Stuart MacGowan

Computational Biologist

An experienced Computational Biologist, I specialise in structural bioinformatics and protein interaction analysis. I leverage extensive knowledge of human genomics and genetic variation data to comprehend protein-protein and protein-ligand interactions, developing insightful models and tools in Python and R. My research, deeply rooted in protein structures, contributes significantly to the understanding of disease processes. I'm dedicated to improving human health through rigorous, innovative research and collaboration.

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Education

2014
PhD in Computational Chemistry
Trinity College Dublin

2010
BSc (Hons) Chemistry with Mathematics
University of the West of Scotland

Expertise

- Protein structural bioinformatics
- Protein sequence analysis
- Python/ R development
- Research software engineering
- Statistics and data analysis
- Scientific reporting

Experience

2018 - Present
University of Dundee I Nethergate, Dundee
Senior Bioinformatics Scientist

As the Senior Bioinformatics Scientist and Manager of Dundee Resource for Sequence Analysis and Structure Prediction (DRSASP), I maintain and develop a comprehensive toolset for analysing protein sequences and structures. I am deeply involved in research, studying the effects of genetic variation on protein structure and function. This includes analysing large-scale data from hundreds of thousands of proteins. I have helped lead collaborations with multidisciplinary teams to identify genetic risk variants in COVID-19. Additionally, I'm focused on expanding DRSASP's capabilities to include genetic variation, enhancing reliability, and ensuring the reproducibility of our analyses.

2014 - 2018
University of Dundee I Nethergate, Dundee
Life Sciences Research Data Analyst

As a Postdoctoral Researcher in the Data Analysis Group (DAG) in Prof. Geoff Barton's lab at the University of Dundee, I worked on a collaboration with Prof. Irwin McLean investigating the genetics of rare skin diseases. In this role I implemented improved variant calling pipelines for trio sequencing data, developed algorithms and workflows for disease gene identification and built a graphical interface driven R/Shiny application to help our experimental collaborators promise variants for diagnosis and assay follow-up.

2010 - 2014
Trinity College Dublin I College Green, Dublin
PhD Researcher

I completed a PhD in Computational Chemistry working in Prof. Mathias Senge's Science Foundation Ireland Tetrapyrrole Laboratory. My project involved studying the conformations of chlorophyll and haem molecules in photosynthetic proteins, cytochromes and globins, I was the sole computational chemist in the SFI Tetrapyrrole Lab, which was focussed on organic synthesis, and this experience taught me how to work independently and communicate effectively with wet-lab researchers outside my specialism. During this time I developed strategies to analyse ligand conformations across multiple crystal structures and gained experience in scripting, statistical methods, and computational chemistry techniques.

References

Prof. Dr. Mathias Senge
Professor of Organic Chemistry,
Trinity College Dublin
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Prof. Geoff Barton
Professor of Computational Biology,
University of Dundee
Phone: +44 1382 385860
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More references available on request

Publications (1 of 2)

2023

Utgés, J. S., **MacGowan, S. A.**, Ives, C. M. & Barton, G. J. Classification of likely functional state for ligand binding sites identified from fragment screening. PREPRINT (Version 1) available at Research Square, doi:10.21203/rs.3.rs-3185838/v1 (2023).

MacGowan, S. A., Madeira, F., Britto-Borges, T. & Barton, G. J. A unified approach to evolutionary conservation and population constraint in protein domains highlights structural features and pathogenic sites. PREPRINT (Version 1) available at Research Square, doi:10.21203/rs.3.rs-3160340/v1 (2023).

Cleghorn, L. A. T., Wall, R. J., Albrecht, S., **MacGowan, S. A.** et al. Development of a 2,4-Diaminothiazole Series for the Treatment of Human African Trypanosomiasis Highlights the Importance of Static-Cidal Screening of Analogues. J Med Chem 66, 8896-8916, doi:10.1021/acs.jmedchem.3c00509 (2023).

2022

MacGowan, S. A. et al. Missense variants in human ACE2 strongly affect binding to SARS-CoV-2 Spike providing a mechanism for ACE2 mediated genetic risk in Covid-19: A case study in affinity predictions of interface variants. PLoS Comput Biol 18, e1009922, doi:10.1371/journal.pcbi.1009922 (2022).

2021

Utges, J. S., Tsenkov, M. I., Dietrich, N. J. M., **MacGowan, S. A.** & Barton, G. J. Ankyrin repeats in context with human population variation. PLoS Comput Biol 17, e1009335, doi:10.1371/journal.pcbi.1009335 (2021).

Barton, M. I., **MacGowan, S. A.** et al. Effects of common mutations in the SARS-CoV-2 Spike RBD and its ligand, the human ACE2 receptor on binding affinity and kinetics. Elife 10, doi:10.7554/eLife.70658 (2021).

2020

Varadi, M. et al. PDBe-KB: a community-driven resource for structural and functional annotations. Nucleic Acids Res 48, D344-D353, doi:10.1093/nar/gkz853 (2020).

MacGowan, S. A. et al. The Dundee Resource for Sequence Analysis and Structure Prediction. Protein Sci 29, 277-297, doi:10.1002/pro.3783 (2020).

MacGowan, S. A. & Barton, G. J. Missense variants in ACE2 are predicted to encourage and inhibit interaction with SARS-CoV-2 Spike and contribute to genetic risk in COVID-19. bioRxiv, doi:10.1101/2020.05.03.074781 (2020).

Llabres, S., Tsenkov, M. I., **MacGowan, S. A.**, Barton, G. J. & Zachariae, U. Disease related single point mutations alter the global dynamics of a tetratricopeptide (TPR) alpha-solenoid domain. J Struct Biol 209, 107405, doi:10.1016/j.jsb.2019.107405 (2020).

Publications (2 of 2)

2018

Portnoi, M. F. et al. Mutations involving the SRY-related gene SOX8 are associated with a spectrum of human reproductive anomalies. Human Molecular Genetics 27, 1228-1240, doi:10.1093/hmg/ddy037 (2018).

2017

MacGowan, S. A. et al. Human Missense Variation is Constrained by Domain Structure and Highlights Functional and Pathogenic Residues. bioRxiv, doi:10.1101/127050 (2017).

2016

MacGowan, S. A. & Senge, M. O. Contribution of bacteriochlorophyll conformation to the distribution of site-energies in the FMO protein. Biochim Biophys Acta 1857, 427-442, doi:10.1016/j.bbabio.2016.02.001 (2016).

2015

Senge, M. O., **MacGowan, S. A.** & O'Brien, J. M. Conformational control of cofactors in nature - the influence of protein-induced macrocycle distortion on the biological function of tetrapyrroles. Chem Commun (Camb) 51, 17031-17063, doi:10.1039/c5cc06254c (2015).

Mercier, S. et al. Expanding the clinical spectrum of hereditary fibrosing poikiloderma with tendon contractures, myopathy and pulmonary fibrosis due to FAM111B mutations. Orphanet J Rare Dis 10, 135, doi:10.1186/s13023-015-0352-4 (2015).

McAleer, M. A. et al. Severe dermatitis, multiple allergies, and metabolic wasting syndrome caused by a novel mutation in the N-terminal plakin domain of desmoplakin. J Allergy Clin Immunol 136, 1268-1276, doi:10.1016/j.jaci.2015.05.002 (2015).

2014

Senge, M. O., Ryan, A. A., Letchford, K. A., **MacGowan, S. A.** & Mielke, T. Chlorophylls, Symmetry, Chirality, and Photosynthesis. Symmetry-Basel 6, 781-843, doi:10.3390/sym6030781 (2014).

2013

MacGowan, S. A. & Senge, M. O. Computational quantification of the physicochemical effects of heme distortion: redox control in the reaction center cytochrome subunit of Blastochloris viridis. Inorg Chem 52, 1228-1237, doi:10.1021/ic301530t (2013).

2011

Senge, M. O. & **MacGowan, S. A.** The Structural Chemistry of Isolated Chlorophylls. Handbook of Porphyrin Science 13, 253-297 (2011).

MacGowan, S. A. & Senge, M. O. Conformational control of cofactors in nature-functional tetrapyrrole conformations in the photosynthetic reaction centers of purple bacteria. Chem Commun 47, 11621-11623, doi:10.1039/c1cc14686f (2011).