Researchers based at the STFC Hartree® Centre 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 were 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.

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 materials discovery.

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Michael Hoptroff
Unilever
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Michael Hoptroff
Unilever

At a glance

- Applying high performance computing technologies to simulate peptide and small molecule synergy for product discovery
- Using in-silico modelling techniques to assess lead materials
- Structural and mechanistic insights as to how natural peptides interact with candidate compounds, explaining why some exert a greater effect than others.

Who we are

- 60+ computational scientists and technologists
- World-leading supercomputing and AI infrastructure
- Bespoke small teams built around your project
- Tailored business development support
- Access to our network of industry, academic and technology partners

What we do

- Boost productivity and enhance innovation for industry
- Big data analytics and artificial intelligence (AI)
- High performance computing and quantum simulation
- Training and skills development
- Insights into emerging technologies

Our impact on UK industry and society

The Hartree Centre was created by UK Government to transform industry by accelerating the adoption of high performance computing (HPC), big data analytics and artificial intelligence (AI) 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.

The Science and Technology Facilities Council (STFC) Hartree Centre is part of UK Research and Innovation.