



A/Professor Ashley Buckle

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Monash Biomedicine Discovery Institute
Infection and Immunity Program

OTHER PROGRAM AFFILIATIONS



Cancer



Cardiovascular Disease

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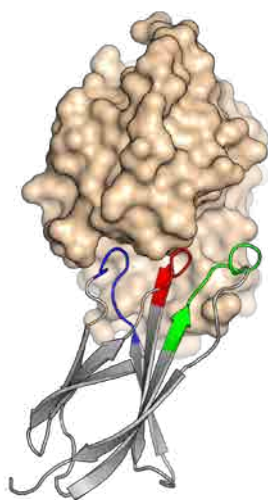
TELEPHONE +61 3 9902 9313

WEB <http://pxgrid.med.monash.edu.au/projects/>

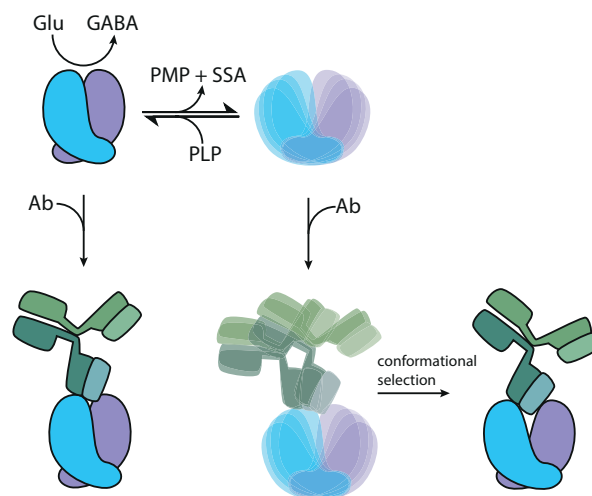
We combine x-ray crystallography and biophysics with molecular simulation to study the structure, folding and dynamics of proteins, with a particular focus on the design and engineering of proteins for medical and biotechnological application. Our team is a unique and exciting mix of experimentalists and computational biologists using modeling and simulation to make predictions that can be tested in the lab.

Research Projects

1. Designing potent protease inhibitors as potential anti-cancer agents
2. Using computational and experimental methods to design and evolve novel proteins
3. The evolution of protein dynamics



Design, engineering and evolution of Adnectins.



Implications of GAD65 autoinactivation for neurotransmitter biosynthesis and autoantigenicity.

Selected significant publications:

1. Porebski BT, Nickson AA, Hoke DE, Hunter MR, Zhu L, McGowan S, Webb GI, and **Buckle AM**. 2015. Structural and dynamic properties that govern the stability of an engineered fibronectin type III domain. *Protein Engineering, Design and Selection* 28 (3): 67-78.
2. Kass I, Hoke DE, Costa MG, Reboul CF, Porebski BT, Cowieson NP, Leh H, Pennacchietti E, McCoe J, Kleinfeld O, Borri Voltattorni C, Langley D, Roome B, Mackay IR, Christ D, Perahia D, Buckle M, Paiardini A, De Biase D and **Buckle AM**. 2014. Cofactor-dependent conformational heterogeneity of GAD65 and its role in autoimmunity and neurotransmitter homeostasis. *Proc. Natl. Acad. Sci. USA*, 111(25):E2524-9.
3. Kass I, Knaupp A, Bottomley S and **Buckle AM**. 2012. Conformational properties of the disease-causing Z variant of α^1 antitrypsin revealed by theory and experiment. *Biophys. Journal*, 102, 2856-65
4. Reboul CF, Meyer GR, Porebski BT, Borg NA and **Buckle AM**. 2012. Epitope Flexibility and Dynamic Footprint Revealed by Molecular Dynamics of a pMHC-TCR Complex. *PLoS Computational Biology*, 8(3):e1002404.
5. Reboul CF, Porebski BT, Griffin MD, Dobson RC, Perugini MA, Gerrard JA, **Buckle AM**. 2012. Structural and dynamic requirements for optimal activity of the essential bacterial enzyme dihydrodipicolinate synthase. *PLoS Comput Biol* 8(6):e1002537.