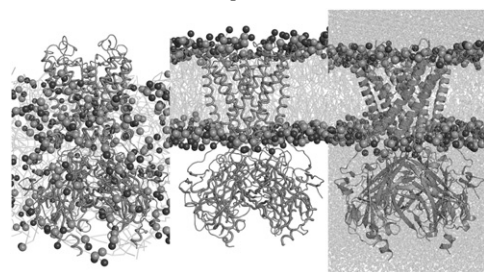


**2390-Pos Board B160****Memprotmd: Adding the Grease to Membrane Protein Structures****Phillip J. Stansfeld**, Mark S.P. Sansom.

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Membrane protein structural biology is one of the key biochemical challenges. With continuous improvements to the methods used by structural biologists there is a predicted exponential growth in the number of membrane proteins structures. Nevertheless, these biological assemblies are usually resolved in the absence of the native lipid environment. Coarse-Grained molecular dynamics (CGMD) simulations provide a means for assessing the assembly and interactions of molecular complexes at a reduced level of representation. This method has been shown to accurately predict the position and orientation of proteins within a cell membrane. The results of these predictions are available in a database (<http://sbc.bioch.ox.ac.uk/cgdb>). We are in the process of pipelining the procedure, so that new membrane protein structures are automatically inserted into

a DPPC lipid bilayer on release from the Protein Data Bank (PDB). The CG simulations are then assessed for protein-lipid interactions, bilayer deformation, lipid diffusion and protein tilt. The resulting models are



then refined to include more physiologically relevant lipid mixtures and subsequently converted to an atomistic resolution [1] to enable more detailed simulations of lipid protein interactions [2].

[1] Stansfeld, JCTC, 7 (2011) 1157-1166.

[2] Stansfeld, Biochemistry, 48 (2009) 10926-33.