

John B. O. Mitchell  
School of Chemistry  
Biomedical Sciences Research Complex

EaSTCHEMA

**Type of address: Postal address.**

School of Chemistry, Biomolecular Sciences Building, North Haugh, St Andrews,  
KY16 9ST, UK

Email: [jbom@st-andrews.ac.uk](mailto:jbom@st-andrews.ac.uk)

Phone: +44 (0)1334 467259

Web address: <https://bsrc.st-andrews.ac.uk/>



## Research overview

Our research covers everything that is broadly both chemical and computational. Some of the main themes are described below, but if you're just after a list of publications, here you are.

### Machine Learning

A substantial part of computational chemistry involves building mathematical models to analyse data. The Machine Learning (ML) part of our work comprises everything that is not an attempt realistically to model the processes by which the real world actually works. In jargon, this is everything that is not physics-based. Such tasks might firstly be regression, that is predicting numerical values such as solubilities. Secondly they might be classification, assigning items such as molecules to classes like "toxic" or "non-toxic". Thirdly, they might be clustering, finding patterns in unlabelled data. In our group, we use such models to predict and calculate properties such as solubility, bioactivity and toxicity.

Such modelling in fact has a long history in chemistry, dating back to the 19th century. However, for much of that time models were limited to simple linear regressions. In the latter part of the 20th century, the field developed through building QSAR (Quantitative Structure-Activity Relationship) and QSPR (ditto, but now it's Structure-Property) models with multi-linear regression, and then onto non-linear methods. The field was usually known as chemoinformatics (or cheminformatics, being unsure how to spell its own name). In the modern era, the sophistication of the models has increased to a point where it's more descriptive, and certainly more widely understood, to call these techniques Machine Learning.

What about Artificial Intelligence (AI) - can we cut a divide between ML and AI? Probably not a clear one. As Google DeepMind executive Mat Veloso said: "*If it is written in Python, it's probably machine learning. If it is written in PowerPoint, it's probably AI.*" While there's clearly a substantial overlap between the categories, we tend to refer to souped up non-linear regression models as ML, but to LLMs as AI. Nonetheless, under the lid, LLMs are just large neural networks doing neural network things like optimising weights.

### Molecular Simulation

By way of contrast, molecular simulation is definitely a physics-based approach. We set up in the computer a mathematical representation of the molecules involved, one that typically includes the chemical nature and spatial coordinates of each constituent atom. The computer then produces a possible future of that molecular system, calculating its response to its physical and chemical environment at each timestep to create a trajectory, in a process known as Molecular Dynamics.

If carried out intelligently, such methods can provide great scientific insight into the behaviour of the system, covering things such as structure, energy, interactions with other molecules, phase changes and much more. Typically, simulations are carried out with the molecules contained in 3-dimensional boxes that are stacked together without limit in all directions and fill space with no gaps, a scenario described as having "periodic boundary conditions." Our group use such methods for structural studies of the interactions between enzymes and their substrates, with applications like plastic-eating enzymes and new medicines.

The forces, or more explicitly the interaction energies, between molecules are defined by a "force field", which has little to do with science fiction but a lot to do with the fundamental physical processes governing the attractive and repulsive interactions amongst atoms and molecules. This forms a major part of the scientific input into simulations. Historically, force fields have been either fitted to experiment or parameterised via theoretical calculation, but increasingly they are now being generated through ML.

### Quantum Chemistry

For all the usefulness of simulations, typically their force fields know nothing about covalent bond making or breaking, which means that they can't be used to study chemical reactions, molecular orbitals or even the vibrational motions of molecules. Instead, a more chemically intelligent approach is required, and this is provided by the electronic structure methods of quantum chemistry. Such approaches are known as "first principles," due to their sound basis in atomic and molecular quantum mechanics.

The most foundational such method historically has been Hartree-Fock self-consistent field theory (HF). However, in this century, Density Functional Theory (DFT) has become a much more widely known and used alternative, largely because it generally gives a more accurate result at a lesser cost.

We use quantum chemical methods such as HF and DFT for a variety of applications, including the energetics of chemical reactions, development of force fields, physics-based calculation of solubility and the prediction of crystal structures. While our group are very much users rather than developers of quantum chemical methods, we appreciate their central role in computational chemistry.

## Bioinformatics

The sequential and alphabetical nature of both DNA and proteins makes them a rich source of computational research. Study of these essential and foundational biomolecules provides a window into the evolutionary history of life and its chemistry, as well as the impressive structural diversity of protein folds. Our own research frequently occupies the interface between chemistry and biology, the interactions between large biological polymers and smaller molecules being fundamental to processes of life and disease alike.

Much of our work in these areas has centred on enzymes, their chemical functions and their evolutionary histories. In this post-AlphaFold era, we continue to seek out new research questions that can shed light on the rich and diverse repertoire of biochemistry. In this endeavour, we frequently collaborate with colleagues in Biology as well as Chemistry.

Additional information about the current Mitchell Group can be found here: <https://jbomgroup.wp.st-andrews.ac.uk/>

## Qualifications

Doctor of Philosophy, Theoretical Studies of Hydrogen Bonding, University of Cambridge

1 Oct 1987 → 30 Sept 1990

Award Date: 2 Feb 1991

## Employment

### Reader

School of Chemistry

University of St Andrews

St Andrews, United Kingdom

1 Aug 2009 → present

### Biomedical Sciences Research Complex

University of St Andrews

United Kingdom

1 Aug 2009 → present

### EaSTCHEMA

University of St Andrews

United Kingdom

1 Aug 2009 → present

## Research outputs

### Revisiting the application of machine learning approaches in predicting aqueous solubility

Zheng, T., Mitchell, J. B. O. & Dobson, S. A., 13 Aug 2024, In: ACS Omega. 9, 32, p. 35209-35222 14 p.

### Robust identification of interactions between heat-stress responsive genes in the chicken brain using Bayesian networks and augmented expression data

Videla Rodriguez, E. A., Mitchell, J. B. O. & Smith, V. A., 19 Apr 2024, In: Scientific Reports. 14, 8 p., 9019.

### Allosteric activation unveils protein-mass modulation of ATP phosphoribosyltransferase product release

Read, B., Mitchell, J. B. O. & da Silva, R. G., 6 Apr 2024, In: Communications Chemistry. 7, 13 p., 77.

### Crystal structure, steady-state and pre-steady-state kinetics of *Acinetobacter baumannii* ATP phosphoribosyltransferase

Read, B., Cadzow, A., Alphey, M. S., Mitchell, J. B. O. & da Silva, R. G., 16 Jan 2024, In: Biochemistry. 63, 2, p. 230-240 11 p.

### Computational insights into the catalytic mechanism of *is*-PETase: an enzyme capable of degrading poly(ethylene) terephthalate

Shrimpton-Phoenix, E., Mitchell, J. B. O. & Buehl, M., 15 Dec 2022, In: Chemistry - A European Journal. 28, 70, 7 p., e202201728.

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Mann, P. S., Smith, V. A., Mitchell, J. B. O. & Dobson, S. A., 20 Jul 2022, In: Physical Review. E, Statistical, nonlinear, and soft matter physics. 106, 1, 20 p., 014304.

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**Exact formula for bond percolation on cliques**

Mann, P. S., Smith, V. A., Mitchell, J. B. O., Jefferson, C. A. & Dobson, S. A., 4 Aug 2021, In: Physical Review E - Statistical, Nonlinear, and Soft Matter Physics. 104, 2, 10 p., 024304 .

**Symbiotic and antagonistic disease dynamics on clustered networks using bond percolation**

Mann, P. S., Smith, V. A., Mitchell, J. B. O. & Dobson, S. A., 3 Aug 2021, In: Physical Review. E, Statistical, nonlinear, and soft matter physics. 104, 2, 9 p., 024303 .

**Two-pathogen model with competition on clustered networks**

Mann, P. S., Smith, V. A., Mitchell, J. B. O. & Dobson, S. A., 17 Jun 2021, In: Physical Review. E, Statistical, nonlinear, and soft matter physics. 103, 6, 8 p., 062308.

**Toward physics-based solubility computation for pharmaceuticals to rival informatics**

Fowles, D. J., Palmer, D. S., Guo, R., Price, S. L. & Mitchell, J. B. O., 8 Jun 2021, In: Journal of Chemical Theory and Computation. 17, 6, p. 3700-3709 10 p.

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**The natural history of biocatalytic mechanisms**

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Nigsch, F., Bender, A., van Buuren, B., Tissen, J., Nigsch, E. & Mitchell, J. B. O., 27 Nov 2006, In: *Journal of Chemical Information and Modeling*. 46, 6, p. 2412-2422 11 p.

**Classification of enzyme reaction mechanisms**

O'Boyle, N. M., Holliday, G. L., Almonacid, D. E., Murray-Rust, P., Mitchell, J. B. O. & Thornton, J. M., 26 Mar 2006, In: *Abstracts of Papers of the American Chemical Society*. 231, p. - 1 p.

**Classifying the world anti-doping agency's 2005 prohibited list using the Chemistry Development Kit fingerprint**

Cannon, E. O. & Mitchell, J. B. O., 2006, *Computational Life Sciences II: Second International Symposium, CompLife 2006, Cambridge, UK, September 27-29, 2006, Proceedings*. Berthold, M. R., Glen, R. & Fischer, I. (eds.). Springer, p. 173-182 10 p. (Lecture Notes in Computer Science; vol. 4216).

**MACiE: a database of enzyme reaction mechanisms**

Holliday, G. L., Bartlett, G. J., Almonacid, D. E., O'Boyle, N. M., Murray-Rust, P., Thornton, J. M. & Mitchell, J. B. O., Dec 2005, In: Bioinformatics. 21, 23, p. 4315-4316 2 p.

**Communication and re-use of chemical information in bioscience**

Murray-Rust, P., Mitchell, J. B. O. & Rzepa, H. S., 18 Jul 2005, In: BMC Bioinformatics. 6, 15 p., 180.

**Chemistry in Bioinformatics**

Murray-Rust, P., Mitchell, J. B. O. & Rzepa, H. S., 7 Jun 2005, In: BMC Bioinformatics. 6, 4 p., 141.

**Knowledge based potentials: the reverse Boltzmann methodology, virtual screening and molecular weight dependence**

Kirtay, C. K., Mitchell, J. B. O. & Lumley, J. A., Jun 2005, In: QSAR and Combinatorial Science. 24, 4, p. 527-536 10 p.

**CMLSnap: Animated reaction mechanisms**

Holliday, G. L., Mitchell, J. B. O. & Murray-Rust, P., 26 Oct 2004, In: Internet Journal of Chemistry. 7, 4, 6 p.

**Comparative evaluation of five scoring functions for accurate prediction of protein-ligand binding energy.**

Puvanendrampillai, D., Marsden, P. M., Mitchell, J. B. O. & Glen, R. C., 28 Mar 2004, In: Abstracts of Papers of the American Chemical Society. 227, p. U1018-U1018 1 p.

**A structure-odour relationship study using EVA descriptors and hierarchical clustering**

Takane, S. Y. & Mitchell, J. B. O., 2004, In: Organic & Biomolecular Chemistry. 2, 22, p. 3250-3255 6 p.

**Predicting protein-ligand binding affinities: a low scoring game?**

Marsden, P. M., Puvanendrampillai, D., Mitchell, J. B. O. & Glen, R. C., 2004, In: Organic & Biomolecular Chemistry. 2, 22 , p. 3267-3273 7 p.

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**Can we predict lattice energy from molecular structure?**

Ouvrard, C. & Mitchell, J. B. O., Oct 2003, In: Acta Crystallographica. Section B, Structural Science. 59, p. 676-685 10 p.

**Protein Ligand Database (PLD): additional understanding of the nature and specificity of protein-ligand complexes**

Puvanendrampillai, D. & Mitchell, J. B. O., 22 Sept 2003, In: Bioinformatics. 19, 14, p. 1856-1857 2 p.

**D-amino acid residues in peptides and proteins**

Mitchell, J. B. O. & Smith, J., 1 Mar 2003, In: Proteins: Structure, Function and Bioinformatics. 50, 4, p. 563-571 9 p.

**Anisotropic repulsion potentials for cyanuric chloride (C<sub>3</sub>N<sub>3</sub>Cl<sub>3</sub>) and their application to modeling the crystal structures of azaaromatic chlorides**

Mitchell, J. B. O., Price, S. L., Leslie, M., Buttar, D. & Roberts, R. J., 1 Nov 2001, In: Journal of Physical Chemistry A. 105 , 43, p. 9961-9971 11 p.

**The determination of the crystal structure of anhydrous theophylline by X-ray powder diffraction with a systematic search algorithm, lattice energy calculations, and C-13 and N-15 solid-state NMR: A question of polymorphism in a given unit cell**

Smith, E. D. L., Hammond, R. B., Jones, M. J., Roberts, K. J., Mitchell, J. B. O., Price, S. L., Harris, R. K., Apperley, D. C., Cherryman, J. C. & Docherty, R., 21 Jun 2001, In: Journal of Physical Chemistry B. 105, 24, p. 5818-5826 9 p.

**Evaluation of a knowledge-based potential of mean force for scoring docked protein-ligand complexes**

Nobel, I., Mitchell, J. B. O., Alex, A. & Thornton, J. M., May 2001, In: Journal of Computational Chemistry. 22, 7, p. 673-688 16 p.

**The relationship between the sequence identities of alpha helical proteins in the PDB and the molecular similarities of their ligands**

Mitchell, J. B. O., 2001, In: Journal of Chemical Information and Computer Sciences. 41, 6, p. 1617-1622 6 p.

**A systematic nonempirical method of deriving model intermolecular potentials for organic molecules: Application to amides**

Mitchell, J. B. O. & Price, S. L., 23 Nov 2000, In: Journal of Physical Chemistry A. 104, 46, p. 10958-10971 14 p.

**BLEEP - Potential of mean force describing protein-ligand interactions: I. Generating potential**

Mitchell, J. B. O., Laskowski, R. A., Alex, A. & Thornton, J. M., Aug 1999, In: Journal of Computational Chemistry. 20, 11, p. 1165-1176 12 p.

**BLEEP - Potential of mean force describing protein-ligand interactions: II. Calculation of binding energies and comparison with experimental data**

Mitchell, J. B. O., Laskowski, R. A., Alex, A., Forster, M. J. & Thornton, J. M., Aug 1999, In: Journal of Computational Chemistry. 20, 11, p. 1177-1185 9 p.

**Electrostatic factors in DNA intercalation**

Medhi, C., Mitchell, J. B. O., Price, S. L. & Tabor, A. B., 1999, In: Biopolymers. 52, 2, p. 84-93 10 p.

**SATIS: Atom typing from chemical connectivity**

Mitchell, J. B. O., Alex, A. & Snarey, M., 1999, In: Journal of Chemical Information and Computer Sciences. 39, 4, p. 751-757 7 p.

**Protein folds and functions**

Martin, A. C., Orengo, C. A., Hutchinson, E. G., Jones, S., Karmirantzou, M., Laskowski, R. A., Mitchell, J. B. O., Taroni, C. & Thornton, J. M., 15 Jul 1998, In: Structure. 6, 7, p. 875-884 10 p.

**Design, synthesis and structure of a zinc finger with an artificial beta-turn**

Viles, J. H., Patel, S. U., Mitchell, J. B. O., Moody, C. M., Justice, D. E., Uppenbrink, J., Doyle, P. M., Harris, C. J., Sadler, P. J. & Thornton, J. M., 19 Jun 1998, In: Journal of Molecular Biology. 279, 4, p. 973-986 14 p.

**Non-randomness in side-chain packing: The distribution of interplanar angles**

Mitchell, J. B. O., Laskowski, R. A. & Thornton, J. M., Nov 1997, In: Proteins: Structure, Function and Bioinformatics. 29, 3, p. 370-380 11 p.

**Multiple solution conformations of the integrin-binding cyclic pentapeptide cyclo(-Ser-D-Leu-Asp-Val-Pro-) Analysis of the (phi,psi) space available to cyclic pentapeptides**

Viles, J. H., Mitchell, J. B. O., Gough, S. L., Doyle, P. M., Harris, C. J., Sadler, P. J. & Thornton, J. M., 1 Dec 1996, In: European Journal of Biochemistry. 242, 2, p. 352-362 11 p.

**Protein recognition of adenylate: An example of a fuzzy recognition template**

Moodie, S. L., Mitchell, J. B. O. & Thornton, J. M., 1 Nov 1996, In: Journal of Molecular Biology. 263, 3, p. 486-500 15 p.

**Multipole-based calculation of the polarization energy**

Mitchell, J. B. O., Nov 1996, In: Theoretica Chimica Acta. 94, 5, p. 287-295 9 p.

**Modelling the interactions of protein side-chains**

Mitchell, J. B. O., THORNTON, J. M. & PRICE, S. L., 1995, *Modelling of biomolecular structures and mechanisms: proceedings of the Twenty-seventh Jerusalem symposium on quantum chemistry and biochemistry held in Jerusalem, Israel, May 23-26, 1994*. Pullman, A., Jortner , J. & Pullman, B. (eds.). Kluwer Academic Publishers, p. 119-135 17 p. (Jerusalem symposia on quantum chemistry and biochemistry ; vol. 27).

**GAUSSIAN MULTipoles IN PRACTICE - ELECTROSTATIC ENERGIES FOR INTERMOLECULAR POTENTIALS**  
WHEATLEY, R. J. & Mitchell, J. B. O., Nov 1994, In: Journal of Computational Chemistry. 15, 11, p. 1187-1198 12 p.

**AMINO/AROMATIC INTERACTIONS IN PROTEINS - IS THE EVIDENCE STACKED AGAINST HYDROGEN-BONDING**  
Mitchell, J. B. O., NANDI, C. L., MCDONALD, I. K., THORNTON, J. M. & PRICE, S. L., 3 Jun 1994, In: Journal of Molecular Biology. 239, 2, p. 315-331 17 p.

#### **AMINO AROMATIC INTERACTIONS**

Mitchell, J. B. O., NANDI, C. L., ALI, S., MCDONALD, J. K., THORNTON, J. M., PRICE, S. L. & SINGH, J., 2 Dec 1993, In: Nature. 366, 6454, p. 413-413 1 p.

#### **Protein Structures and Complexes: What they Reveal about the Interactions that Stabilize them**

THORNTON, J. M., MACARTHUR, M. W., MCDONALD, I. K., JONES, D. T., Mitchell, J. B. O., NANDI, C. L., PRICE, S. L. & ZVELEBIL, M. J. J. M., 15 Oct 1993, In: Philosophical Transactions of the Royal Society of London. Series A, Physical Sciences and Engineering. 345, 1674, p. 113-129 17 p.

#### **A comparison of three theoretical approaches to the study of side-chain interactions in proteins**

Mitchell, J. B. O., NANDI, C. L., THORNTON, J. M., PRICE, S. L., SINGH, J. & SNAREY, M., 7 Aug 1993, In: Journal of the Chemical Society, Faraday Transactions. 89, 15, p. 2619-2630 12 p.

#### **TOWARDS AN UNDERSTANDING OF THE ARGININE ASPARTATE INTERACTION**

Mitchell, J. B. O., THORNTON, J. M., SINGH, J. & PRICE, S. L., 5 Jul 1992, In: Journal of Molecular Biology. 226, 1, p. 251-262 12 p.

#### **ON THE RELATIVE STRENGTHS OF AMIDE ... AMIDE AND AMIDE ... WATER HYDROGEN-BONDS**

Mitchell, J. B. O. & PRICE, S. L., 7 Jun 1991, In: Chemical Physics Letters. 180, 6, p. 517-523 7 p.

#### **THE NATURE OF THE N-H O=C HYDROGEN-BOND - AN INTERMOLECULAR PERTURBATION-THEORY STUDY OF THE FORMAMIDE FORMALDEHYDE COMPLEX**

Mitchell, J. B. O. & PRICE, S. L., 1990, In: Journal of Computational Chemistry. 11, 10, p. 1217-1233 17 p.

#### **ON THE ELECTROSTATIC DIRECTIONALITY OF N-H...O=C HYDROGEN-BONDING**

Mitchell, J. B. O. & PRICE, S. L., 20 Jan 1989, In: Chemical Physics Letters. 154, 3, p. 267-272 6 p.

#### **DIISOPHORONE AND RELATED-COMPOUNDS .19. SYNTHESIS AND REACTIONS OF 6,8-DIBROMODIISOPHORONES**

KURZER, F., Mitchell, J. B. O. & PATEL, J. N., Feb 1988, In: Monatshefte für Chemie. 119, 2, p. 195-213 19 p.

## **Activities**

### **Scientific Writing**

Mitchell, J. B. O. (Speaker)  
28 Oct 2024

### **Machine Learning & AI in Chemistry**

Mitchell, J. B. O. (Speaker)  
18 Jul 2024

### **Fifty years of Bioinformatics**

Mitchell, J. B. O. (Participant)  
15 Dec 2023

### **Kaggle Competition Review: Novozymes Enzyme Stability**

Mitchell, J. B. O. (Speaker)

18 Aug 2023

**Machine Learning & Artificial Intelligence in Chemistry**

Mitchell, J. B. O. (Speaker)

21 Jul 2023

**Talking Statistics: Random Forest**

Mitchell, J. B. O. (Speaker)

18 Jun 2019

**EastBio DTP Symposium 2019**

Mitchell, J. B. O. (Participant)

13 Jun 2019 → 14 Jun 2019

**Methods and Applications of Crystal Structure Prediction**

Mitchell, J. B. O. (Participant)

11 Jul 2018 → 13 Jul 2018

**Sutton Trust Summer School**

Mitchell, J. B. O. (Invited speaker)

5 Jul 2018

**International Science Summer School**

Mitchell, J. B. O. (Invited speaker)

3 Jul 2018

**ScotCHEM Computational Chemistry Symposium 2018**

Mitchell, J. B. O. (Organiser)

14 Jun 2018 → 15 Jun 2018

**CECAM Solubility Prediction Workshop.**

Mitchell, J. B. O. (Participant)

14 May 2018 → 15 May 2018

**Internal PhD Examiner**

Mitchell, J. B. O. (External examiner)

10 Apr 2018

**External PhD Examiner, University College London**

Mitchell, J. B. O. (External examiner)

25 Oct 2017

**Internal MPhil Examiner**

Mitchell, J. B. O. (External examiner)

4 Sept 2017

**Sutton Trust Summer School**

Mitchell, J. B. O. (Invited speaker)

4 Jul 2017

**External MPhil Examiner**

Mitchell, J. B. O. (External examiner)

28 Jun 2017

**Enzyme Informatics**

Mitchell, J. B. O. (Speaker)  
18 Oct 2016

**International Science Summer School**

Mitchell, J. B. O. (Invited speaker)  
5 Jul 2016

**10th European Conference on Computational Chemistry**

Mitchell, J. B. O. (Invited speaker)  
31 Aug 2015 → 3 Sept 2015

**International Science Summer School**

Mitchell, J. B. O. (Invited speaker)  
9 Jul 2015

**Internal PhD Examiner**

Mitchell, J. B. O. (External examiner)  
25 Jun 2015

**Seminar, College of Life Sciences, Dundee**

Mitchell, J. B. O. (Invited speaker)  
30 Mar 2015

**External PhD Examiner**

Mitchell, J. B. O. (External examiner)  
3 Mar 2015

**External EngD Examiner**

Mitchell, J. B. O. (External examiner)  
7 Jan 2015

**External DPhil Examiner**

Mitchell, J. B. O. (External examiner)  
6 Jan 2015

**External PhD Examiner**

Mitchell, J. B. O. (External examiner)  
29 Aug 2014

**International Science Summer School**

Mitchell, J. B. O. (Invited speaker)  
22 Jul 2014

**BSRC Seminar**

Mitchell, J. B. O. (Invited speaker)  
22 Nov 2013

**Open Drug Discovery, Strathclyde, 2013**

Mitchell, J. B. O. (Keynote/Plenary speaker)  
15 Oct 2013

**International Science Summer School**

Mitchell, J. B. O. (Invited speaker)

23 Jul 2013

**Sutton Trust Summer School**

Mitchell, J. B. O. (Invited speaker)

1 Jul 2013

**ScotCHEM Computational Symposium 2013**

Mitchell, J. B. O. (Organiser)

13 Jun 2013 → 14 Jun 2013

**Discovery Chemistry Congress, Munich, 2013**

Mitchell, J. B. O. (Invited speaker)

19 Mar 2013 → 20 Mar 2013

**COST CM1103 WG Meeting, Madrid**

Mitchell, J. B. O. (Invited speaker)

24 Nov 2012 → 25 Nov 2012

**BSRC seminar**

Mitchell, J. B. O. (Invited speaker)

2 Nov 2012

**St Andrews Bioinformatics Research Symposium 2012**

Mitchell, J. B. O. (Organiser)

22 Aug 2012

**Sutton Trust Summer School**

Mitchell, J. B. O. (Invited speaker)

6 Jul 2012

**Computational Chemogenomics, Geneva**

Mitchell, J. B. O. (Invited speaker)

14 May 2012 → 16 May 2012

**Fife Science Festival**

Mitchell, J. B. O. (Participant)

10 Mar 2012

**iGEM 2012**

Mitchell, J. B. O. (Participant)

1 Jan 2012 → 7 Oct 2012

**BMS Seminar, University of St Andrews**

Mitchell, J. B. O. (Invited speaker)

25 Nov 2011

**SULSA Research Symposium, Glasgow**

Mitchell, J. B. O. (Invited speaker)

7 Jun 2011

**Physical Chemical Aspects of Biomolecular Solvation, Leipzig**

Mitchell, J. B. O. (Invited speaker)

23 May 2011 → 24 May 2011

**Fife Science Festival**

Mitchell, J. B. O. (Participant)  
12 Mar 2011

**Computational Chemistry Seminar, University of St Andrews**

Mitchell, J. B. O. (Speaker)  
8 Feb 2011

**External Doctoral (D.Eng.) Examiner for the University of Manchester**

Mitchell, J. B. O. (External examiner)  
27 Jan 2011

**iGEM 2011**

Mitchell, J. B. O. (Participant)  
1 Jan 2011 → 2 Oct 2011

**Editorial board of Journal of Molecular Graphics and Modelling (External organisation)**

Mitchell, J. B. O. (Participant)  
2011 → ...

**BMS Seminar, University of St Andrews**

Mitchell, J. B. O. (Invited speaker)  
26 Nov 2010

**External PhD examiner for the University of Nottingham**

Mitchell, J. B. O. (External examiner)  
5 Nov 2010

**UK-QSAR Spring 2010, Glasgow**

Mitchell, J. B. O. (Speaker)  
12 May 2010 → 13 May 2010

**ADMET Europe 2010, Munich**

Mitchell, J. B. O. (Invited speaker)  
8 Apr 2010 → 9 Apr 2010

**Dyers Brae Lab Chat, St Andrews**

Mitchell, J. B. O. (Invited speaker)  
26 Feb 2010

**Departmental Seminar, Department of Chemistry, University of Aberdeen**

Mitchell, J. B. O. (Invited speaker)  
3 Feb 2010

**Solvation of Bioactive Compounds: Bridging Theory, Computation & Experiment, Leipzig**

Mitchell, J. B. O. (Invited speaker)  
7 Jan 2010 → 9 Jan 2010

**iGEM 2010**

Mitchell, J. B. O. (Participant)  
1 Jan 2010 → 8 Nov 2010

**Computational Chemistry Seminar, University of St Andrews**

Mitchell, J. B. O. (Invited speaker)

1 Dec 2009

**SULSA Translational Biology Theme Directorate (External organisation)**

Mitchell, J. B. O. (Participant)

16 Nov 2009 → ...

**BMS Seminar, University of St Andrews**

Mitchell, J. B. O. (Invited speaker)

30 Oct 2009

**ADMET 2009, London**

Mitchell, J. B. O. (Invited speaker)

1 Jul 2009 → ...

**Improving Solubility 2009, London.**

Mitchell, J. B. O. (Invited speaker)

30 Jun 2009 → ...

**SULSA Research Symposium, Edinburgh**

Mitchell, J. B. O. (Invited speaker)

10 Jun 2009 → ...

**ScotCHEM Computational Chemistry Symposium, Heriot-Watt**

Mitchell, J. B. O. (Invited speaker)

13 May 2009

**Improving Solubility 2008, London**

Mitchell, J. B. O. (Invited speaker)

24 Jun 2008

**Seminar at Imperial College London**

Mitchell, J. B. O. (Invited speaker)

2 Jun 2008

**National Service for Computational Chemistry Software, London 2008**

Mitchell, J. B. O. (Invited speaker)

16 Apr 2008

**British Crystallographic Association, York**

Mitchell, J. B. O. (Invited speaker)

10 Apr 2008

**Chem@Cam**

Mitchell, J. B. O. (Interviewee)

2008

**High Throughput Technologies 4 Chemists, Cambridge**

Mitchell, J. B. O. (Invited speaker)

22 Mar 2007

**Comp Life 2006, Cambridge**

Mitchell, J. B. O. (Speaker)

27 Sept 2006 → 29 Sept 2006

### **Chemoinformatics in Drug Research, Copenhagen**

Mitchell, J. B. O. (Invited speaker)  
31 Oct 2005

### **External PhD examiner for the University of Manchester**

Mitchell, J. B. O. (External examiner)  
24 Aug 2005

### **Seminar at University of Manchester**

Mitchell, J. B. O. (Invited speaker)  
24 Aug 2005 → ...

### **Member of Thesis Advisory Committee for three students from EMBL-EBI**

Mitchell, J. B. O. (External examiner)  
2003 → ...

### **Seminar at University of Cambridge**

Mitchell, J. B. O. (Invited speaker)  
6 Feb 2002

### **Peter Kollman memorial conference, Biomolecular Interactions, Bristol**

Mitchell, J. B. O. (Invited speaker)  
2002 → ...

### **Royal Society of Chemistry (External organisation)**

Mitchell, J. B. O. (Participant)  
2000 → ...

## **Prizes**

### **iGEM Bronze Medal**

Mitchell, J. B. O. (Recipient), Melo Czekster, C. (Recipient), Stokes, V. A. (Recipient), Ferreira, H. C. (Recipient) & Hooley, C. A. (Recipient), 28 Oct 2018

### **iGEM Gold Medal**

Mitchell, J. B. O. (Recipient), 8 Nov 2010

### **iGEM Gold Medal**

Mitchell, J. B. O. (Recipient), 2 Oct 2011

### **iGEM Gold Medal**

Mitchell, J. B. O. (Recipient), 7 Oct 2012

### **iGEM Gold Medal**

Mitchell, J. B. O. (Recipient), Smith, V. A. (Recipient), Melo Czekster, C. (Recipient), Schwarz-Linek, U. (Recipient), Hooley, C. (Recipient) & Bentley, K. (Recipient), 4 Nov 2019

## **Press/Media**

### **AI in drug discovery**

Mitchell, J. B. O.  
14/09/20

1 Media contribution

#### **Ethical Dilemmas That Artificial Intelligence Raises in the Lab**

Mitchell, J. B. O.

2/07/19

1 Media contribution

## **Awards**

### **Machine Learning Approaches to Predict: Machine Learning Approaches to Predict Enzyme Function**

Mitchell, J. B. O. (PI)

BBSRC: £247,960.46

1/09/11 → 31/12/14

## **Projects**

### **Wellcome Trust 091959/Z/10/Z: International Genetically Engineered Machine Competition Student Stipends**

Mitchell, J. B. O. (PI)

The Wellcome Trust

1/03/10 → 31/12/10

### **Machine Learning Approaches to Predict: Machine Learning Approaches to Predict Enzyme Function**

Mitchell, J. B. O. (PI) & De Ferrari, L. (Researcher)

BBSRC

1/09/11 → 31/12/14

## **Datasets/Software**

### **Additional file 1 of Practical application of a Bayesian network approach to poultry epigenetics and stress**

Videla Rodriguez, E. A. (Creator), Pértille, F. (Creator), Guerrero-Bosagna, C. (Creator), Mitchell, J. B. O. (Creator), Jensen, P. (Creator) & Smith, V. A. (Creator), Figshare, 2022

DOI: 10.6084/m9.figshare.20219738.v1

### **Computational Insights into the Catalytic Mechanism of Is-PETase: An Enzyme Capable of degrading poly(ethylene) terephthalate (dataset)**

Shrimpton-Phoenix, E. (Creator), Mitchell, J. B. O. (Creator) & Buehl, M. (Creator), University of St Andrews, 27 Oct 2022

DOI: 10.17630/486acc90-3be5-43c2-aa08-17c02096bb85

### **Data underpinning : Greedy and linear ensembles of machine learning methods outperform single approaches for QSPR regression problems**

Kew, W. (Creator) & Mitchell, J. B. O. (Creator), University of St Andrews, 2015

### **Data underpinning: Is Experimental Data Quality the Limiting Factor in Predicting the Aqueous Solubility of Druglike Molecules?**

Mitchell, J. B. O. (Creator) & Palmer, D. (Creator), University of St Andrews, 11 Jun 2014

DOI: 10.17630/1a4dbdf0-b2ba-42f6-9408-e5895ccb9faf

### **Data underpinning: One origin for metallo-β-lactamase activity, or two? An investigation assessing a diverse set of reconstructed ancestral sequences based on a sample of phylogenetic trees, Journal of Molecular Evolution, 79, 117-129 (2014)**

Mitchell, J. B. O. (Creator), Barker, D. (Creator) & Alderson, R. G. (Creator), University of St Andrews, 1 Oct 2014

DOI: 10.17630/46100988-896f-4d05-9800-3f44060aa4bd

### **Data underpinning: Probing the average distribution of water in organic hydrate crystal structures with radial distribution functions (RDFs)**

Skyner, R. E. (Creator), Mitchell, J. B. O. (Creator) & Groom, C. (Contributor), Royal Society of Chemistry, 19 Dec 2016

<https://doi.org/10.1039/C6CE02119K>

**Data Underpinning: Toward physics-based solubility computation for pharmaceuticals to rival informatics**  
Fowles, D. (Creator), Palmer, D. (Creator), Guo, R. (Creator), Price, S. (Creator) & Mitchell, J. B. O. (Creator), University of St Andrews, 2021  
DOI: 10.17630/4a3b4fba-1e62-46d5-af7a-6eedfb517c67, <https://doi.org/10.1021/acs.jctc.1c00130.s001>

**Data underpinning: Why do sequence signatures predict enzyme mechanism? Homology versus Chemistry**  
Beattie, K. (Creator), De Ferrari, L. (Creator) & Mitchell, J. B. O. (Creator), SAGE Publications Ltd STM, 2015  
<http://www.la-press.com/why-do-sequence-signatures-predict-enzyme-mechanism-homology-versus-ch-article-a5293>

**DLS-100 Solubility Dataset**  
Mitchell, J. B. O. (Creator) & McDonagh, J. (Contributor), University of St Andrews, 31 Oct 2017  
DOI: 10.17630/3a3a5abc-8458-4924-8e6c-b804347605e8

**Practical application of a Bayesian network approach to poultry epigenetics and stress (dataset)**  
Videla Rodriguez, E. A. (Creator) & Mitchell, J. B. O. (Creator), European Nucleotide Archive (ENA), 2022  
<https://www.ebi.ac.uk/ena/browser/view/PRJEB34868?show=reads>

**Read 2024 Mass Specs Raw Data, kinetics raw data, and Sequence Alignments**  
Read, B. (Creator), Guimaraes da Silva, R. (Creator) & Mitchell, J. (Creator), Figshare, 2024  
DOI: 10.6084/m9.figshare.24631194.v2

**The natural history of biocatalytic mechanisms (dataset)**  
Nath, N. (Creator), Mitchell, J. B. O. (Creator) & Caetano-Anolles, G. (Creator), University of St Andrews, 29 May 2014  
DOI: 10.17630/9ea8f970-c3bb-4fed-b6a2-db95e1148d8a