

# Neil Swainston

BSc (Hons) MSc PhD MRSB MRSC

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## Summary

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- Bioinformatics, cheminformatics, machine learning, software engineering, computational systems and synthetic biology in academic and industrial environments.
- BSc Chemistry with Industrial Experience (first class); MSc Computing Science; PhD Computer Science.
- Professional software engineering skills.
- Team Leading and Project Management in industry.
- International research experience in Germany and France.
- Lecturing and undergraduate and postgraduate student supervision.
- Well published and cited (40 peer-reviewed articles, 5 with >100 citations; h-index: 22).
- Conference organising experience.
- Multiple successful grant applications (>£1.4M funding).

## Employment

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04/06 - **Manchester Institute of Biotechnology** Senior Experimental Officer  
*Centre for Synthetic Biology of Fine and Specialty Chemicals (SYNBIOCHEM)*

I work in an interdisciplinary role focussing on 'omics experimental data analysis and interpretation through its integration with systems and synthetic biology approaches, driven by software development. My areas of expertise in experimental data cover quantitative proteomics, metabolomics and enzyme kinetics. I co-lead an international community focussed on the development of comprehensive predictive models of metabolism in human, yeast and other organisms, and this work has been both highly cited and publicised. Further work includes the improvement of metabolic modelling predictions through integration of experimental data. More recent work has covered computational synthetic biology, gene design and synthesis, and directed evolution as applied to enzyme optimisation and biocatalysis. Current work involves application of machine learning and neural networks to protein structure prediction.

I am also involved in teaching and PhD student supervision responsibilities, and have successful grant writing experience. I recently received BBSRC funding of £700k for a three-year collaborative project in cheminformatics and metabolic modelling with the European Bioinformatics Institute, and a further £650k from the BBSRC to develop an integrated model building and text-mining platform.

04/99 – 04/06 **Waters Corporation** Bioinformatics Team Manager

I have seven years experience in commercial software development, as applied to bioinformatics, proteomics and mass spectrometry. During my time at Waters, I quickly developed from a software engineer, through to a team leader and ultimately a project manager, directly managing a group of five people and being responsible for a software release involving the work of nine developers.

This role was also interdisciplinary, covering all facets of the software development life cycle, from requirements gathering, software design, development and documentation, through to testing and support. Due to the focus on requirements gathering from users, and providing software support, I was frequently involved in customer site visits, user training, and conference speaking; tasks which greatly developed my skills of collaborating with biologists and chemists.

10/98 - 04/99 **AstraZeneca** Graduate Trainee

Graduate Trainee in IT problem management and data analysis.

09/94 - 08/95 **Dow Chemical Company, Stade, Germany** Student Placement

Year long placement in a varied role involving polycarbonate synthesis and analytical chemistry. Duties involved lab research, plant visits, provision of analytical chemistry support, and development of a searchable database resource of spectra of chemical standards, presentation giving in both

English and German.

## Education

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03/12	<b>PhD</b> "Systems biology informatics for the development and utility of genome-scale metabolic models". <i>University of Manchester</i>
09/97 – 10/98	<b>MSc Computing Science</b> <i>University of Newcastle-upon-Tyne; IRISA, Rennes, France.</i> Year long conversion course including Masters project in bioinformatics (DNA sequence analysis), undertaken in Rennes, France.
09/92 – 06/96	<b>BSc (Hons) Chemistry with Industrial Experience</b> <i>University of Manchester</i> First class honours; industrial experience in analytical chemistry with Dow Deutschland Inc., Stade, Germany.

## Selected publications

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- Recon 2.2: from reconstruction to model of human metabolism. **Swainston N**, et al. *Metabolomics*. 2016, **12**, 1-7.
  - Synthetic biology for the directed evolution of protein biocatalysts: navigating sequence space intelligently. Currin A, **Swainston N**, Day PJ, Kell DB. *Chem Soc Rev*. 2015, **44**, 1172-239.
  - GeneGenie: optimised oligomer design for directed evolution. **Swainston N**, et al. *Nucleic Acids Res*. 2014, **42**:W395-400.
  - A community-driven global reconstruction of human metabolism. Thiele I, **Swainston N**, et al. *Nat Biotechnol*. 2013, **31**, 419-25.
  - Improving metabolic flux predictions using absolute gene expression data. Lee D, Smallbone K, Dunn WB, Murabito E, Winder CL, Kell DB, Mendes P, **Swainston N**. *BMC Syst Biol*. 2012, **6**:73.
  - A consensus yeast metabolic network obtained from a community approach to systems biology. Herrgård MJ, **Swainston N**, et al. *Nat Biotechnol*. 2008, **26**, 1155-1160.

## Funding

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- Continued development of ChEBI towards better usability for the systems biology and metabolic modelling community. *BBSRC; Bioinformatics and biological resources fund; 2013. £682,950.* (BB/K019783/1; Co-Investigator).
  - Enriching Metabolic PATHwaY models with evidence from the literature (EMPATHY). *BBSRC; Responsive mode; 2014. £659,535.* (BB/M006891/1; Co-Investigator).
  - Modelling and sensitivity analysis of metabolic networks in diabetic neuropathy. *Faculty of Life Sciences, University of Manchester, Interdisciplinary Projects in Quantitative Biology; 2014. £46,798.*
  - Hackathon on Resources for Modelling in Biology 2014 (HARMONY 2014). *BBSRC; International workshops; 2014. £9047.* (BB/L026325/1; Co-Applicant).
  - The relationship of clusters of gene expression associated with development in childhood disease in the ageing adult. *Manchester Institute for Collaborative Research on Ageing (MICRA) Seedcorn Funding; 2014. £6000.*
  - Iron metabolism and its role in neurodegenerative disease. *University of Manchester; Faculty of Engineering and Physical Sciences Strategic Fund; 2013. £5200.*
  - Towards an integrated model of human metabolism, cell signalling and gene expression. *University of Manchester; Faculty of Engineering and Physical Sciences Strategic Fund; 2014. £4000.*

## Teaching and student supervision

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- **Teaching:** Bioinformatics, Proteomics, Systems Biology. Systems Biology Doctoral Training Centre, MRes Translational Medicine, University of Manchester, 2006-10, 2015. Systems Biology. MSc (Res) Translational Oncology, University of Sheffield, 2014-16. Data integration and Interaction Networks. MSc Applied Bioinformatics, MSc Molecular Medicine, Cranfield University, 2011-15.
  - **Tutor:** In Silico Systems Biology: Network Reconstruction, Analysis and Network-based Modelling. EBI-EMBL, Hinxton, Cambridge, 23-26 May 2011.

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- **Student supervisor:** Systems Biology Doctoral Training Centre, University of Manchester, 2007-12; MSc Applied Bioinformatics, Cranfield University, 2013; MSc Advanced Computer Science, University of Manchester, 2014; ALM Biotechnology, Harvard University Extension School, 2014.
  - **Advisor:** University of Manchester iGEM Advisor, 2013-15.

### Scientific responsibilities

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- Lead conference organiser, HARMONY 2014, Manchester, 22-25 April 2014.
- Associate Editor, BMC Systems Biology.
- Invited member, Synthetic Biology Open Language (SBOL) Developers Group.
- Invited member, STREDA Commission.
- Session chair. COMBINE 2010, Edinburgh.
- Scientific Committee member, International Symposium on Integrative Bioinformatics, 2010-14.
- Course Office member, FEBSX-SysBio2011: From Molecules To Function. Innsbruck, Austria.
- Nominated for election to position of SBML Editor, 2010-12 and 2011-13.
- Journal reviews, including: Bioinformatics, BMC Bioinformatics, BMC Genomics, BMC Systems Biology, BMC Biotechnology, Database, Metabolites, Nature Protocols, npj Systems Biology and Applications, PLOS Computational Biology, PLOS ONE.
- Funding reviews: BBSRC, Breast Cancer Campaign.
- PhD external examiner: "Critical examination of an existing genome-scale mouse metabolic network from a bioprocessing perspective", Al-Hussein Nasrullah Abutaleb; University of Sheffield, March 2017.

### Computational and software development skills

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- Languages: Java (Certified Programmer), Python, Matlab, C/C++.
- Web development: Javascript, AJAX, JQuery, AngularJS, Bootstrap, Google Web Toolkit, Flask.
- Data science: Deep Learning, neural networks, theano, theanets.
- Data management: XML, JSON, relational, XML and graph (neo4j) databases.
- Semantic web: RDF.
- Cloud computing: Google Compute Engine.
- Software engineering: source code control (svn, git), build and deployment scripts (ant, Maven, Docker), software design with UML.
- Operating systems: OS X, Windows, Linux.

### Courses and training

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- **University of Manchester:** Academic career planning; Practical project management for PIs and academics; Collaboration: the hidden research skill; Communicating with your teams; Getting the best out of yourself and others; Coaching and mentoring skills for supervisors; Practical application of supervision skills; How to shine at fellowship interviews
- **Coursera:** Introduction to Genetics and Evolution; Calculus One; Astrobiology and the Search for Extraterrestrial Life; Machine Learning
- **Peter Kenyon:** The Front Line Manager
- **Pentland Training:** Project Management Fundamentals

### References

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#### Prof Douglas B Kell CBE

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#### Prof Hans V Westerhoff

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## Publications

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1. SpeedyGenes: Exploiting an Improved Gene Synthesis Method for the Efficient Production of Synthetic Protein Libraries for Directed Evolution. Currin A, et al. *Methods Mol Biol*, 2017, **1472**, 63-78.
2. SYNBIOCHEM Synthetic Biology Research Centre, Manchester—A UK foundry for fine and speciality chemicals production. Le Feuvre RA, et al. *Biochem Soc Trans*. 2016, **44**, 675-7.
3. Recon 2.2: from reconstruction to model of human metabolism. Swainston N, et al. *Metabolomics*. 2016, **12**, 1-7.
4. SYNBIOCHEM—a SynBio foundry for the biosynthesis and sustainable production of fine and speciality chemicals. Carbonell P, et al. *Biochem Soc Trans*. 2016, **44**, 675-7.
5. Bioinformatics for the synthetic biology of natural products: Integrating across the Design-Build-Test cycle. Carbonell P, et al. *Nat Prod Rep*. 2016, **33**, 925-32.
6. libChEBI: an API for accessing the ChEBI database. Swainston N, et al. *J Cheminform*. 2016, **8**:11.
7. ChEBI in 2016: Improved services and an expanding collection of metabolites. Hastings J, et al. *Nucleic Acids Res*. 2016, **44**, D1214-9.
8. SBOL Visual: A Graphical Language for Genetic Designs. Quinn JY, et al. *PLoS Biol*. 2015, **13**:e1002310.
9. Membrane transporter engineering in industrial biotechnology and whole-cell biocatalysis. Kell DB, et al. *Trends Biotechnol*. 2015, **33**, 237-246.
10. RobOKoD: microbial strain design for (over)production of target compounds. Stanford NJ, et al. *Front Cell Dev Biol*. 2015, **3**:17.
11. Synthetic biology for the directed evolution of protein biocatalysts: navigating sequence space intelligently. Currin A, et al. *Chem Soc Rev*. 2015, **44**, 1172-239.
12. A 'rule of 0.5' for the metabolite-likeness of approved pharmaceutical drugs. O'Hagan S, et al. *Metabolomics*. 2015, **11**, 323-339.
13. SpeedyGenes: an improved gene synthesis method for the efficient production of error-corrected, synthetic protein libraries for directed evolution. Currin A, et al. *Protein Eng Des Sel*. 2014, **27**, 273-80.
14. Enzyme characterisation and kinetic modelling of the pentose phosphate pathway in yeast. Messiha et al. *PeerJ PrePrints* 2014, **2**:e146v4.
15. GeneGenie: optimised oligomer design for directed evolution. **Swainston N**, et al. *Nucleic Acids Res*. 2014, **42**, W395-400.
16. Path2Models: Large-scale generation of computational models from biochemical pathway maps. Büchel B, Rodriguez N, **Swainston N**, Wrzodek C, et al. *BMC Syst Biol*. 2013, **7**:116.
17. An analysis of a 'community-driven' reconstruction of the human metabolic network. **Swainston N**, et al. *Metabolomics*. 2013, **9**, 757-764.
18. A model of yeast glycolysis based on a consistent kinetic characterization of all its enzymes. Smallbone K, Messiha H, et al. *FEBS Lett*. 2013, **587**, 2832-41.
19. A community-driven global reconstruction of human metabolism. Thiele I, **Swainston N**, et al. *Nat Biotechnol*. 2013, **31**, 419-25.
20. Improving metabolic flux predictions using absolute gene expression data. Lee D, Smallbone K, Dunn WB, Murabito E, Winder CL, Kell DB, Mendes P, **Swainston N**. *BMC Syst Biol*. 2012, **6**:73.
21. The SuBliMinaL Toolbox: automating steps in the reconstruction of metabolic networks. **Swainston N**, et al. *J Integr Bioinform*. 2011, **8**:186.
22. Sustainable Model Building: The Role of Standards and Biological Semantics. Krause F, et al. *Methods Enzymol*. 2011, **500**, 371-95.
23. A community effort towards a knowledge-base and mathematical model of human pathogen *Salmonella Typhimurium* LT2. Thiele I, et al. *BMC Syst Biol*. 2011, **5**:8.
24. A QconCAT informatics pipeline for the analysis, visualization and sharing of absolute quantitative proteomics data. **Swainston N**, et al. *Proteomics* 2011, **11**, 329–333.
25. Systematic integration of experimental data and models in systems biology. Li P, et al. *BMC Bioinformatics* 2010, **11**:582.
26. Further developments towards a genome-scale metabolic model of yeast. Dobson PD, Smallbone K, et al. *BMC Syst Biol*. 2010, **4**:145.
27. Enzyme kinetics informatics: from instrument to browser. **Swainston N**, Golebiewski M, et al.

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*FEBS J.* 2010, **77**, 3769–3779.

28. Integrative Information Management for Systems Biology. **Swainston N**, et al. *In proceedings of the 7th International workshop on Data Integration in the Life Sciences 2010 (DILS'10)*, Gothenburg, Sweden. *Lecture Notes in Computer Science* 2010, **6254**, 164-178.
29. Integration of metabolic databases for the reconstruction of genome-scale metabolic networks. Radrich K, et al. *BMC Syst Biol.* 2010, **4**:114.
30. Towards a genome-scale kinetic model of cellular metabolism. Smallbone K, et al. *BMC Syst Biol.* 2010, **4**:6.
31. Information management for high content live cell imaging. Jameson D, et al. *BMC Bioinformatics* 2009, **10**:226.
32. Mass spectrometry tools and metabolite-specific databases for molecular identification in metabolomics. Brown MC, et al. *Analyst* 2009, **134**, 1322–1332.
33. libAnnotationSBML: a library for exploiting SBML annotations. **Swainston N**, Mendes P. *Bioinformatics* 2009, **25**, 2292–2293.
34. A consensus yeast metabolic network obtained from a community approach to systems biology. Herrgård MJ, **Swainston N**, et al. *Nat Biotechnol.* 2008, **26**, 1155-1160.
35. Capture and analysis of quantitative proteomics data. Lau K, et al. *Proteomics* 2007, **7**, 2787-99.
36. Growth control of the eukaryote cell: A systems biology study in yeast. Castrillo JI, et al. *J Biol.* 2007, **6**:4.
37. An informatic pipeline for the data capture and submission of quantitative proteomic data using iTRAQ. Siepen JA, **Swainston N**, et al. *Proteome Sci.* 2007, **5**:4.
38. Model-driven User Interfaces for Bioinformatics Data Resources: Regenerating the Wheel as an Alternative to Reinventing It. Garwood K, et al. *BMC Bioinformatics* 2006, **7**:532.
39. Synthesis and redox properties of the cycloheptatrienylmolybdenum complexes  $[\text{MoX}(\text{N-N})(\text{h-C}_7\text{H}_7)]^{z+}$ , (N-N = 2,2'-bipyridine or 1,4-Bu<sub>2</sub>t-1,3-diazabutadiene; z = 0, X = Br or Me; z = 1, X = NCMe, CNBut or CO). Disley SPM, et al. *J. Organomet. Chem.* 1998, **566**, 151-158.

## Presentations

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- †Genome-wide modelling. *University of Sheffield, 13 January 2017.*
- Go-faster enzymes: improved biocatalysis through intelligent directed evolution. *University of Edinburgh, 5 September 2016.*
- PathwayGenie - pathway design from selection to plasmid. *8th International Workshop on Bio-Design Automation (IWBDA), Newcastle-upon-Tyne, 17 August 2016*
- Design Tools and Data in Synthetic Biology. *FAIRDOM webinar series, 27 June 2016.*
- †Genome scale modelling. *University of Sheffield, 2 February 2016.*
- GeneGenie: Enzyme Variant Libraries For Directed Evolution. *ESSEC Symposium, Ruedesheim-am-Rhein, DE, 16 September 2015.*
- GeneGenie: Optimized Oligomer Design For Directed Evolution. *Cell Factories and Biosustainability, Favrholt, DK, 19 May 2015.*
- †Genome-wide modelling in systems biology. *University of Sheffield, 3 February 2015.*
- †Integrative Informatics for Metabolic Systems Biology. *Cranfield University, 19 January 2015.*
- GeneGenie: Optimized Oligomer Design For Directed Evolution. *C1net Conference, Nottingham, 16 January 2015.*
- Modelling human metabolism with Recon 2. *FMHS – MIB Symposium. University of Manchester, 12 November 2014.*
- \*Standardisation of stoichiometric models: how and why. *Stoichiometric modelling (SM) of microbial metabolism, Isaac Newton Institute, Cambridge, 4 November 2014.*
- \*Modelling cellular metabolism. *Cancer Research UK Manchester Institute, 8 October 2014.*
- \*Genome-scale modelling of human metabolism through 'omics data constraints. *Workshop on Synergising Clinical Proteomics & Metabolomics. University of Manchester, 10 July 2014.*
- \*Mapping Life. *SupraBiology: Supercomputing for Systems Biology. Manchester Institute for Biotechnology, Manchester, 16-17 June 2014.*
- Modelling of human metabolism with the genome-scale metabolic reconstruction Recon 2. *Beilstein Bozen Symposium "Chemistry and Time", Prien am Chiemsee, DE, 19-23 May 2014.*
- \*Continued development of ChEBI towards better usability for the systems biology and metabolic modelling community. *3rd ChEBI User Workshop. EMBL-EBI, Hinxton, 25 March 2014.*
- †Genome-wide modelling in systems biology. *University of Sheffield, 18 February 2014.*
- †Integrative Informatics for Metabolic Systems Biology. *Cranfield University, 20 January 2014.*
- \*Modelling of human metabolism with the genome-scale metabolic reconstruction Recon 2. *Systems Medicine. Manchester, 30 September 2013.*
- \*Modelling of human metabolism with the genome-scale metabolic reconstruction Recon 2. *Molecular Interactions. Berlin, DE, 14-16 August 2013.*
- †Integrative Informatics for Metabolic Systems Biology. *Cranfield University, 7 January 2013.*
- \*Manchester Institute of Biotechnology. *AllBio Networking Meeting. Amsterdam, NL, 29-30 November 2012.*
- Path2Models: automated generation of genome-scale metabolic reconstructions from pathway databases. *International Workshop of Systems and Synthetic Biology. Illetes, Mallorca, ES, 16-20 October 2012.*
- Human Metabolic Network Reconstructions: Past, Present and Future. *Future Challenges for Systems Medicine. Nowgen Centre, Manchester, 27 June 2012.*
- \*Integrative Informatics for Metabolic Systems Biology. *Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Belval, LU, 5 April 2012.*
- †Integrative Informatics for Metabolic Systems Biology. *Cranfield University, 23 January 2012.*
- The Subliminal Toolbox: automating steps in the reconstruction of metabolic networks. *1st Conference on Constraint-based Reconstruction and Analysis. Reykjavik, IS, 24-26 June 2011.*
- †Using metadata to develop and integrate models. *In Silico Systems Biology: Network Reconstruction, Analysis and Network-based Modelling. EMBL-EBI, Hinxton, 26 May 2011.*
- \*Data Integration, Mass Spectrometry Proteomics Software Development. *Bitesize Bio. 6 April 2011.*
- \*Encoding genome-wide models. *EBI Industry Workshop: Foundations for Biomedical Data and Model Interoperability. EMBL-EBI, Hinxton, Cambridge, 29 March 2011.*

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- The Subliminal Toolbox: automating steps in the reconstruction of metabolic networks. *Integrative Bioinformatics 2011, Wageningen, NL, 21-23 March 2011.*
  - \*Exploiting semantics in metabolic systems biology. *EMBL-EBI, Hinxton, 8 March 2011.*
  - †Integrative Informatics for Metabolic Systems Biology. *Cranfield University, 24 January 2011.*
  - \*Integrative Informatics for Metabolic Systems Biology. *Beatson Institute for Cancer Research, Glasgow, 30 November 2010.*
  - The SBML Level 3 Annotation package: an initial proposal. *COMBINE 2010, Edinburgh, 7-10 October 2010.*
  - Integrative Information Management for Systems Biology. *7th International workshop on Data Integration in the Life Sciences 2010 (DILS'10). Gothenburg, SE, 25-27 August 2010.*
  - \*ChEBI and genome-scale metabolic reconstructions. *2<sup>nd</sup> ChEBI User Group Workshop 2010. EMBL-EBI, Hinxton, Cambridge, 23-24 June 2010.*
  - libAnnotationSBML. *BioModels Meeting 2009. EMBL-EBI, Hinxton, 28-30 March 2009.*
  - Parameterisation of SBML models and visualization of experimental data through CellDesigner plugins. *3<sup>rd</sup> FEBS Advanced Lecture Course on Systems Biology: from Molecules to Life, Alpbach, AT, 7-13 March 2009.*
  - Development of an extensible system for the data capture and storage of enzyme kinetics experimental data. *Experimental Standard Conditions of Enzyme Concentrations, Rüdesheim-am-Rhein, DE, 23-26 September 2007.*
  - \*Development of an extensible system for the data capture and storage of enzyme kinetics experimental data. *Storage and Annotation of Reaction Kinetics Data, Heidelberg, DE, 21-23 May 2007.*

\* *Invited presentation.*

† *Guest lecture.*