

Sam Hay

Manchester Institute of Biotechnology (MIB) and School of Chemistry
131 Princess St
M1 7DN
Manchester
United Kingdom
Email: Sam.Hay@manchester.ac.uk
Phone: +44 (0)161 306 5141

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

An Active Site Tyr Residue Guides the Regioselectivity of Lysine Hydroxylation by the Nonheme Iron Lysine-4-Hydroxylase enzymes: Through Proton-Coupled-Electron-Transfer

Cao, Y., Hay, S. & De Visser, S., 18 Apr 2024, In: Journal of the American Chemical Society.

Arginine Kinase Activates Arginine for Phosphorylation by Pyramidalization and Polarization

Falcioni, F., Robert W. Molt, J., Jin, Y., Waltho, J. P., Hay, S., Richards, N. G. J. & Blackburn, G. M., 16 Apr 2024, In: ACS Catalysis.

A Non-Canonical Nucleophile Unlocks a New Mechanistic Pathway in a Designed Enzyme

Hutton, A. E., Foster, J., Crawshaw, R., Hardy, F., Johannissen, L., Lister, T., Gerard, E., Birch - Price, Z., Obexer, R., Hay, S. & Green, A., 9 Feb 2024, (Accepted/In press) In: Nature Communications.

Redox driven B₁₂-ligand switch drives CarH photoresponse

Poddar, H., Rios-Santacruz, R., Heyes, D. J., Shanmugam, M., Brookfield, A., Johannissen, L. O., Levy, C. W., Jeffreys, L. N., Zhang, S., Sakuma, M., Colletier, J. P., Hay, S., Schirò, G., Weik, M., Scrutton, N. S. & Leys, D., Dec 2023, In: Nature Communications. 14, 1, 5082.

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

Bertran, A., Morbiato, L., Sawyer, J., Dalla Torre, C., Heyes, D. J., Hay, S., Timmel, C. R., Di Valentin, M., De Zotti, M. & Bowen, A., 25 Oct 2023, In: Journal of the American Chemical Society. 145, 42, p. 22859-22865

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

Camacho, I. S., Wall, E., Sazanovich, I. V., Gozzard, E., Towrie, M., Hunt, N. T., Hay, S. & Jones, A. R., 13 Oct 2023, (E-pub ahead of print) In: Chem. Comm.. 87

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

Fisher, K., Halliwell, T., Payne, K., Ragala, G., Hay, S., Rigby, S. & Leys, D., 1 Sept 2023, In: Journal of Biological Chemistry. 299, 9, 105086.

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

Natrajan, L., Thornton, M., Hemsworth, J., Hay, S., Parkinson, P. & Faulkner, S., 31 Jul 2023, In: Frontiers in Chemistry. 11, 1232690.

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

Gerard, E., Mokkaes, T., Johannissen, L., Warwicker, J., Spiess, R., Blanford, C. F., Hay, S., Heyes, D. & De Visser, S., 19 May 2023, (Accepted/In press) In: ACS Catalysis.

Reactivity Differences of Trigonal Pyramidal Nonheme Iron(IV)-Oxo and Iron(III)-Oxo Complexes: Experiment and Theory. Cao, Y., Valdez-Moreira, J. A., Hay, S., Smith, J. M. & De visser, S. P., 9 May 2023, (E-pub ahead of print) In: Chemistry – A European Journal.

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

Speirs, M., Hardman, S., Iorgu, A. I., Johannissen, L., Heyes, D., Scrutton, N., Sazanovich, I. V. & Hay, S., 23 Mar 2023, (Accepted/In press) In: Journal of Physical Chemistry Letters.

A Vitamin B2-Photocatalysed Approach to Methionine Analogues

Knowles, O. J., Johannissen, L. O., Crisenza, G. E. M., Hay, S., Leys, D. & Procter, D. J., 5 Dec 2022, In: Angewandte Chemie. International Edition. 61, 50

How a 10-epi-cubebol Synthase Avoids Premature Reaction Quenching to Form a Tricyclic Product at High Purity

Whitehead, J. N., Leferink, N. G. H., Komati Reddy, G., Levy, C. W., Hay, S., Takano, E. & Scrutton, N. S., 7 Oct 2022, In: ACS Catalysis. 12, 19, p. 12123–12131

Combined pulsed electron double resonance EPR and molecular dynamics investigations of calmodulin suggest effect of crowding agents on protein structure

Shanmugam, M., Kutta, R., Scrutton, N., Lovett, J. & Hay, S., 9 Aug 2022, (Accepted/In press) In: Biochemistry.

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

Kantakevičius, P., Mathiah, C., Johannissen, L. & Hay, S., 10 Mar 2022, (Accepted/In press) In: Journal of Chemical Theory and Computation.

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

Johannissen, L., Taylor, A., Hardman, S., Heyes, D., Scrutton, N. & Hay, S., 8 Mar 2022, (Accepted/In press) In: ACS Catalysis.

Molecular determinants of carbocation cyclisation in bacterial monoterpene synthases

Leferink, N., Escorcia, A. M., Ouwensloot, B. R., Johannissen, L. O., Hay, S., van der Kamp, M. W. & Scrutton, N., 10 Jan 2022, In: CHEMBIOCHEM.

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

Crawshaw, R., Crossley, A., Johannissen, L., Burke, A., Hay, S., Levy, C., Baker, D., Lovelock, S. & Green, A., 16 Dec 2021, In: Nature Chemistry.

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

Roberts, A., Whittall, D., Breitling, R., Takano, E., Blaker, J., Hay, S. & Scrutton, N., 3 Sept 2021, (Accepted/In press) In: Materials Today Bio.

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

Ortmayer, M., Hardy, F. J., Quesne, M. G., Fisher, K., Levy, C., Heyes, D. J., Catlow, C. R. A., Visser, S. P. D., Rigby, S. E. J., Hay, S. & Green, A. P., 26 Jul 2021, In: JACS Au.

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

Camacho, I., Black, R., Heyes, D., Johannissen, L. O., Ramakers, L. A. I., Bellina, B., Barran, P., Hay, S. & Jones, A. R., 5 May 2021, In: Chemical Science.

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

Ortmayer, M., Hardy, F., Quesne, M., Fisher, K., Levy, C., Heyes, D., Catlow, C. R. A., De Visser, S., Rigby, S., Hay, S. & Green, A., 23 Apr 2021, (Accepted/In press) In: JACS Au.

Photocatalysis as the 'master switch' of photomorphogenesis in early plant development

Heyes, D., Zhang, S., Taylor, A., Johannissen, L., Hardman, S., Hay, S. & Scrutton, N., 8 Mar 2021, In: Nature Plants.

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

Payne, K. A. P., Marshall, S. A., Fisher, K., Rigby, S. E. J., Cliff, M. J., Spiess, R., Cannas, D. M., Larrosa, I., Hay, S. & Leys, D., 5 Mar 2021, In: ACS Catalysis. 11, 5, p. 2865-2878 14 p.

Predicting New Protein Conformations from Molecular Dynamics Simulation Conformational Landscapes and Machine Learning

Jin, Y., Johannissen, L. & Hay, S., 25 Feb 2021, (E-pub ahead of print) In: Proteins: structure, function, and bioinformatics

Structure and mechanism of *Pseudomonas aeruginosa* PA0254/HudA, a prFMN-dependent pyrrole-2-carboxylic acid decarboxylase linked to virulence

Payne, K., Marshall, S., Fisher, K., Rigby, S., Cliff, M., Spiess, R., Cannas, D., Larrosa, I., Hay, S. & Leys, D., 5 Feb 2021, (Accepted/In press) In: ACS Catalysis.

Quantum Biology: An Update and Perspective

Kim, Y., Bertagna, F., D'Souza, E. M., Heyes, D. J., Johannissen, L. O., Nery, E. T., Pantelias, A., SanchezPedreno, A., Slocombe, L., Spencer, M. G., Al-Khalili, J., Engel, G. S., Hay, S., Hingley-Wilson, S. M., Jeevaratnam, K., Jones, A., Kattnig, D., Lewis, R., Sacchi, M., Scrutton, N., & 2 others Silva, S. R. P. & McFadden, J., 26 Jan 2021, In: Quantum Reports. 3, 1, p. 80-126

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

Burgess, L., Wilson, H., Jones, A. R., Hay, S. & Natrajan, L. S., 21 Dec 2020, In: Frontiers in Chemistry. 8, 613334.

How do vanadium chloroperoxidases generate hypochlorite from hydrogen peroxide and chloride? A computational study.

Bin Mubarak, M. Q. E., Gerard, E., Blanford, C. F., Hay, S. & De Visser, S., 4 Dec 2020, In: ACS Catalysis. 10, 23, p. 14067-14079 13 p.

Enzymatic C-H activation of aromatic compounds through CO₂ fixation

Aleku, G., Saaret, A., Bradshaw Allen, R., Derrington, S., Titchiner, G., Gostimskaya, I., Gahloth, D., Parker, D. A., Hay, S. & Leys, D., 1 Nov 2020, In: Nature chemical biology. 16, 11, p. 1255-1260 6 p.

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

Zhang, S., Godwin, A., Taylor, A., Hardman, S., Jowitt, T., Johannissen, L., Hay, S., Baldock, C., Heyes, D. & Scrutton, N., 31 Aug 2020, (E-pub ahead of print) In: The FEBS Journal.

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

Roberts, A., Finnigan, W., Kelly, P., Faulkner, M., Breitling, R., Takano, E., Scrutton, N., Blaker, J. & Hay, S., 10 Jul 2020, In: Materials Today Bio. 7, p. 100068

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

Burgess, L., Wilson, H., Jones, A., Hay, S. & Natrajan, L., 7 Jul 2020, (Accepted/In press) In: Methods and Applications in Fluorescence.

Ultrafast Vibrational Energy Transfer between Protein and Cofactor in a Flavoenzyme

Hardman, S. J. O., Iorgu, A. I., Heyes, D. J., Scrutton, N. S., Sazanovich, I. V. & Hay, S., 4 Jun 2020, (E-pub ahead of print) In: The Journal of Physical Chemistry B.

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

Natrajan, L., Hay, S., Burgess, L., Harvey, P. & Jones, A., 31 May 2020, In: Chemistry – A European Journal.

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

Phillips, R. S., Craig, S., Kovalevsky, A. Y., Gerlits, O. O., Weiss, K. L., Iorgu, A. I., Heyes, D. J. & Hay, S., 2020, In: ACS Catalysis.

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

Ortmayer, M., Fisher, K., Basran, J., Wolde-Michael, E. M., Heyes, D. J., Levy, C., Lovelock, S. L., Anderson, J. L. R., Raven, E. L., Hay, S., Rigby, S. E. J. & Green, A. P., 2020, In: ACS Catalysis. 10, 4, p. 2735-2746 12 p.

Taming the reactivity of monoterpene synthases to guide regioselective product hydroxylation

Leferink, N., Ranaghan, K. E., Battye, J., Johannissen, L., Hay, S., Kamp, M. W. V. D., Mulholland, A. J. & Scrutton, N., 2020, In: CHEMBIOCHEM. 20, p. 1-7 7 p.

Structural basis for enzymatic photocatalysis in chlorophyll biosynthesis

Zhang, S., Heyes, D. J., Feng, L., Sun, W., Johannissen, L. O., Liu, H., Levy, C. W., Li, X., Yang, J., Yu, X., Lin, M., Hardman, S. J. O., Hoeven, R., Sakuma, M., Hay, S., Leys, D., Rao, Z., Zhou, A., Cheng, Q. & Scrutton, N. S., 23 Oct 2019, In: Nature. 574, p. 722-725

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

Bailey, S., Payne, K., Saaret, A., Marshall, S., Gostimskaya, I., Kosov, I., Fisher, K., Hay, S. & Leys, D., 16 Sept 2019, In: Nature Chemistry. 11, p. 1049-1057

Graphene–aramid nanocomposite fibres via superacid co-processing

Roberts, A., Kelly, P., Bain, J., Morrison, J., Wimpenny, I., Barrow, M., Woodward, R. T., Gresil, M., Blanford, C. F., Hay, S., Blaker, J., Yeates, S. & Scrutton, N., 11 Sept 2019, In: Chemical Communications.

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

Czarnota, S., Johannissen, L. O., Baxter, N. J., Rummel, F., Wilson, A., Cliff, M. J., Levy, C. W., Scrutton, N. S., Waltho, J. P. & Hay, S., 2019, In: ACS Catalysis. 9, 5, p. 4394-4401 8 p.

Isotopically labeled flavoenzymes and their uses in probing reaction mechanisms

Iorgu, A. I., Cliff, M., Waltho, J., Scrutton, N. & Hay, S., 2019, In: Methods in Enzymology.

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

Matthews, S., Pacholarz, K., France, A., Jowitt, T., Hay, S., Barran, P. & Munro, A., 2019, In: ACS Infectious Diseases. 8, 5(11), p. 1855-1866 12 p., doi: 10.1021/acsinfecdis.9b00181.

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

Iorgu, A. I., Hedison, T., Hay, S. & Scrutton, N., 2019, In: The FEBS Journal.

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

Roberts, A., Finnigan, W., Wolde-Michael, E., Kelly, P., Blaker, J., Hay, S., Breitling, R., Takano, E. & Scrutton, N., 2019, In: MRS Communications.

The Photochemical Spin Dynamics of the Vitamin B12 Derivative, Methylcobalamin

Lukinović, V., Woodward, J. R., Marrafa, T. C., Shanmugam, M., Heyes, D. J., Hardman, S. J. O., Scrutton, N. S., Hay, S., Fielding, A. J. & Jones, A. R., 2019, In: The Journal of Physical Chemistry B.

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

Hedison, T., Shenoy, R., Iorgu, A. I., Heyes, D., Fisher, K., Wright, G., Hay, S., Eady, R. R., Antonyuk, S., Hasnain, S. S. & Scrutton, N. S., 2019, In: ACS Catalysis.

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

Johannissen, L. O., Iorgu, A. I., Scrutton, N. & Hay, S., 2019, In: Faraday Discussions.

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

Iorgu, A. I., Baxter, N. J., Cliff, M. J., Levy, C., Waltho, J. P., Hay, S. & Scrutton, N. S., 7 Dec 2018, In: ACS Catalysis. 8, 12, p. 11589-11599 11 p.

Trapping methods for probing functional intermediates in nitric oxide synthases and related enzymes

Hedison, T., Hay, S. & Scrutton, N., 1 Jun 2018, In: Frontiers in Bioscience. 23, 10, p. 1874-1888 14 p.

H-1, N-15 and C-13 backbone resonance assignments of pentaerythritol tetranitrate reductase from *Enterobacter cloacae* PB2

Iorgu, A. I., Baxter, N. J., Cliff, M. J., Waltho, J. P., Hay, S. & Scrutton, N. S., Apr 2018, In: Biomolecular NMR Assignments. 12, 1, p. 79-83 5 p.

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

Plasch, K., Hofeř, G., Keller, W., Hay, S., Heyes, D., Dennig, A., Glueck, S. M. & Faber, K., 2018, In: Green Chemistry.

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

Hay, S., 20 Sept 2017, *Methods in Enzymology: Measurement and Analysis of Kinetic Isotope Effects*. Vol. 596.

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

Natrajan, L., Hay, S., Jones, A., Harvey, P., Oakland, C., Burgess, L. & Andrews, M., 3 Aug 2017, In: European Journal of Inorganic Chemistry. 10 p.

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

Liu, K-C., Hughes, J., Hay, S. & Scrutton, N., 17 Jul 2017, In: The FEBS Journal. 284, 14, p. 2302-2319 18 p.

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

Appel, E. A., Biedermann, F., Hoogland, D., del Barrio, J., Driscoll, M. D., Hay, S., Wales, D. J. & Scherman, O. A., 29 Jun 2017, In: Journal of the American Chemical Society. 139, 37, p. 12985-12993

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

Czarnota, S., Baxter, N. J., Cliff, M. J., Waltho, J. P., Scrutton, N. S. & Hay, S., Apr 2017, In: Biomolecular NMR Assignments. 11, 1, p. 57-61 5 p.

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

Hedison, T., Hay, S. & Scrutton, N., 28 Feb 2017, In: Nitric Oxide: Biology and Chemistry. 63, p. 61-67 7 p.

A common mechanism for coenzyme cobalamin-dependent reductive dehalogenases

Johannissen, L., Leys, D. & Hay, S., 2017, In: Physical Chemistry Chemical Physics. 19, 8, p. 6090-6094 5 p.

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

Delgado, M., Gorlich, S., Longbotham, J. E., Scrutton, N., Hay, S., Moliner, V. & Tuñón, I., 2017, In: ACS Catalysis. 7, p. 3190-3198

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

Karupiah, V., Ranaghan, K. E., Leferink, N., Johannissen, L., Shanmugam, M., Ni Cheallaigh, A., Bennett, N. J., Takano, E., Gardiner, J., van der Kamp, M. W., Hay, S., Mulholland, A. J., Leys, D. & Scrutton, N., 2017, In: ACS Catalysis.

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

Ortmayer, M., Lafite, P., Menon, B. R. K., Tralau, T., Fisher, K., Denkhaus, L., Scrutton, N., Rigby, S., Munro, A., Hay, S. & Leys, D., 16 Nov 2016, In: Nature. 539, 7630, p. 593-597 5 p.

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

Longbotham, J. E., Hardman, S., Gorlich, S., Scrutton, N. & Hay, S., 27 Sept 2016, In: Journal of the American Chemical Society. 138, 41, p. 13693–13699

Correlating calmodulin landscapes with chemical catalysis in neuronal nitric oxide synthase using time-resolved FRET and a 5- deazaflavin thermodynamic trap.

Hedison, T., Leferink, N., Hay, S. & Scrutton, N., 5 Aug 2016, In: ACS Catalysis. 6, 8, p. 5170–5180 11 p.

A 'Plug and Play' Platform for the Production of Diverse Monoterpene Hydrocarbon Scaffolds in Escherichia coli

Leferink, N., Jervis, A., Zebec, Z., Toogood, H., Hay, S., Takano, E. & Scrutton, N., Jun 2016, In: ChemistrySelect . 1, 9, p. 1893-1896 4 p.

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

Morra, R., Shankar, J., Robinson, C., Halliwell, S., Butler, L., Upton, M., Hay, S., Micklefield, J. & Dixon, N., 18 Feb 2016, In: Nucleic acids research. 44, 3, e21.

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

Miwa, S., Treumann, A., Bell, A., Vistoli, G., Nelson, G., Hay, S. & von Zglinicki, T., 1 Jan 2016, In: Free radical biology & medicine. 90, p. 173-183

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

Geddes, A., Paul, C. E., Hay, S., Hollmann, F. & Scrutton, N., 2016, In: Journal of the American Chemical Society. 138, 35

Ground-state Destabilization by Phe⁴⁴⁸ and Phe⁴⁴⁹ Contributes to Tyrosine Phenol-lyase Catalysis

Phillips, R. S., Vita, A., Spivey, J. B., Rudloff, A. P., Driscoll, M. & Hay, S., 2016, In: ACS Catalysis. 6, 10, p. 6770-6779 9 p.

Time course analysis of enzyme-catalyzed DNA polymerization

Rentergent, J., Driscoll, M. & Hay, S., 2016, In: Biochemistry. 55, 39, p. 5622–5634 13 p.

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

Johannissen, L., Hay, S. & Scrutton, NS., 18 Nov 2015, In: Physical Chemistry Chemical Physics. 17, 46, p. 30775-30782 8 p.

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

Hedison, T. M., Hay, S. & Scrutton, N., 16 Sept 2015, In: The FEBS Journal. 282, 22, p. 4357–4375 19 p.

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

Hoeven, R., Heyes, D. J., Hay, S. & Scrutton, NS., 2015, In: The FEBS Journal. 282, 16, p. 3243-3255 12 p.

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

Jones, A. R., Rentergent, J., Scrutton, NS. & Hay, S., 2015, In: Chemistry. 21, 24, p. 8826-8831 5 p.

Structure and Mechanism of a Viral Collagen Prolyl Hydroxylase

Longbotham, J. E., Levy, C., Johannissen, L. O., Tarhonskaya, H., Jiang, S., Loenarz, C., Flashman, E., Hay, S., Schofield, C. J. & Scrutton, N. S., 2015, In: *Biochemistry*. 54, 39, p. 6093-6105 13 p.

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

Leferink, N., Hay, S., Rigby, S. E. J. & Scrutton, N. S., 2015, In: *The FEBS Journal*. 282, 16, p. 3016-3029 13 p.

Energy landscapes and catalysis in nitric-oxide synthase

Sobolewska-Stawiarz, A., Leferink, N. G. H., Fisher, K., Heyes, D. J., Hay, S., Rigby, S. E. J. & Scrutton, N. S., 25 Apr 2014, In: *Journal of Biological Chemistry*. 289, 17, p. 11725-11738 13 p.

Ratiometric detection of enzyme turnover and flavin reduction using rare-earth upconverting phosphors

Harvey, P., Oakland, C., Driscoll, M. D., Hay, S. & Natrajan, L. S., 14 Apr 2014, In: *Dalton Transactions*. 43, 14, p. 5265-5268 3 p.

A quantitative fluorescence-based steady-state assay of DNA polymerase

Driscoll, M. D., Rentergent, J. & Hay, S., Apr 2014, In: *FEBS Journal*. 281, 8, p. 2042-2050 9 p.

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

Kandathil, S. M., Driscoll, M. D., Dunn, R. V., Scrutton, N. S. & Hay, S., 14 Feb 2014, In: *Physical Chemistry Chemical Physics*. 16, 6, p. 2256-2259 3 p.

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

Pudney, C. R., Hay, S., Scrutton, N. S., Weber, S. (ed.) & Schleicher, E. (ed.), 2014, In: *Methods in Molecular Biology*. 1146, p. 161-175

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

Hardman, S. J. O., Pudney, C. R., Hay, S. & Scrutton, N. S., 3 Dec 2013, In: *BIOPHYSICAL JOURNAL*. 105, 11, p. 2549-2558 9 p.

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

Russell, H. J., Hardman, S. J. O., Heyes, D. J., Hough, M. A., Greetham, G. M., Towrie, M., Hay, S. & Scrutton, N. S., Dec 2013, In: *FEBS Journal*. 280, 23, p. 6070-6082 12 p.

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

Chen, Z. G., Zietek, M. A., Russell, H. J., Tait, S., Hay, S., Jones, A. R. & Scrutton, N. S., Sept 2013, In: *ChemBioChem: a European journal of chemical biology*. 14, 13, p. 1529-1533 4 p.

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

Jones, A. R., Levy, C., Hay, S. & Scrutton, N. S., Jul 2013, In: *FEBS Journal*. 280, 13, p. 2997-3008 11 p.

Enzymatic single-molecule kinetic isotope effects

Pudney, C. R., Lane, R. S. K., Fielding, A. J., Magennis, S. W., Hay, S. & Scrutton, N. S., 13 Mar 2013, In: *Journal of the American Chemical Society*. 135, 10, p. 3855-3864 9 p.

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

Pudney, C. R., Guerriero, A., Baxter, N. J., Johannissen, L. O., Waltho, J. P., Hay, S. & Scrutton, N. S., 20 Feb 2013, In: *Journal of the American Chemical Society*. 135, 7, p. 2512-2517 5 p.

Protein motions are coupled to the reaction chemistry in coenzyme B 12-dependent ethanolamine ammonia lyase
Russell, H. J., Jones, A., Hay, S., Greetham, G. M., Towrie, M. & Scrutton, N., 10 Sept 2012, In: *Angewandte Chemie International Edition*. 51, 37, p. 9306-9310 4 p.

Evidence of preorganization in quinonoid intermediate formation from I-Trp in H463F mutant Escherichia coli tryptophan indole-lyase from effects of pressure and pH
Phillips, R. S., Kalu, U. & Hay, S., 21 Aug 2012, In: *Biochemistry*. 51, 33, p. 6527-6533 6 p.

Pressure effects on enzyme-catalyzed quantum tunneling events arise from protein-specific structural and dynamic changes
Hay, S., Johannissen, L. O., Hothi, P., Sutcliffe, M. J. & Scrutton, N. S., 13 Jun 2012, In: *Journal of the American Chemical Society*. 134, 23, p. 9749-9754 5 p.

Ultrafast infrared spectral fingerprints of Vitamin B12 and related cobalamins
Jones, A., Russell, H. J., Greetham, G. M., Towrie, M., Hay, S. & Scrutton, N., 21 May 2012, In: *Journal of Physical Chemistry A*. 116, 23, p. 5586-5594 9 p.

Preparation and photophysical properties of a caged kynurenine
Maitrani, C., Heyes, D. J., Hay, S., Arumugam, S., Popik, V. V. & Phillips, R. S., 15 Apr 2012, In: *Bioorganic and Medicinal Chemistry Letters*. 22, 8, p. 2734-2737 3 p.

Good vibrations in enzyme-catalysed reactions
Hay, S. & Scrutton, N. S., Mar 2012, In: *Nature Chemistry*. 4, 3, p. 161-168 7 p.

Experimental approaches towards proton-coupled electron transfer reactions in biological redox systems
Brenner, S., Hay, W. S., Heyes, D. J. & Scrutton, N. S., 2012, *RSC Catalysis Series/RSC Catal. Ser.*. Cambridge, UK: Royal Society of Chemistry, p. 57-88 31 p.

Is there a dynamic protein contribution to the substrate trigger in coenzyme B 12-dependent ethanolamine ammonia lyase?
Jones, A. R., Hardman, S. J. O., Hay, S. & Scrutton, N. S., 11 Nov 2011, In: *Angewandte Chemie - International Edition*. 50, 46, p. 10843-10846 3 p.

Electrochemical and structural properties of a protein system designed to generate tyrosine pourbaix diagrams
Martínez-Rivera, M. C., Berry, B. W., Valentine, K. G., Westerlund, K., Hay, S. & Tommos, C., 9 Nov 2011, In: *Journal of the American Chemical Society*. 133, 44, p. 17786-17795 9 p.

Examining the importance of dynamics, barrier compression and hydrogen tunnelling in enzyme catalysed reactions
Hay, S. & Scrutton, N. S., 2011, In: *Procedia Chemistry*. 3, 1, p. 306-315 9 p.

Direct analysis of donor-acceptor distance and relationship to isotope effects and the force constant for barrier compression in enzymatic H-tunneling reactions
Pudney, C., Johannissen, L., Sutcliffe, M. J., Hay, S. & Scrutton, N. S., 18 Aug 2010, In: *Journal of the American Chemical Society*. 132, 32, p. 11329-11335 6 p.

Probing active site geometry using high pressure and secondary isotope effects in an enzyme-catalysed 'deep' H-tunnelling reaction
Hay, S., Pudney, C. R., Sutcliffe, M. J. & Scrutton, N. S., Jul 2010, In: *Journal of Physical Organic Chemistry*. 23, 7, p. 696-701 5 p.

Barrier compression and its contribution to both classical and quantum mechanical aspects of enzyme catalysis
Hay, S., Johannissen, L. O., Sutcliffe, M. J. & Scrutton, N. S., 6 Jan 2010, In: *BIOPHYSICAL JOURNAL*. 98, 1, p. 121-128 7 p.

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

Pudney, C., Hay, S., Levy, C., Pang, J., Sutcliffe, M. J., Leys, D. & Scrutton, N. S., 2 Dec 2009, In: Journal of the American Chemical Society. 131, 47, p. 17072-17073 1 p.

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

Hay, S., Evans, R. M., Levy, C., Loveridge, E. J., Wang, X., Leys, D., Allemann, R. K. & Scrutton, N. S., 21 Sept 2009, In: ChemBioChem: a European journal of chemical biology . 10, 14, p. 2348-2353 5 p.

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

Brenner, S., Heyes, D. J., Hay, S., Hough, M. A., Eady, R. R., Hasnain, S. S. & Scrutton, N. S., 18 Sept 2009, In: Journal of Biological Chemistry. 284, 38, p. 25973-25983 10 p.

Bipartite recognition and conformational sampling mechanisms for hydride transfer from nicotinamide coenzyme to FMN in pentaerythritol tetranitrate reductase

Pudney, C. R., Hay, S. & Scrutton, N. S., Sept 2009, In: FEBS Journal. 276, 17, p. 4780-4789 9 p.

Structural and mechanistic aspects of flavoproteins: Probes of hydrogen tunnelling

Hay, S., Pudney, C. R. & Scrutton, N. S., Aug 2009, In: FEBS Journal. 276, 15, p. 3930-3941 11 p.

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

Pudney, C. R., McGrory, T., Lafite, P., Pang, J., Hay, S., Leys, D., Sutcliffe, M. J. & Scrutton, N. S., 25 May 2009, In: ChemBioChem: a European journal of chemical biology . 10, 8, p. 1379-1384 5 p.

Barrier compression enhances an enzymatic hydrogen-transfer reaction

Hay, S., Pudney, C. R., McGrory, T. A., Pang, J., Sutcliffe, M. J. & Scrutton, N. S., 9 Feb 2009, In: Angewandte Chemie - International Edition. 48, 8, p. 1452-1454 2 p.

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

Hay, S., Sutcliffe, M. & Scrutton, N. S., 2009, *Quantum tunnelling in enzyme-catalysed reactions*. London: Royal Society of Chemistry, p. 199-218 20 p.

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

Hay, S., Pudney, C. R., Hothi, P. & Scrutton, N. S., 18 Dec 2008, In: Journal of Physical Chemistry A. 112, 50, p. 13109-13115 6 p.

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

Hothi, P., Hay, S., Roujeinikova, A., Sutcliffe, M. J., Lee, M., Leys, D., Cullis, P. M. & Scrutton, N. S., 24 Nov 2008, In: ChemBioChem: a European journal of chemical biology . 9, 17, p. 2839-2845 6 p.

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

Westerlund, K., Moran, S. D., Privett, H. K., Hay, S., Jarvet, J., Gibney, B. R. & Tommos, C., Nov 2008, In: Protein Engineering, Design and Selection. 21, 11, p. 645-652 7 p.

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

Hay, S. & Scrutton, N. S., Oct 2008, In: Photosynthesis Research. 98, 1-3, p. 169-177 8 p.

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

Hay, S. & Scrutton, N. S., 16 Sept 2008, In: Biochemistry. 47, 37, p. 9880-9887 7 p.

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

Hay, S., Pudney, C. R., Sutcliffe, M. J. & Scrutton, N. S., 15 Sept 2008, In: ChemPhysChem. 9, 13, p. 1875-1881 6 p.

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

Brenner, S., Hay, S., Munro, A. W. & Scrutton, N. S., Sept 2008, In: FEBS Journal. 275, 18, p. 4540-4557 17 p.

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

Hay, S., Pang, J., Monaghan, P. J., Wang, X., Evans, R. M., Sutcliffe, M. J., Allemann, R. K. & Scrutton, N. S., 4 Aug 2008, In: ChemPhysChem. 9, 11, p. 1536-1539 3 p.

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

Pang, J., Hay, S., Scrutton, N. S. & Sutcliffe, M. J., 4 Jun 2008, In: Journal of the American Chemical Society. 130, 22, p. 7092-7097 5 p.

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

Hay, S., Pudney, C., Hothi, P., Johannissen, L. O., Masgrau, L., Pang, J., Leys, D., Sutcliffe, M. J. & Scrutton, N. S., Feb 2008, In: Biochemical Society Transactions. 36, 1, p. 16-21 5 p.

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

Hay, S., Pudney, C. R., Sutcliffe, M. J. & Scrutton, N. S., 2008, In: Angewandte Chemie - International Edition. 47, 3, p. 537-540 3 p.

Promoting motions facilitate nuclear tunneling in flavoprotein enzymes

Hay, S., Pudney, C. R., Pang, J., Leys, D., Sutcliffe, M. J. & Scrutton, N. S., 2008, *Flavins and Flavoproteins 2008*. Prentice Hall, p. 415-426

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

Jones, A. R., Hay, S., Woodward, J. R. & Scrutton, N. S., 19 Dec 2007, In: Journal of the American Chemical Society. 129, 50, p. 15718-15727 9 p.

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

Pudney, C. R., Hay, S., Pang, J., Costello, C., Leys, D., Sutcliffe, M. J. & Scrutton, N. S., 14 Nov 2007, In: Journal of the American Chemical Society. 129, 45, p. 13949-13956 7 p.

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

Gong, M., Hay, S., Marshall, K. R., Munro, A. W. & Scrutton, N. S., 12 Oct 2007, In: Journal of Biological Chemistry. 282, 41, p. 30331-30340 9 p.

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

Brenner, S., Hay, S., Girvan, H. M., Munro, A. W. & Scrutton, N. S., 12 Jul 2007, In: Journal of Physical Chemistry B. 111, 27, p. 7879-7886 7 p.

Redox characteristics of a de novo quinone protein

Hay, S., Westerlund, K. & Tommos, C., 5 Apr 2007, In: Journal of Physical Chemistry B. 111, 13, p. 3488-3495 7 p.

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

Johannissen, L. O., Hay, S., Scrutton, N. S. & Sutcliffe, M. J., 15 Mar 2007, In: Journal of Physical Chemistry B. 111, 10, p. 2631-2638 7 p.

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

Hay, S., Sutcliffe, M. J. & Scrutton, N. S., 9 Jan 2007, In: Proceedings of the National Academy of Sciences of the United States of America. 104, 2, p. 507-512 5 p.

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

Pudney, C. R., Hay, S., Sutcliffe, M. J. & Scrutton, N. S., 1 Nov 2006, In: Journal of the American Chemical Society. 128, 43, p. 14053-14058 5 p.

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

Hay, S., Westerlund, K. & Tommos, C., 6 Sept 2005, In: Biochemistry. 44, 35, p. 11891-11902 11 p.

Conversion of the Escherichia coli cytochrome b562 to an archetype cytochrome b: A mutant with bis-histidine ligation of heme iron

Hay, S. & Wydrzynski, T., 11 Jan 2005, In: Biochemistry. 44, 1, p. 431-439 8 p.

Protein engineering of cytochrome b562 for quinone binding and light-induced electron transfer

Hay, S., Wallace, B. B., Smith, T. A., Ghiggino, K. P. & Wydrzynski, T., 21 Dec 2004, In: Proceedings of the National Academy of Sciences of the United States of America. 101, 51, p. 17675-17680 5 p.