505>

[Faculty of Life Sciences](#) AZ Seminar series

Pharmacy <http://www.pharmacy.manchester.ac.uk/aboutus/events/seminars2010/>

School of Chemical Engineering and Analytical Science <http://www.ceas.manchester.ac.uk/research/seminar/>

School of Chemistry <http://www.chemistry.manchester.ac.uk/research/seminars/>

School of Computer Science <http://www.cs.manchester.ac.uk/research/seminars/school/>

School of Materials <http://www.materials.manchester.ac.uk/aboutus/events/>

School of Mathematics <http://www.mims.manchester.ac.uk/events/>

School of Physics and Astronomy <http://www.physics.manchester.ac.uk/aboutus/events/>

School of Mechanical, Aerospace and Civil Engineering <http://www.mace.manchester.ac.uk/>

School of Electrical and Electronic Engineering <http://www.eee.manchester.ac.uk/aboutus/news/>

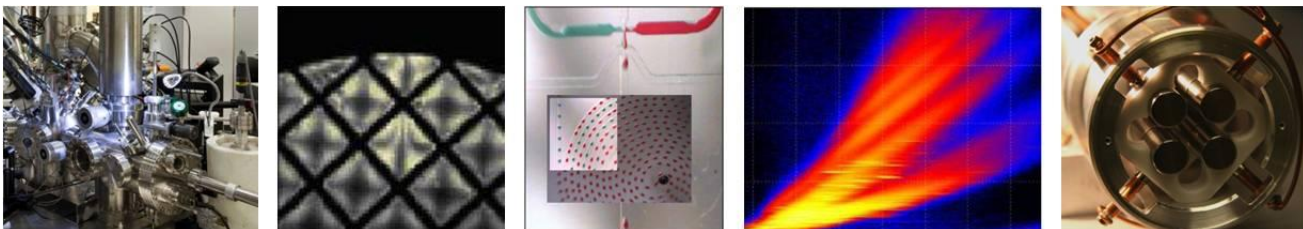
School of Earth, Atmospheric and Environmental Sciences

<http://www.seaes.manchester.ac.uk/aboutus/events/>

Events/Symposia/Meetings

[TOP](#)

Enabling technologies for quantitative bioscience



The MIB will host a free one day “*Enabling technologies for quantitative bioscience*” event on the 14th June. Confirmed Speakers include: Peter Fielden (MIB, University of Manchester (UoM)), Stephen Haswell (University of Hull), Ian Wilson (AZ), Ern Edmonds (Solvay), Jeremy Lea (Bruker), Eric McInnes (UoM), Mike White (UoM), Andreas Manz (KIST Europe), John Shockcor (Waters Corp), Martin Packer (AZ), Alan Dickson (UoM), Christiane Hertz-Fowler (University of Hull) and Jon Waltho (MIB, UoM). The aim of the day is to have a variety of talks across enabling technologies to discuss their application towards quantitative bioscience.

Register now: [registration form](#)

Pathways: Career Options for PhD Researchers and Research Staff

10, 13 & 15 June 2011, Renold Building. Now in its fifth year, this university wide event is designed to help our PhDs and Research Staff (post-docs) make some potentially difficult life and career choices. All four Faculties and the Careers Service are collaborating to attract panellists who have completed their PhDs within the last 10 years and are now working in a wide range of careers to talk to our current PhDs and research staff, over 500 of whom attended last year. <<http://www.manchester.ac.uk/pathways>>

Panel sessions run in 40 minute slots, throughout Day 1 (Friday, 10 June 2011) and panellists can come for all or part of the day. In addition to the Day 1 discussion panels, Day

2 (Monday, 13 June) will involve interactive workshops offering practice in interviews and assessment centres. Day 3 (Wednesday, 15 June) will be part of a larger Graduate Recruitment Fair [at GMex] with a specific “PhD Zone” of PhD recruiters. There will also be specialist CV advice on the day.

For more information and registration site see the [website](#)

Diversity Week

The University of Manchester recognizes the diverse make up of its staff and students and acknowledges this in Goal 3 of ‘Advancing the 2015 Agenda’. There are a number of strategies for social responsibility, which extend to the wider community, and commits the University to understand the challenges facing our society.

‘Personally, I am deeply committed to the principles of Equality and Diversity and I am proud to be President and Vice-Chancellor of a University that champions these principles as part of its approach to every aspect of its work.’ (Nancy Rothwell- President & Vice Chancellor)

To celebrate the rich diversity we have at The University of Manchester there will be a number of events between 23 – 27 May. These will range from ‘Trees of Diversity’ to an ‘International Song Contest’ to a diversity walk of Manchester. All events are free and open to staff, students and their friends & relatives.

A full timetable can be found on the Equality & Diversity Intranet Pages:

- [Diversity Week Timetable](http://www.campus.manchester.ac.uk/equalityanddiversity/) <http://www.campus.manchester.ac.uk/equalityanddiversity/>

Come along, join in and celebrate your own diversity!

Research Impact Showcase

This year the School of Chemical Engineering and Analytical Science is introducing a new event on the skills training calendar aimed primarily for, and organised by, PGR students. The research impact showcase is a two day event for postgraduate and postdoctoral researchers to explore how to identify, understand and communicate the potential economic, social and cultural impacts of research.

The dates for the events are Friday 24th June and Wednesday 6th July. The first day is focused on providing a series of interactive workshops to prepare the researchers for the presentation and pitch day on day 2. Workshops include: creating, realising and choosing ideas, preparing for commercialisation, networking and developing business plan and pitching it.



The poster for the Research Impact Showcase features the University of Manchester logo at the top left. The main title is "What is the impact of your research?" in large, bold, black and green text. Below the title, a short paragraph describes the event as a two-day event for postgraduate and postdoctoral researchers to explore how to identify, understand and communicate the potential economic, social or cultural impacts of their research. The poster is divided into two columns: "Day 1 - Friday 24 June" and "Day 2 - Wednesday 6 July". Each column lists workshops and training, invited speakers and activities, and prizes and awards. The poster is decorated with red starburst graphics and a globe icon.

What is the impact of your research?

The CEAS impact showcase is a two day event for postgraduate and postdoctoral researchers to explore how to identify, understand and communicate the potential economic, social or cultural impacts of your research.

Day 1 - Friday 24 June

Workshops and training:

- Identifying research opportunities
- Market analysis
- IP and licensing
- Funding for research commercialisation
- Developing and pitching a business plan
- Networking

Day 2 - Wednesday 6 July

Invited speakers and activities:

- Social impact of research
- Commercial impact of research
- Presentations of pitches by postgraduate and postdoctoral researchers
- Group discussions and feedback sessions
- Prizes and awards

Both days will take place in the MIB Lecture Theatre

To register and get more information, go to <http://tinyurl.com/ceasimpact>
This event is free to attend. Lunch and refreshments will be provided.

Sponsored by Graduate and Researcher Development, in the Faculty of Engineering and Physical Sciences.

This event will complement the school’s existing annual PGR Conference, which focuses on the technical presentation of PhD research, by providing a further opportunity for communication and networking.

Further details and to register to participate in this event, please go to: <http://www.tinyurl.com/ceasimpact>

Challenges in Chemical Biology (ISACS5)

International symposia on advancing the Chemical Sciences

26-29th July, University of Manchester.

Early bird registration deadline: 27th May 2011!

Gain a state-of-the-art review of current research developments and identify future challenges in a comprehensive plenary programme. See www.rsc.org/isacs5



Challenges in Chemical Biology (ISACS5)

26-29 July 2011 • Manchester, UK

Plenary Speakers:

- Donna Blackmond (Scripps)
- Ben Davis (Oxford)
- Andrew Ellington (Texas at Austin)
- Hermann Gaub (Ludwig-Maximilians)
- Reza Ghadiri (Scripps)
- Nathanael Gray (Harvard)
- Andrew Griffiths (Strasbourg)
- Bartosz Grzybowski (Northwestern)
- Johan Hofkens (KU Leuven)
- Philip Holliger (MRC)
- Clyde Hutchison (J. Craig Venter Institute)
- Stefan Knapp (Oxford)
- Stephen Mann (Bristol)
- David Rees (Astex Therapeutics Ltd)
- Hugh Rosen (Scripps)
- William Shih (Harvard)
- Hiroaki Suga (Tokyo)
- Erik Winfree (Caltech)

RSC Advancing the Chemical Sciences

www.rsc.org/isacs5

Publications

Publication Highlight

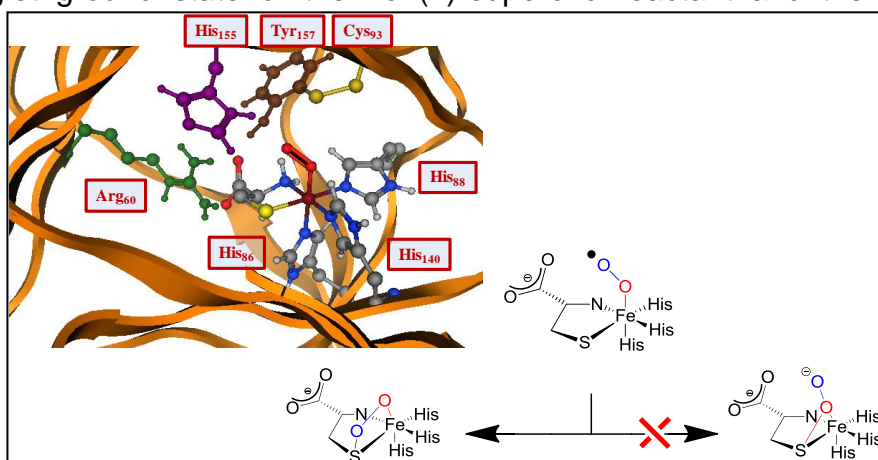
Theoretical Study on the Mechanism of the Oxygen Activation Process in Cysteine Dioxygenase Enzymes – Sam de Visser

Devesh Kumar, Walter Thiel, & Sam P. de Visser, *J. Am. Chem. Soc.* **2011**, *133*, 3869–3882.

Cysteine dioxygenase (CDO) is a vital enzyme for human health involved in the biodegradation of toxic cysteine and thereby regulation of the cysteine concentration in the body. The enzyme belongs to the group of nonheme iron dioxygenases, which contain a transition metal active center (iron) that is linked to the protein via interactions with three histidine side chains. This is an unusual feature, since most nonheme iron dioxygenases contain a 2-His-1-Asp ligand system.

CDO utilizes molecular oxygen to transfer its both oxygen atoms to cysteinate to form cysteine sulfinic acid products. The mechanism for this reaction is currently disputed, with crystallographic studies implicating a persulfenate intermediate in the catalytic cycle, while density functional theory models preferred a mechanism initiating by an iron(III)-superoxo structure. To resolve the dispute we have performed quantum mechanics/molecular mechanics (QM/MM) calculations on substrate activation by CDO enzymes for both mechanisms using an enzyme monomer and a large QM active region.¹ We find a stepwise mechanism, whereby the distal oxygen atom of the iron(II)-superoxo complex attacks the sulfur atom of cysteinate to form a ring structure, followed by dioxygen bond breaking and the formation of a sulfoxide bound to an iron(IV)-oxo complex. A sulfoxide rotation precedes the second oxygen atom transfer to the substrate to give cysteine sulfinic acid products. The reaction takes place on several low-lying spin state surfaces via multistate reactivity patterns. It starts in the singlet ground state of the iron(II)-superoxo reactant and then

proceeds mainly on the quintet and triplet surfaces. The initial and rate-determining attack of the peroxy group on the cysteinate sulfur atom involves a spin state crossing from singlet to quintet. We have also investigated an alternative mechanism via a persulfenate intermediate,



with a realignment of hydrogen bonding interactions in the substrate binding pocket. However, this alternative mechanism of proximal oxygen atom attack on the sulfur atom of cysteinylate is computed to be a high-energy pathway, and therefore, the persulfenate intermediate is unlikely to participate in the catalytic cycle of CDO enzymes.

Figure 1. Established reaction mechanism for oxygen activation by cysteine dioxygenase enzymes.

Publications

S-linked sugars lost and found – Sardzik, R., Both, P & Flitsch, S.L. Nature Chemical Biology, 7: Feb 2011 – [Paper](#)

The vast majority of core structures of protein and peptide glycosylation motifs belong to either O-linked or N-linked glycans. A recent publication describes the structure and biosynthesis of an unusual S-linked glycans linkage in the antibacterial glycopeptides sublancin.

Wu M, Zampini M, Bussiek M, Hoischen C, Diekmann S, Hayes F (2011) Segrosome assembly at the pliable parH centromere. Nucleic Acids Res., in press [Paper](#)

Hayes F (2011) Moving in for the kill: activation of an endoribonuclease toxin by a quorum-sensing peptide. Mol. Cell 41:617-618. [Paper](#)

Kulinska A, Cao Y, Macioszek M, Hayes F, Jagura-Burdzy G (2011) The centromere site of the segregation cassette of broad host range plasmid RA3 is located at the border of the maintenance and conjugative transfer modules. Appl. Environ. Microbiol. 77:2414-2427. [Paper](#)

Lockyer NP. Bioimaging of elements and small molecules using MS. Bioanalysis. 2011 May;3(10):1047-51. [Paper](#)

Harding AP, Popelier PL. pK(a) prediction from an ab initio bond length: Part 3-benzoic acids and anilines. Phys Chem Chem Phys. 2011 May 13. [Paper](#)

Harding AP, Popelier PL. pK(a) Prediction from an ab initio bond length: part 2-phenols. Phys Chem Chem Phys. 2011 May 13. [Paper](#)

Taylor PN, Baier G. A spatially extended model for macroscopic spike-wave discharges. J Comput Neurosci. 2011 May 10. [Paper](#)

Rannes JB, Ioannou A, Willies SC, Grogan G, Behrens C, Flitsch SL, Turner NJ. Glycoprotein Labeling Using Engineered Variants of Galactose Oxidase Obtained by Directed Evolution. J Am Chem Soc. 2011 May 12. [Paper](#)

Gardiner JD, Dimitriadis G, Codd JR, Nudds RL. A potential role for bat tail membranes in flight control. PLoS One. 2011 Mar 30;6(3):e18214. [Paper](#)

Hardwick HC, Royal DS, Helliwell M, Pope SJ, Ashton L, Goodacre R, Sharrad CA. Structural, spectroscopic and redox properties of uranyl complexes with a maleonitrile containing ligand. Dalton Trans. 2011 Apr 28. [Epub ahead of print] [Paper](#)

Rigby SE, Lou X, Toogood HS, Wolthers KR, Scrutton NS. ELDOR Spectroscopy Reveals that Energy Landscapes in Human Methionine Synthase Reductase are Extensively Remodelled Following Ligand and Partner Protein Binding. ChemBiochem. 2011 Apr 11;12(6):863-7. Epub 2011 Feb 25. No abstract available. [Paper](#).

Leferink NG, Han C, Antonyuk SV, Heyes DJ, Rigby SE, Hough MA, Eady RR, Scrutton NS, Hasnain SS. Proton-Coupled Electron Transfer in the Catalytic Cycle of Alcaligenes xylosoxidans Copper-Dependent Nitrite Reductase. *Biochemistry*. 2011 Apr 19. [Epub ahead of print] [Paper](#)

de Visser SP. Van der waals equation of state revisited: importance of the dispersion correction. *J Phys Chem B*. 2011 Apr 28;115(16):4709-17. Epub 2011 Apr 6. [Paper](#)

Sardzík R, Sharma R, Kaloo S, Voglmeir J, Crocker PR, Flitsch SL. Chemoenzymatic synthesis of sialooligosaccharides on arrays for studies of cell surface adhesion. *Chem Commun (Camb)*. 2011 May 21;47(19):5425-7. Epub 2011 Apr 5. [Paper](#)

Ananiadou S, Sullivan D, Black W, Levow GA, Gillespie JJ, Mao C, Pyysalo S, Kolluru B, Tsujii J, Sobral B. Named Entity Recognition for Bacterial Type IV Secretion Systems. *PLoS One*. 2011 Mar 29;6(3):e14780. [Paper](#)

Griffin M, Iqbal SA, Bayat A. Exploring the application of mesenchymal stem cells in bone repair and regeneration. *J Bone Joint Surg Br*. 2011 Apr;93(4):427-34. [Paper](#)

Rabbani S, Barber AM, Fletcher JS, Lockyer NP, Vickerman JC. TOF-SIMS with Argon Gas Cluster Ion Beams: A Comparison with C(60)(+). *Anal Chem*. 2011 Apr 15. [Epub ahead of print] [Paper](#)

Vickerman JC. Molecular imaging and depth profiling by mass spectrometry-SIMS, MALDI or DESI? *Analyst*. 2011 Apr 4. [Epub ahead of print] [Paper](#)

Brown BC, McKenna SP, Bayat A. Reply: patient assessments of scarring: patient-reported impact of scars measure or patient scar assessment questionnaire? *Plast Reconstr Surg*. 2011 Apr;127(4):1745-6. No abstract available. [Paper](#)

de Cogan F, Gough JE, Webb SJ. Adhesive interactions between cells and biotinylated phospholipid vesicles in alginate: towards new responsive biomaterials. *J Mater Sci Mater Med*. 2011 Apr;22(4):1045-51. Epub 2011 Mar 23. [Paper](#)

Waltham TN, Girvan HM, Butler CF, Rigby SR, Dunford AJ, Holt RA, Munro AW. Analysis of the oxidation of short chain alkynes by flavocytochrome P450 BM3. *Metallomics*. 2011 Apr 1;3(4):369-78. Epub 2011 Mar 23. [Paper](#)

Kocbek S, Sætre R, Stiglic G, Kim JD, Pernek I, Tsuruoka Y, Kokol P, Ananiadou S, Tsujii AGRA: Analysis of Gene Ranking Algorithms. *J.Bioinformatics*. 2011 Feb 23. [Epub ahead of print] [Paper](#)

Heyes DJ, Levy C, Sakuma M, Robertson DL, Scrutton NS. A twin-track approach has optimised proton and hydride transfer by dynamically-coupled tunnelling during the evolution of protochlorophyllide oxidoreductase. *J Biol Chem*. 2011 Feb 11. [Epub ahead of print] [Paper](#)

Bella H, Heise M, Yagi KI, Black G, McGrouther DA, Bayat A. A clinical characterization of familial keloid disease in unique african tribes reveals distinct keloid phenotypes. *Plast Reconstr Surg*. 2011 Feb;127(2):689-702. [Paper](#)

Dada JO, Mendes P. Multi-scale modelling and simulation in systems biology. *Integr Biol (Camb)*. 2011 Feb 8;3(2):86-96. Epub 2011 Jan 6. [Paper](#)

Ismail F, Schoenleber M, Mansour R, Bastani B, Fielden P, Goddard NJ. Strength of interactions between immobilized dye molecules and sol-gel matrices. *Analyst*. 2011 Feb 21;136(4):807-15. Epub 2010 Dec 1. [Paper](#)

Xu Y, Cheung W, Winder CL, Dunn WB, Goodacre R. Metabolic profiling of meat: assessment of pork hygiene and contamination with *Salmonella typhimurium*. *Analyst*. 2011 Feb 7;136(3):508-14. Epub 2010 Nov 29. [Paper](#)

Hindocha S, Iqbal SA, Farhatullah S, Paus R, Bayat A. Characterization of stem cells in Dupuytren's disease. *Br J Surg*. 2011 Feb;98(2):308-15. [Paper](#)

O'Connell MD, Roberts SA, Srinivas-Shankar U, Tajar A, Connolly MJ, Adams JE, Oldham JA, Wu FC. Do the effects of testosterone on muscle strength, physical function, body composition, and quality of life persist six months after treatment in intermediate-frail and frail elderly men? *J Clin Endocrinol Metab*. 2011 Feb;96(2):454-8. Epub 2010 Nov 17. [Paper](#)

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