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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Websites

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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 l 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 l 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 l 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
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Prof. Geoff Barton
Professor of Computational Biology,
University of Dundee
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More references available on request

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).

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2022

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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).

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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).

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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).

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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).

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