Development of interfacial models to understand preservation through Neutron Reflection

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Evidence of humans using preservation techniques spans over 100,000 years, from the first evidence of wood polishing 750,00 years ago to use of beeswax as an antimicrobial in cosmetics ancient Rome [1,2]. However since the widespread acceptance of germ theory we have seen vast advances in preservative technology including chemical synthesis and refrigeration. Preservation is vital today for the prevention of disease and protection of human health but also to reduce production waste or recalls, which present both environmental and industrial costs. Despite the widespread use and importance of chemical preservatives today very little is known about the mechanisms of action on molecular scales, which is key preservative development and understanding risk.

In this work we study phenoxyethanol (PE), which is the most widespread preservative used in personal care products today. PE has been shown to cause some cytoplasmic leakage in bacteria, but this study has been the first to directly structural and mechanical changes induced at the membrane interface [3]. Safety and environmental concerns have encouraged development of boosting molecules, which show no efficacy alone, to work synergistically with PE enabling reduced concentrations in products. These include propylene glycol monocaprylate (PGMC).

This work has been an interdisciplinary study teasing out biocidal mechanisms of PE and PE+PGMC mixtures. These include microbiology work demonstrating improvement in PE efficacy against E. coli under addition of PGMC, and increased membrane depolarisation and leakage (Fig 1. A,B,C). Rheological study using the Langmuir Trough with phospholipid monolayer models of gram-negative bacteria inner membranes revealed PGMC creates a more elastic membrane enabling easier incorporation of PE and under mixture membrane become more rigid and easier to rupture (Fig .1 D). Neutron Reflection techniques using same membrane model directly observe the structural changes to model membranes revealing PE and more significantly PE+PGMC cause lipid loss from monolayer and PGMC causes PE retention under pressure fluctuations (Fig 1. E,F). We have also performed molecular dynamics simulations to tease out more details from this neutron work. Much work has been done to explore effects of antibiotic drugs on model microbe membranes using neutron techniques however this is the first work to explore the effects of preservatives, demonstrating neutron techniques as a very powerful tool in preservative science [4].

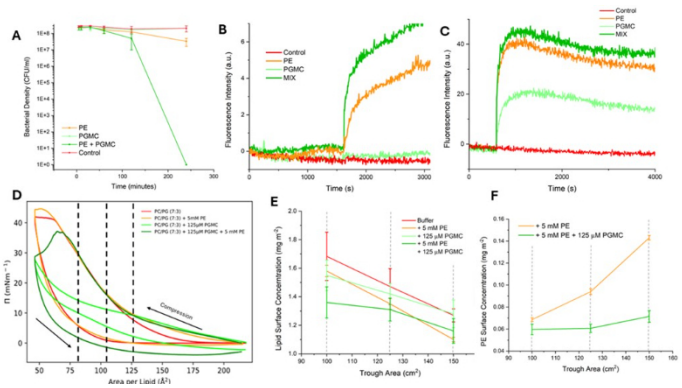

Fig 1. A. E.coli Dynamic killing B. E. coli NPN Uptake C. E. coli Membrane Depolarization (DiSC3) D. Langmuir Isotherms E,F. Surface Concentrations from Neutron Fitting

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