David Wright

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About Me

I am a molecular modeller and software engineer, with a wide range of problem solving skills and experience running and maintaining IT infrastructure. I have also led small development teams and collaborated in large multi-national projects.

Skills

- Molecular Simulation
- High Performance Computing
- Programming: Python, R, Fortran, C
- Data Analysis
- Presentation Delivery
- Project Management
- System Administration
- Containerization: Docker, Singularity
- Cloud: Kubernetes, Azure, AWS, Google

References

Available upon request

Experience

I have fulfilled a variety of roles in my postdoctoral career, combining both modelling and software development, published 29 articles in leading journals and conference proceedings (a list of which are provided below). I have presented work at major conferences such as the Biophysical Society Annual Meeting, in 2012, 2013 and 2015, and International Supercomputing Conference (ISC) in 2018. During this time I have additionally worked on industrial projects on a consultancy basis.

2016 - present **Research Associate** — **Centre for Computational Science, UCL**

- Develop molecular simulation approaches to predict the strength of small molecule binding to protein targets for drug discovery applications.
- Process and analyze large quantities of simulation, experimental and clinical data.
- Lead team of developers on BAC 2.0 tool designed to automate molecular simulations using multiple applications and HTBAC workflow management tool.
- Lead development of the EasyVVUQ tool to automate verification, validation and uncertainty quantification for high performance computing applications.
- Research representative on the UCL Research Data Repository project board, involving collating and communicating user needs and providing feedback on project design and implementation.
- Contribute to reviews and panels informing strategic decisions in the European HPC (through the EXDCI project and PRACE scientific steering committee).
- Supervision of Masters and Ph.D. students, including both day to day direction of research, deadline management and coordination with primary supervisors.
- Organization of the "Free Energy Calculations from Molecular Simulation" workshop - in collaboration with the CompBioMed and BioExcel projects.
- Named investigator on the INSPIRE project (supported by the US department of INCITE program) combining molecular dynamics and machine learning to study cancer drug resistance.
- Contributing to writing of grant proposals, including those successfully approved for the CompBioMed2 (€8m) and VECMA (€4m) EU projects.

2017 - present **Chief Scientific Officer** — **EnsembleMD**

- Development and deployment of cloud based (SaaS) molecular simulation tools for multiple providers.
- Structural modelling of antibodies from small angle scattering data for pharmaceutical companies.
- Liaise with clients to determine their requirements and design solutions to fulfill them.

2013 - 2016 **Research Associate** — **Structural Immunology Group, UCL**

- Modelling and simulation of antibodies and other immune system proteins with the aim of understanding structural data.
- Lead developer of SCT, a Python package for the comparison of atomistic models to small angle scattering data.
- Head UK developer within the joint UK-US project CCP-SAS. Developed structural modelling packages (PDBRx, PDBScan), and contributed to underlying libraries (SASSIE, SasMol) and a common web interface for all project software (made available at sassie-web.chem.utk.edu).
- Trained users in the use of CCP-SAS tools, including teaching at a summer school at ILL in Grenoble, France.

2011 - 2013 **Research Associate** **Centre for Computational Science, UCL**

- Use of molecular dynamics simulations to understand the influence of protein mutations on drug binding.
- Administrator for network of 12 desktop machines and small cluster.
- Liaison with experimental groups in multinational medical and experimental project (CHAIN).

2010 - 2011 **Biomedical Simulation Consultant**

- Creation and testing of high performance computing workflow tools for Louisiana State University.
- Development (C and Fortran) of advanced simulation software for Fujitsu Laboratories of Europe.

Education

2011 **Ph.D., Chemistry** **UCL**
Molecular Dynamics Simulation of Drug Resistance in HIV-1 Protease and Reverse Transcriptase
Advisor: Prof. Peter V. Coveney

2006 **M Res (Distinction), CoMPLEX** **UCL**
Modelling Biological Complexity

2003 **M Phys (1st), Computational Physics** **University of York**

Publications

A live list of my publications can be found on **Google scholar**.

J. Dakka, M. Turilli, **D. W. Wright** *et al.*, High-throughput binding affinity calculations at extreme scales, BMC Bioinformatics, 2018, 19 (18), DOI: 10.1186/s12859-018-2506-6

W. Zhang, S. C. Howell, **D. W. Wright** *et al.*, Combined Monte Carlo/torsion-angle molecular dynamics for ensemble modeling of proteins, nucleic acids and carbohydrates, Journal of Molecular Graphics and Modelling, 2017, 73, DOI: 10.1016/j.jmgm.2017.02.010

N. A. Altwaijry, M. Baron, **D. W. Wright** *et al.*, An Ensemble-Based Protocol for the Computational Prediction of Helix–Helix Interactions in G Protein-Coupled Receptors using Coarse-Grained Molecular Dynamics, Journal of chemical theory and computation, 2017, 13 (5), DOI: 10.1021/acs.jctc.6b01246

R. Nan, C. M. Furze, **D. W. Wright** *et al.*, Flexibility in mannan-binding lectin-associated serine proteases-1 and-2 provides insight on lectin pathway activation, Structure, 2017, 25 (2), DOI: 10.1016/j.str.2016.12.014

A. P. Bhati, S. Wan, **D. W. Wright** and P. V. Coveney, Rapid, accurate, precise, and reliable relative free energy prediction using ensemble based thermodynamic integration, Journal of chemical theory and computation, 2016, 13 (1), DOI: 10.1021/acs.jctc.6b00979

S. J. Perkins, **D. W. Wright**, H. Zhang *et al.*, Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS), Journal of applied crystallography, 2016, 49 (6), DOI: 10.1107/S160057671601517X

K. W. Fung, **D. W. Wright**, J. Gor *et al.*, Domain structure of human complement C4b extends with increasing NaCl concentration: implications for its regulatory mechanism, Biochemical Journal, 2016, 473 (23), DOI: 10.1042/BCJ20160744

G. K. Hui, **D. W. Wright**, O. L. Vennard *et al*, The solution structures of native and patient monomeric human IgA1 reveal asymmetric extended structures: implications for function and IgAN disease, Biochemical Journal, 2015, 471 (2), DOI: 10.1042/BJ20150612

S. Wan, B. Knapp, **D. W. Wright** *et al.*, "Rapid, Precise, and Reproducible Prediction of Peptide–MHC Binding Affinities from Molecular Dynamics That Correlate Well with Experiment", Journal of Chemical Theory and Computation, 2015, 11 (7), DOI: 10.1021/acs.jctc.5b00179

D. W. Wright and S. J. Perkins, SCT: a suite of programs for comparing atomistic models with small-angle scattering data, *Journal of Applied Crystallography*, 2015, 48 (3), DOI: 10.1107/S1600576715007062

J. B. Swadling, **D. W. Wright**, J. L. Suter and P. V. Coveney, Structure, Dynamics, and Function of the Hammerhead Ribozyme in Bulk Water and at a Clay Mineral Surface from Replica Exchange Molecular Dynamics, Langmuir 31 (8), 2493-2501, DOI: 10.1021/la503685t

I. P. Deuzing, C. Charpentier, **D. W. Wright** *et al.*, Mutation V111I in HIV-2 reverse transcriptase increases the fitness of the nucleoside analogue resistant K65R and Q151M viruses, *Journal of Virology*, 2014, 89 (1), 833-843, DOI: 10.1128/JVI.02259-14

D. W. Wright, B. A. Hall, Owain A. Kenway, Shantenu Jha and P. V. Coveney, Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors, *Journal of Chemical Theory and Computation*, 2014, 10 (3), DOI: 10.1021/ct4007037

M. B. A. Kunze, **D. W. Wright**, N. D. Werbeck, J. Kirkpatrick, P. V. Coveney, and D. F. Hansen, Loop Interactions and Dynamics Tune the Enzymatic Activity of the Human Histone Deacetylase 8, *Journal of the American Chemical Society*, 2013, 135 (47), DOI: 10.1021/ct4007037

D. W. Wright, I. P. Deuzing, P. Flandre, P. van den Eede, M. Govaert, L. Setiawan, P. V. Coveney, A. Marcelin, V. Calvez, C. A. B. Boucher, N. Beerens, A Polymorphism at Position 400 in the Connection Subdomain of HIV-1 Reverse Transcriptase Affects Sensitivity to NNRTIs and RNaseH Activity, *PLoS One*, 2013, DOI: 10.1371/journal.pone.0074078

D. W. Wright, S. K. Sadiq, G. De Fabritiis and P. V. Coveney, Thumbs down for HIV: Domain level rearrangements do occur in the NNRTI bound HIV-1 Reverse Transcriptase, *Journal of the American Chemical Society*, 2012, 134 (31), DOI: 10.1021/ja301565k

S. Wan, **D. W. Wright** and P.V. Coveney, Mechanism of Drug Efficacy Within the EGF Receptor Revealed by Microsecond Molecular Dynamics Simulation, *Molecular Cancer Therapeutics*, 2012, 11, DOI: 10.1158/1535-7163.MCT-12-0644-T

B. A. Hall, **D. W. Wright**, S. Jha and P. V. Coveney, Quantized water access to the HIV-1 protease active site as a mechanism for cooperative changes in drug affinity, *Biochemistry*, 2012, 51 (33), DOI: 10.1021/bi300432u

D. W. Wright, B. A. Hall, P. Kellam and P. V. Coveney, Global Conformational Dynamics of HIV-1 Reverse Transcriptase Bound to Non Nucleoside Inhibitors, *Biology*, 2012, 1(2), DOI: 10.3390/biology1020222

D. W. Wright, S. Wan, N. Shublaq, S. Zasada and P. V. Coveney, From base pair to bedside: molecular simulation and the translation of genomics to personalised medicine, *WIREs Systems Biology and Medicine*, 2012, 4, 6, DOI: 10.1002/wsbm.1186

D. W. Wright and P. V. Coveney, Resolution of Discordant HIV-1 Protease Resistance Rankings Using Molecular Dynamics Simulations, *Journal of Chemical Information and Modeling*, 2011, 51, DOI: 10.1021/ci200308r

R. S. Saksena, B. Boghosian, L. Fazendeiro, O. A. Kenway, S. Manos, M. D. Mazzeo, S. K. Sadiq, J. L. Suter, **D. W. Wright** and P. V. Coveney, Real Science at the Petascale, *Philosophical Transactions of the Royal Society A*, 2009, 367, DOI: 10.1098/rsta.2009.0049

Preprints

S. K. Sadiq, **D. W. Wright**, O. A. Kenway and P. V. Coveney, Accurate Ensemble Molecular Dynamics Binding Free Energy Ranking of Multidrug-Resistant HIV-1 Proteases, *Journal of Chemical Information and Modeling*, 2009, 50, DOI: 10.1021/ci100007w

S. K. Sadiq, **D. W. Wright**, S. J. Watson, S. J. Zasada, I. Stoica, and P. V. Coveney, Automated Molecular Simulation-Based Binding Affinity Calculator for Ligand-Bound HIV-1 Proteases, *Journal of Chemical Information and Modeling*, 2008, 48, DOI: 10.1021/ci8000937

D. W. Wright, S. Wan, C. Meyer *et al.*, Application of ESMACS Binding Free Energy Protocols to Diverse Datasets: Bromodomain-Containing Protein 4, ChemRxiv (submitted to Scientific Reports) DOI: 10.26434/chemrxiv.7327019.v1

D. W. Wright, E. L. K. Ellison, G. K. Hui and S. J. Perkins, Monte Carlo atomistic modelling of X-ray and neutron scattering data for human IgG1 and IgG4 reveals new insights on antibody solution structure and function, submitted to Biophysical Journal

Conference Proceedings and Posters

D. W. Wright, G. K. Hui, O. L. Vennard, L. E. Rayner *et al.*, The asymmetric solution structures of native and patient monomeric human IgA1 reveal new insights on IgA nephropathy, 2015, *SAS 2015*

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D. W. Wright, B. A. Hall, S. Jha and P. V. Coveney, Multiscale Modelling of the Interplay Between Global and Local Structural Changes in Viral Drug Target Proteins, 2012, *VPH2012*

O. Kenway, **D. W. Wright**, H. Heller *et al.* Towards high-throughput, high-performance computational estimation of binding affinities for patient specific HIV-1 protease sequences, *Proceedings of the 2011 TeraGrid Conference on Extreme Digital Discovery - TG '11*, DOI: 10.1145/2016741.2016746

P. V. Coveney, **D. W. Wright** and S. K. Sadiq, Rapid and Accurate Binding Free Energy Prediction for Inhibitor-Bound HIV-1 Enzymes, 2010, *Biophysical Society 53rd Annual Meeting* (Poster)

D. W. Wright, S. K. Sadiq, O. Kenway *et al.* Computational Estimation of Binding Affinities for Patient Derived HIV-1 Protease Sequences Bound to Lopinavir, *VPH2010*, http://www.vphnoe.eu/vphrepository/doc_download/204-bookofabstractsforvph2010

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I have presented work at major conferences such as the Biophysical Society Annual Meeting, in 2012, 2013 and 2015, and International Supercomputing Conference (ISC) in 2018.