

267-Pos Board B53**Analysing Helix Flexibility in Membrane Proteins using Bendix****A. Caroline E. Dahl**, Matthieu Chavent, Mark S.P. Sansom.

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Alpha helix flexibility plays a key role in the mechanisms of gating of ion channels and solute transporters. Examples of this can be seen in the voltage-gated potassium channel Kv1.2 and the mechanosensitive channel of small conductance, MscS, where molecular hinges within channel-lining helices are important for gating. Kv1.2 and MscS are not exceptional - membrane proteins often feature curved or kinked helices, and dynamics of such non-ideal helices is critical to protein function. However, non-linear helices are compromised by current visualization techniques, and call for better characterization. Bendix is a software that colours, quantifies and simplifies both static structures and dynamic (MD) simulation trajectories, without sacrificing details of local conformation. It also enables visualization of secondary structure in coarse-grained simulations of proteins. It is available as a plugin for the molecular graphics program Visual Molecular Dynamics (VMD, <http://www.ks.uiuc.edu/Research/vmd>) and works under most operating systems. Bendix offers custom colour schemes that highlight relevant helix curvature and allow you to explore protein structures. Generated helix data is easily presented using the in-built 2D or 3D graphing module, alternatively exported to other graphics packages. We will illustrate its application to a number of channel and transport proteins, including MscS, the potassium channel KcsA, the MFS transporter proteins L-fucose permease (FucP) and lactose permease (LacY), and the sodium-hydantoin transporter Mhp1. Bendix is user-friendly, free and available for download at <http://sbc.bioch.ox.ac.uk/dahl.php>.
