

Abstract Submitted  
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**Simulated biophysical experimental techniques for chlorhexidine in dmpc/cholesterol systems** BRAD VAN OOSTEN, THAD HARROUN, Brock University — We have investigated the use of molecular dynamic simulations and the MARTINI force field to simulate isothermal titration calorimetry and differential scanning calorimetry techniques. The goal of these simulations was to observe how well they can reproduce the concentration effects of the addition of the small molecule chlorhexidine (CHX) into a model DMPC membrane containing varying concentrations of cholesterol. We constructed a coarse grained model for CHX compatible with the MARTINI force field. We were able to mimic an isothermal titration calorimetry experiment by repeatedly adding CHX into a DMPC membrane. With the increased concentration, we observed a decreasing affinity between CHX and the membrane as well as a resulting increase in the reaction time before the system was equilibrated. We then performed a controlled cooling of the membrane with various CHX concentrations to mimic a differential scanning calorimetry experiment. A change in membrane structure accompanied by a spike in the specific heat was measured at specific temperature  $T_m$  signaling a phase transition. We then varied the concentration of CHX as well as the addition of varying concentrations of cholesterol to observe trends in the change to  $T_m$  due to the addition of CHX and cholesterol.

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