

James McDonagh

EaStCHEM School of Chemistry
University of St Andrews
North Haugh
St Andrews
KY16 9ST

e-mail: james.l.mcdonagh@gmail.com

Tel: 07872049826

[Link: LinkedIn Profile](#)

[Link: Google Scholar Profile](#)

[Link: Research web page](#)

Education

- **PhD in Computational Chemistry**

- University of St Andrews 2010 - 2014 (Expected)
 - Computing Intrinsic Aqueous Solubility of Organic Drug-like Molecules and Understanding Hydrophobicity. (Supervisors Dr John Mitchell and Dr Tanja van Mourik)

- **MChem Degree**

- University of Wales, Bangor (1st Honours) 2006-2010
 - MChem project: Conformational Analysis of Anthraquinone Based Dyes (Dr R. A. Davies)
 - Third year project: Characterisation and Mutation of Cytochrome *C'* (Dr L. Murphy)
 - Mini-project: Synthetic Analogues of Human Insulin - Application to Diabetes Treatment

Research Interests

Computational chemistry methods, ranging from QSAR models to *ab initio* methods. Pharmaceutical molecules design and property prediction. Polymorphism and crystal structure prediction. Solution phase modelling. Combined computational chemistry and cheminformatics models.

Skills and Competencies

Computing: Linux shell scripting, limit Fortran, R, learning Python, L^AT_EX, regular use of MS Word, Excel and Power Point. Computational chemistry applications: Gaussian 09, ORCA DMACRYS, CASTEP, CRYSTAL09, Ambertools.

Coaching, leadership and outreach: Qualified fencing coach and referee (Sabre). Experienced indoor climbing teacher. I was elected men's captain in Bangor University and the University of St Andrews fencing clubs. I led the St Andrews team to the UK student semi-finals (2011 - 2012). I have assisted in science workshops at the Dundee science centre and summer schools run by the chemistry department for international students ages 16 - 17.

Research Placements

- **Research Collaboration with the Group of Maxim Fedorov**

- Max Planck institute for Mathematics in the Sciences
 - Calculating hydration free energy by the Reference Interaction Site Model.

Leipzig, Germany

September 2011

- **Summer Industry Placement**

- ViewHolographic, OpTIC Technium
 - Optimisation of holographic emulsion for laser light sources.

St Asaph, Wales, UK

June - August 2010

- **Summer Research Placement**

- Oxford Centre for Diabetes, Endocrinology and Metabolism (OCDEM)
 - Investigating enzymatic digestion of extra cellular matrix tissue around human pancreatic islet cells.

Oxford, UK

July - August 2009

Research Presentations

- Oral presentation: *Can we predict solubility accurately and efficiently from theory?* RSC Younger Members Symposium, University of Birmingham, UK, (2014)
- Oral presentation: *Predicting the Solubility and Related Thermodynamic Quantities of Drug-Like Molecules.* Theoretical Chemistry Group (TCG) meeting, University College London, UK, (2014)
- Oral presentation: *Predictions of the Solubility of Drug-like Molecules.* Biomedical Sciences (BMS) graduate student presentation, University of St Andrews, UK (2014).
- Oral presentation: *Predictions of Intrinsic Aqueous Solubility of Crystalline Drug-like Molecules.* ScotChem, University of St Andrews, UK (2013).
- Oral presentation: *Intrinsic Aqueous solubility: Predictions from sublimation and hydration free energies.* Visiting researcher presentation. Max Planck institute for Mathematics in Science, Leipzig, Germany (2011).
- 12 poster presentations, two at international conferences.

Teaching and Demonstrating

Introduction to Computational Chemistry; undergraduate course (Course Demonstrator).

Introducing Gaussian, graphical user interfaces and introductory practical computational chemistry.

Third year undergraduate mini-projects (Course Demonstrator). Introduction to experimental design and calculation - projects: Crowd sourcing chemistry and polymer conformational analysis.

Final Year Student Supervision - Predicting sublimation free energy (Supervisory).

Project conception and supervision, for a student during her final year undergraduate dissertation.

Professional Memberships and Awards

- Best speaker of the physical and analytical session of the RSC-YMS meeting
- NSCCS supercomputer time granted 80,000 CPU hours (2013)
- RSC Associate Member AMRSC (2012 - 2014)
- University of St Andrews Athletic Union half blue and Bangor University Athletic Union Colours

Publications

- [Uniting Cheminformatics and Chemical Theory to Predict the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules.](#) **McDonagh, J. L.**; Nath, N.; De Ferrari, L.; van Mourik, T.; Mitchell, J. B. O. [Journal of Chemical Information and Modelling](#), 54, 844-856, 2014.
- [First-Principles Calculation of the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules.](#) Palmer, D. S.; **McDonagh, J. L.**; van Mourik, T.; Mitchell, J. B. O.; Fedorov, M. V. [Journal of Chemical Theory and Computation](#), 8, 3322-3337, 2012
- [Enzyme Informatics.](#) Alderson R.G.; De Ferrari L.; Mavridis L.; **McDonagh J.L.**; Mitchell J.B.O.; Nath N. [Current Topics in Medicinal Chemistry](#), 12(17), 1911-1923 , 2012.
- [Elemental discoveries.](#) **James L. McDonagh**, [Science - Books et al](#); 345, (6194): 262; July 2014