

Dalton Discussion 8

Metals: Centres of Biological Activity

7-9 September 2005, University of Nottingham, UK

PROGRAMME

Wednesday 7 September 2005

Session 1: Haem Iron: Nature's Most Versatile Redox Centre

Session Chair: Emma Raven

University of Leicester, UK

Keynote 1

Multi-heme cytochromes – new structures, new chemistry

Christopher G. Mowat and Stephen K. Chapman*

University of Edinburgh, UK

Cryoreduction EPR and ^{13}C , ^{19}F ENDOR Study of Substrate-bound substates and solvent kinetic isotope effects in the catalytic cycle of cytochrome P450cam and its T252A mutant

Sun Hee Kim, Tran-Chin Yang, Roshan Perera, Shengxi Jin, Thomas A. Bryson, Masanori Sono, Roman Davydov, John H. Dawson and Brian M. Hoffman*

Northwestern University, USA

QM/MM studies of the electronic structure of the compound I intermediate in cytochrome c peroxidase and ascorbate peroxidase

Christine M. Bathelt, Adrian J. Mulholland and Jeremy N. Harvey*

University of Bristol, UK

Transient species involved in catalytic dioxygen/peroxide activation by hemoproteins: possible involvement of protonated compound I species

Radu Silagh-Dumitrescu* and Christopher E. Cooper

University of Essex, UK

On the formation, nature, stability and biological relevance of the primary reaction intermediates of myoglobins with hydrogen peroxide

Chris E. Cooper*, Mary Jurd, Peter Nicholls, Meebi M. Wankasi, Dimitri A. Svistunenko, Brandon J. Reeder and Michael T. Wilson

University of Essex, UK

Why isn't 'standard' heme good enough for c-type and d₁-type cytochromes?

James W.A. Allen, Paul D. Barker, Oliver Daltrop, Julie M. Stevens, Esther J. Tomlinson, Neeti Sinha, Yoshi Sambongi and Stuart J. Ferguson*

University of Oxford, UK

Cytochrome P450s: creating novel ligand sets

Harriet E. Seward*, Hazel M. Girvan and Andrew W. Munro

University of Leicester, UK

Exploring the redox reactions between heme and tetrahydrobiopterin in the nitric oxide synthases

Dennis J. Stuehr*, Chin-Chuan Wei, Zhiqiang Wang and Russ Hille
Ohio State University, USA

Geminate carbon monoxide rebinding to a c-type haem

Gary Silkstone*, A. Jasaitis, M.H. Vos and M.T. Wilson, *University of Essex, UK*

Probing the function of *Mycobacterium tuberculosis* catalase-peroxidase by site-directed mutagenesis

Nigel A.J. Eady, J. Jesmin, Spiros Servos, Anthony E.G. Cass, Judit M. Nagy and Katherine A. Brown*
Imperial College London, UK

Thursday 8 September 2005

Session 2: Multi-Copper Enzymes and their Chemical Analogues

Session Chair: Paul Walton
University of York, UK

Keynote 2

The quest for the particulate methane monooxygenase active site

Raquel L. Lieberman and Amy C. Rosenzweig*
Northwestern University, USA

Formation of a cytochrome c-nitrous oxide reductase complex is obligatory for N₂O reduction by *Paracoccus pantotrophus*

Tim Rasmussen, Thomas Brittain, Ben C. Berks, Nicholas J. Watmough and Andrew J. Thompson*
University of East Anglia, UK

Dioxygen reduction by multi-copper oxidases; a structural perspective

Isabel Bento*, Lgia O. Martins, Gonalo Gato Lopes, Maria Armnia Carrondo and Peter F. Lindley
Universidade Nova de Lisboa, Portugal

Ligand and loop variations at type 1 copper sites: influence on structure and reactivity

Christopher Dennison*
University of Newcastle upon Tyne, UK

Structure and dioxygen-reactivity of copper(I) complexes supported by bis(6-methylpyridin-2-ylmethyl)amine tridentate ligands

Takao Osako, Shohei Terada, Takehiko Tosha, Shigenori Nagatomo, Hideki Furutachi, Shuhei Fujinami, Teizo Kitagawa, Masatatsu Suzuki and Shinobu Itoh*
Osaka City University, Japan

Oxygen binding and activation by the complexes of PY2- and TPA-appended diphenylglycoluril receptors with copper and other metals

Vera S.I. Sprakel, Martin C. Feiters*, Wolfram Meyer-Klaucke, Marten Klopstra, Jelle Brinksma, Ben L. Feringa, Kenneth D. Karlin and Roeland J.M. Nolte
Radboud University Nijmegen, The Netherlands

Selective copper(II)-mediated oxidative coupling of a nucleophilic reagent to the *para*-methyl group of 2,4,6-trimethylphenol

Christophe Boldron, Şeniz Özalp-Yaman, Patrick Gamez*, Duncan M. Tooke, Anthony L. Spek and Jan Reedijk, *Leiden University, The Netherlands*

Session 3: Hydrogen Cycling by Enzymes: Electrocatalysis and Implications for Future Energy Technology

Session Chair: Jon McMaster
University of Nottingham, UK

Keynote 3

Hydrogen cycling by enzymes: electrocatalysis and implications for future energy technology

Kylie A. Vincent, James A. Cracknell, Alison Parkin and Fraser A. Armstrong*
University of Oxford, UK

Structural bases for the catalytic mechanism of Ni-containing carbon monoxide dehydrogenases

Anne Volbeda and Juan C. Fontecilla-Camps*, *Institut de Biologie Structurale J.P. Ebel CEA-CNRS-UJF, France*

Urea decomposition facilitated by a urease model complex: a theoretical investigation

Chad Beddie, Charles Edwin Webster and Michael B. Hall*
Texas A&M University, USA

On the mechanism of methyl-coenzyme M reductase

Ulrich Ermler*
Max-Planck-Institute für Biophysik, Germany

Friday 9 September 2005

Session 4: Molybdenum and Tungsten Enzymes: Nature and Function

Session Chair: David Garner
University of Nottingham, UK

Keynote 4

Molybdenum: biological activity and metabolism

Ralf R. Mendel*, *Technical University of Braunschweig, Germany*

Structural analysis of missense mutations causing isolated sulfite oxidase deficiency

Erkan Karakas and Caroline Kisker*

State University of New York at Stony Brook, USA

Reductive activation of nitrate reductases

Sarah J. Field, Nicholas P. Thornton, Lee J. Anderson, Andrew J. Gates, Ann Reilly, Brian J.N. Jepson, David J. Richardson, Simon J. George, Myles R. Cheesman and Julea N. Butt*

University of East Anglia, UK

The nature and function of the catalytic centres of the DMSO reductases

Jonathan P. McNamara, Ian H. Hillier*, Tanjeet S. Bhachu and C. David Garner

University of Manchester, UK

Synthesis and characterisation of second-generation metallodithiolene complexes of the type [Tp*ME(dithiolene)] (M = Mo, W; E = O, S) and a novel 'organoscorpionate' complex of tungsten

Stephen A. Sproules*, Hugh T. Morgan, Christian J. Doonan, Jonathan M. White and Charles G. Young

University of Melbourne, Australia

A new series of molybdenum-(IV), -(V), and -(VI) dithiolate compounds as active site models of molybdoenzymes: preparation, crystal structures, spectroscopic/electrochemical properties and reactivity in oxygen atom transfer

Hideki Sugimoto*, Makoto Tarumizu, Koji Tanaka, Hiroyuki Miyake and Hiroshi Tsukube

Osaka City University, Japan

Synthesis and characterization of molybdenum oxo complexes of two tripodal ligands: reactivity studies of a functional model for molybdenum oxotransferases

Anders Thapper, Axel Behrens, Jacob Fryxelius, Maria H. Johansson, Fabio Prestopino, Miklos Czaun, Dieter Rehder and Ebbe Nordlander*

Lund University, Sweden