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Biography
Sam received a first class honours degree in biochemistry from the University of Otago, New Zealand (2000), and his PhD in biophysics from the Australian National University (2004). He then spent a year at Stockholm University as a Wenner-Gren visiting postdoctoral fellow (2004-2005) before moving to the University of Manchester to work with Nigel Scrutton as a postdoctoral research associate. Sam was a recipient of the RSC Rita and John Cornforth Award in 2009 and in 2010 he received a BBSRC David Phillips fellowship. In 2014 he was made a lecturer, in 2017 senior lecturer, in 2019 reader and in 2021 he became Professor of Biophysical Chemistry.

Publications
Tuning of B₁₂ Photochemistry in the CarH photoreceptor to avoid radical photoproducts  

Direct comparison between Förster Resonance Energy Transfer and Light-Induced Triplet–Triplet Electron Resonance Spectroscopy  

Efficient NADPH-dependent dehalogenation afforded by a self-sufficient reductive dehalogenase  

Redox driven B₁₂ ligand switch drives CarH photoresponse  

Heterometallic lanthanide complexes with site-specific binding that enable simultaneous visible and NIR-emission  

How is substrate halogenation triggered by the vanadium haloperoxidase from Curvularia inaequalis?  

Reactivity Differences of Trigonal Pyramidal Nonheme Iron(IV)-Oxo and Iron(III)-Oxo Complexes: Experiment and Theory.  

Photoinduced Electron Transfer from a 1,4,5,6-Tetrahydro Nicotinamide Adenine Dinucleotide (Phosphate) Analog to Oxidized Flavin in an Ene-Reductase Flavoenzyme  

A Vitamin B2-Photocatalysed Approach to Methionine Analogues  

How a 10-epi-cubebol Synthase Avoids Premature Reaction Quenching to Form a Tricyclic Product at High Purity  
Combined pulsed electron double resonance EPR and molecular dynamics investigations of calmodulin suggest effect of crowding agents on protein structure

Chelator-based parameterization of the 12-6-4LJ molecular mechanics potential for more realistic metal ion-protein interactions

How Photoactivation Triggers Protochlorophyllide Reduction: Computational Evidence of a Stepwise Hydride Transfer During Chlorophyll Biosynthesis

Molecular determinants of carbocation cyclisation in bacterial monoterpene synthases

Engineering an Efficient and Enantioselective Enzyme for the Morita-Baylis-Hillman Reaction

Blood, sweat and tears: extraterrestrial regolith biocomposites with in vivo binders

A Noncanonical Tryptophan Analogue Reveals an Active Site Hydrogen Bond Controlling Ferryl Reactivity in a Heme Peroxidase

Interplay Between Chromophore-Binding and Domain Assembly by the B12-Dependent Photoreceptor Protein, CarH

A non-canonical tryptophan analogue reveals an active site hydrogen bond controlling ferryl reactivity in a heme peroxidase

Photocatalysis as the ‘master switch’ of photomorphogenesis in early plant development

Structure and Mechanism of Pseudomonas aeruginosa PA0254/HudA, a prFMN-Dependent Pyrrole-2-carboxylic Acid Decarboxylase Linked to Virulence

Predicting New Protein Conformations from Molecular Dynamics Simulation Conformational Landscapes and Machine Learning
Structure and mechanism of Pseudomonas aeruginosa PA0254/HudA, a prFMN-dependent pyrrole-2-carboxylic acid decarboxylase linked to virulence

Quantum Biology: An Update and Perspective

Assessing the Covalent Attachment and Energy Transfer Capabilities of Upconverting Phosphors With Cofactor Containing Bioactive Enzymes

How do vanadium chloroperoxidases generate hypochlorite from hy-drogen peroxide and chloride? A computational study.

Enzymatic C-H activation of aromatic compounds through CO2 fixation

Dual Role of the Active Site 'Lid' Regions of Protochlorophyllide Oxidoreductase in Photocatalysis and Plant Development

Non-covalent protein-based adhesives for transparent substrates – bovine serum albumin vs. recombinant spider silk

Evaluating spectral overlap with the degree of quenching in UCP luminescence energy transfer systems

Ultrafast Vibrational Energy Transfer between Protein and Cofactor in a Flavoenzyme

Covalent attachment of active enzymes to upconversion phosphors allows ratiometric detection of substrates

Pressure and temperature effects on formation of aminoacrylate intermediates of tyrosine phenol-lyase demonstrate reaction dynamics

Rewiring the ‘Push-Pull’ Catalytic Machinery of a Heme Enzyme using an Expanded Genetic Code

Taming the reactivity of monoterpene synthases to guide regioselective product hydroxylation
Structural basis for enzymatic photocatalysis in chlorophyll biosynthesis

Enzymatic control of cycloadduct conformation ensures reversible 1,3 dipolar cycloaddition in a prFMN dependent decarboxylase

Graphene–aramid nanocomposite fibres via superacid co-processing

Equatorial active site compaction and electrostatic reorganization in catechol-O-methyltransferase

Isotopically labeled flavoenzymes and their uses in probing reaction mechanisms

MhuD from Mycobacterium tuberculosis - probing a dual role in heme storage and degradation

Selectivity through discriminatory induced fit enables switching of NAD(P)H coenzyme specificity in Old Yellow Enzyme reductases

Synthetic biology for fibres, adhesives and active camouflage materials in protection and aerospace

The Photochemical Spin Dynamics of the Vitamin B12 Derivative, Methylcobalamin

Unexpected Roles of a Tether Harboring a Tyrosine Gatekeeper Residue in Modular Nitrite Reductase Catalysis

What are the signatures of tunnelling in enzyme-catalysed reactions?

Non-equivalence of second sphere 'non-catalytic' residues in pentaerythritol tetranitrate reductase in relation to local dynamics linked to H-transfer in reactions with NADH and NADPH coenzymes

Trapping methods for probing functional intermediates in nitric oxide synthases and related enzymes
H-1, N-15 and C-13 backbone resonance assignments of pentaerythritol tetranitrate reductase from Enterobacter cloacae PB2

Pressurized CO₂ as Carboxylating Agent for the Biocatalytic ortho-Carboxylation of Resorcinol

Extracting Kinetic Isotope Effects From a Global Analysis of Reaction Progress Curves

Expanding the scope of biomolecule monitoring with ratiometric signaling from rare-earth upconverting phosphors

Liver microsomal lipid enhances the activity and redox coupling of colocalized cytochrome P450 reductase-cytochrome P450 3A4 in nanodiscs

Decoupled Associative and Dissociative Processes in Strong yet Highly Dynamic Host-Guest Complexes

1H, 15N, 13C backbone resonance assignments of human soluble catechol Omethyltransferase in complex with S-adenosyl-L-methionine and 3,5-dinitrocatechol

A perspective on conformational control of electron transfer in nitric oxide synthases

A common mechanism for coenzyme cobalamin-dependent reductive dehalogenases

Convergence of Theory and Experiment on the Role of Preorganization, Quantum Tunneling, and Enzyme Motions into Flavoenzyme-Catalyzed Hydride Transfer

Structural basis of catalysis in the bacterial monoterpene synthases linalool synthase and 1,8-cineole synthase

An oxidative N-demethylase reveals PAS transition from ubiquitous sensor to enzyme

Untangling heavy protein and cofactor isotope effects on enzyme catalyzed hydride transfer

Correlating calmodulin landscapes with chemical catalysis in neuronal nitric oxide synthase using time-resolved FRET and a 5-deazaflavin thermodynamic trap.
A 'Plug and Play' Platform for the Production of Diverse Monoterpene Hydrocarbon Scaffolds in Escherichia coli

Dual transcriptional-translational cascade permits cellular level tunable expression control.

Carboxylesterase converts Amplex red to resorufin: Implications for mitochondrial H2O2 release assays.

Donor–Acceptor Distance Sampling Enhances the Performance of "Better than Nature" Nicotinamide Coenzyme Biomimetics.

Ground-state Destabilization by Phe-448 and Phe-449 Contributes to Tyrosine Phenol-lyase Catalysis

Time course analysis of enzyme-catalyzed DNA polymerization

Nuclear quantum tunnelling in enzymatic reactions - an enzymologist's perspective.

Real time analysis of conformational control in electron transfer reactions of human cytochrome P450 reductase with cytochrome c

Does the pressure dependence of kinetic isotope effects report usefully on dynamics in enzyme H-transfer reactions?

Probing reversible chemistry in coenzyme B12-dependent ethanolamine ammonia lyase with kinetic isotope effects

Structure and Mechanism of a Viral Collagen Prolyl Hydroxylase

Towards the free energy landscape for catalysis in mammalian nitric oxide synthases

Energy landscapes and catalysis in nitric-oxide synthase

Ratiometric detection of enzyme turnover and flavin reduction using rare-earth upconverting phosphors
A quantitative fluorescence-based steady-state assay of DNA polymerase

Proton tunnelling and promoting vibrations during the oxidation of ascorbate by ferricyanide?

Practical aspects on the use of kinetic isotope effects as probes of flavoprotein enzyme mechanisms.

Excited state dynamics can be used to probe donor-acceptor distances for H-tunneling reactions catalyzed by flavoproteins

Modulation of ligand-heme reactivity by binding pocket residues demonstrated in cytochrome c over the femtosecond-second temporal range

Dynamic, Electrostatic Model for the Generation and Control of High-Energy Radical Intermediates by a Coenzyme B12-Dependent Enzyme

Relating localized protein motions to the reaction coordinate in coenzyme B12-dependent enzymes

Fast protein motions are coupled to enzyme H-transfer reactions.

Protein motions are coupled to the reaction chemistry in coenzyme B 12-dependent ethanamine ammonia lyase

Evidence of preorganization in quinonoid intermediate formation from l-Trp in H463F mutant Escherichia coli tryptophan indole-lyase from effects of pressure and pH

Pressure effects on enzyme-catalyzed quantum tunneling events arise from protein-specific structural and dynamic changes

Ultrafast infrared spectral fingerprints of Vitamin B12 and related cobalamins
Preparation and photophysical properties of a caged kynurenine

Good vibrations in enzyme-catalysed reactions

Experimental approaches towards proton-coupled electron transfer reactions in biological redox systems

Is there a dynamic protein contribution to the substrate trigger in coenzyme B 12-dependent ethanolamine ammonia lyase?

Electrochemical and structural properties of a protein system designed to generate tyrosine pourbaix diagrams

Examining the importance of dynamics, barrier compression and hydrogen tunnelling in enzyme catalysed reactions

Direct analysis of donor-acceptor distance and relationship to isotope effects and the force constant for barrier compression in enzymatic H-tunneling reactions

Probing active site geometry using high pressure and secondary isotope effects in an enzyme-catalysed ‘deep’ H-tunnelling reaction

Barrier compression and its contribution to both classical and quantum mechanical aspects of enzyme catalysis

Evidence to support the hypothesis that promoting vibrations enhance the rate of an enzyme catalyzed H-tunneling reaction

Are the catalytic properties of enzymes from piezophilic organisms pressure adapted?

Demonstration of proton-coupled electron transfer in the copper-containing nitrite reductases

Bipartite recognition and conformational sampling mechanisms for hydride transfer from nicotinamide coenzyme to FMN in pentaerythritol tetranitrate reductase
Structural and mechanistic aspects of flavoproteins: Probes of hydrogen tunnelling

Parallel pathways and free-energy landscapes for enzymatic hydride transfer probed by hydrostatic pressure

Barrier compression enhances an enzymatic hydrogen-transfer reaction

Parallel pathways and free-energy landscapes for enzymatic hydride transfer probed by hydrostatic pressure

Barrier compression enhances an enzymatic hydrogen-transfer reaction

Probing coupled motions in enzymatic hydrogen tunnelling reactions: beyond temperature-dependence studies of kinetic isotope effects

Correction of pre-steady-state KIEs for isotopic impurities and the consequences of kinetic isotope fractionation

Driving force analysis of proton tunnelling across a reactivity series for an enzyme-substrate complex.

Making a single-chain four-helix bundle for redox chemistry studies

H-transfers in Photosystem II: What can we learn from recent lessons in the enzyme community?

Incorporation of hydrostatic pressure into models of hydrogen tunneling highlights a role for pressure-modulated promoting vibrations

Solvent as a probe of active site motion and chemistry during the hydrogen tunnelling reaction in morphinone reductase

Inter-flavin electron transfer in cytochrome P450 reductase - Effects of solvent and pH identify hidden complexity in mechanism

Secondary kinetic isotope effects as probes of environmentally-coupled enzymatic hydrogen tunneling reactions

Deep tunneling dominates the biologically important hydride transfer reaction from NADH to FMN in morphinone reductase

Atomistic insight into the origin of the temperature-dependence of kinetic isotope effects and H-tunnelling in enzyme systems is revealed through combined experimental studies and biomolecular simulation

Are environmentally coupled enzymatic hydrogen tunneling reactions influenced by changes in solution viscosity?

Promoting motions facilitate nuclear tunneling in flavoprotein enzymes

Magnetic field effect studies indicate reduced geminate recombination of the radical pair in substrate-bound adenosylcobalamin-dependent ethanolamine ammonia lyase

Mutagenesis of morphinone reductase induces multiple reactive configurations and identifies potential ambiguity in kinetic analysis of enzyme tunneling mechanisms

DNA binding suppresses human AIF-M2 activity and provides a connection between redox chemistry, reactive oxygen species, and apoptosis

Conformational dynamics of the cytochrome P450 BM3/N-palmitoylglycine complex: The proposed "proximal-distal" transition probed by temperature-jump spectroscopy

Redox characteristics of a de novo quinone protein

Proton tunneling in aromatic amine dehydrogenase is driven by a short-range sub-picosecond promoting vibration: Consistency of simulation and theory with experiment

Promoting motions in enzyme catalysis probed by pressure studies of kinetic isotope effects

α-secondary isotope effects as probes of "tunneling-ready" configurations in enzymatic H-tunneling: Insight from environmentally coupled tunneling models

Moving a phenol hydroxyl group from the surface to the interior of a protein: Effects on the phenol potential and pKA

Conversion of the Escherichia coli cytochrome b562 to an archetype cytochrome b: A mutant with bis-histidine ligation of heme iron
Protein engineering of cytochrome b562 for quinone binding and light-induced electron transfer