

Improving personal care products with advanced simulation

We are working with Unilever, using advanced in-silico modelling capabilities to drive understanding into antimicrobial peptide interactions for future product development.

Challenge

For personal care products like deodorant, shampoo or toothpaste to be effective, we need to be able to modulate the growth or activity of some of the body's natural micro-organisms. Our bodies have already evolved ways to do this through the production of antimicrobial peptides (AMPs). Keratinocytes – present in our normal, healthy skin cells – produce AMPs which contribute to the skin's ability to deter the overgrowth of undesirable micro-organisms. Discovering how AMPs exert their antimicrobial effect and translating this knowledge into consumer products which work in partnership with natural defence peptides is important to Unilever when identifying innovative sustainable technologies for consumers.

Approach

Researchers at the Hartree Centre built upon the existing laboratory testing work at Unilever by using advanced in-silico modelling techniques to identify strategies that work in harmony with natural AMPs. The team was able to simulate how AMPs and novel potentiator molecules interact with simulated bacterial members to control microbial growth in great detail. To demonstrate the specificity of the interaction to bacterial membranes, similar work was completed on model non-bacterial membranes.

“The ability to collaborate with the Hartree Centre and benefit from their expertise in high performance computing and simulation has provided fresh insights, advancing our understanding of antimicrobial peptides.”

Michael Hoptroff

Unilever



Credit: Unsplash

Benefits

This approach – developed as part of the collaborative Innovation Return on Research (IROR) programme with IBM Research – generated new structural and mechanistic insights that help answer why some small molecules display a synergy in working with the natural peptide to exert a greater effect and why others do not. Ultimately, this work has helped to generate a lead for a pipeline of new candidate materials with enhanced properties to be investigated further. This learning will help reap benefits from molecules currently under investigation and will help inform the pipeline of new material's discovery.

At a glance

- Conducted simulations that enhanced understanding of how microbial growth can be controlled through interactions between bacteria versus AMPs and their analogues
- Delivered new insights on how small molecules interact with natural AMPs
- Generated a lead for a pipeline of Unilever's next generation materials
- Enhanced the company's understanding of digital technologies
- Valued working with the STFC Hartree Centre as a trusted partner

Who we are

The Hartree Centre was created by UK Government to help businesses and public sector organisations accelerate the adoption of high performance computing (HPC), big data analytics, artificial intelligence (AI) and quantum technologies. We play a key role in realising UK Government's Industrial Strategy by stimulating applied digital research and innovation, creating value for the organisations we work with and generating economic and societal impact for the UK. We are proud to be part of UK Research and Innovation.

What we do

- Boost productivity and innovation for industry
- Offer training and skills development
- Provide insights into future technologies
- Give tailored business development support
- Build bespoke small teams around your project

