Interactions of Antimicrobial Polyelectrolytes with Bacterial Model Membranes

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Widespread use of antibiotics is leading towards increased resistance to common anti-microbial drugs. This justifies the need for more research in new antibiotics. Among the new potentially useful compounds, polyelectrolytes are particularly interesting because they are cheap, commercially available and easy to prepare.

To understand their antibacterial function we focus on the study of a particular family of polyelectrolytes, named polyhexamethylene biguanide (PHMB) developing the first MARTINI model for such polyelectrolyte (Fig. 1). The model has been validated by comparison with all-atom simulations, and it reproduces a number of experimental properties of the polymer.

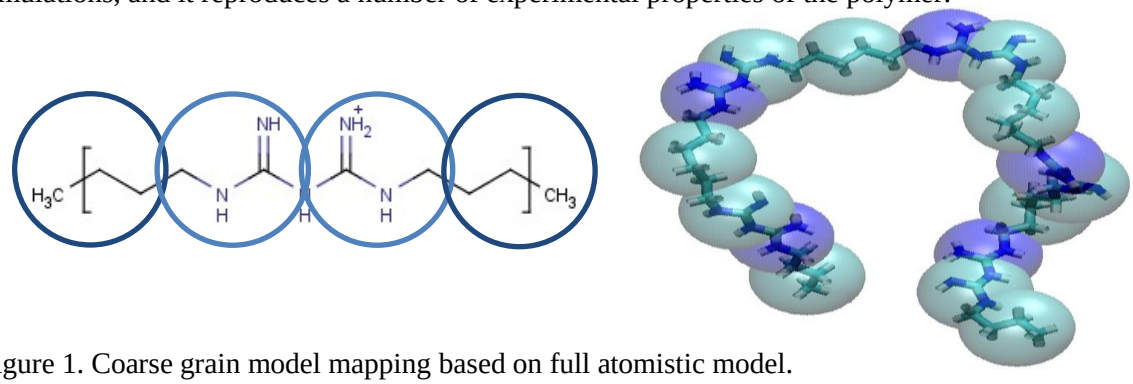

Figure 1. Coarse grain model mapping based on full atomistic model.

We characterise the interaction of PHMB with model lipid membranes of two different types: POPC membranes, very common in the plasma membrane of animal cells, and mixed POPC/POPG membranes, which hold a negative charge and mimic some properties of bacterial membranes[1]. Our preliminary results provide an unprecedented insight into the mechanism of anti-microbial activity shown by these synthetic polymers (Fig. 2).

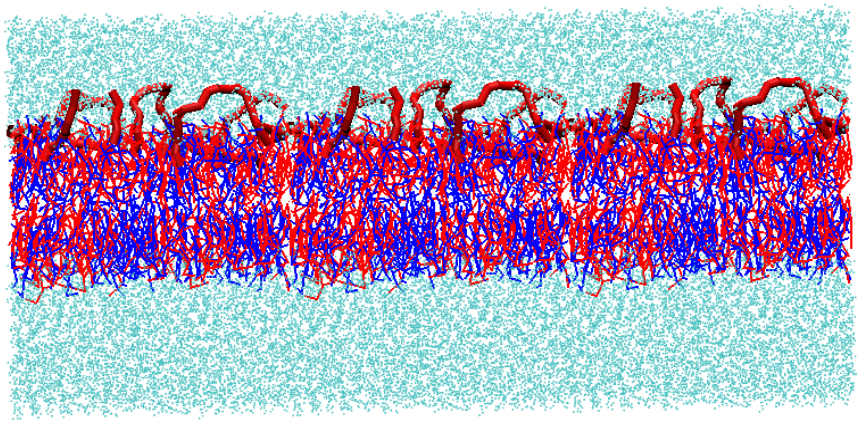

Figure 2. A model bacterial bilayer membrane containing POPC (thin red molecules) and POPG lipids (thin dark blue molecules). The dark red tubular molecules represent the PHMB polyelectrolytes adsorbed onto the membrane surface. The cyan beads on both outer regions are water molecules in the system.

[1]Murzyn, K.; Róg, T.; Pasenkiewicz-Gierula, M., Phosphatidylethanolamine-Phosphatidylglycerol Bilayer as a Model of the Inner Bacterial Membrane. *Biophysical journal* **2005,** *88* (2), 1091-1103.