Science and Technology Facilities Council

Scientific Computing

Using computers to boost the skin's natural defences

Acne breakouts, blocked pores, dandruff, eczema and body odour are all universal problems resulting from imbalances in the skin's microbial environment. A major challenge is to find products that will boost our natural defences to treat these problems.

The challenge

The cosmetics industry has experimented and produced many products that aim to fix the damage caused by bacterial imbalances in the skin. However, there is one ingredient that is particularly desirable for its versatility and efficacy: the vitamin B3 derivative known as niacinamide.

Building on an earlier research collaboration, scientists from Unilever, the Science and Technology Facilities Council (STFC) and IBM Research, embarked on an investigation to understand the mechanism behind niacinamide's power.

Scientists at Unilever had, some years earlier, observed that niacinamide enhanced antimicrobial activity. They wanted to find out more about it so asked colleagues from STFC Hartree Centre, STFC Scientific Computing and IBM Research to help.

To understand niacinamide, we first need to understand how it interacts with antimicrobial peptides (AMPs). These are small proteins that occur naturally as part of our skin's immune system, regulating its bacterial balance and protecting us against harmful bacteria.

When such bacteria do come into contact with our skin, the AMPs are attracted to it, clustering on the bacterial membrane and eventually inserting themselves into it. This ultimately causes the bacterial cell to burst and die.

Our approach

Scientific Computing's Dr Valeria Losasso created computational models of the components involved in the process: AMP, niacinamide, and the bacterial cell membrane.

Because the software is pre-programmed with general 'rules', such as how bonds form between certain atoms or protein structures, the software can accurately determine and model the structure of niacinamide and AMPs.

She used software specialising in membrane modelling to model the bacterial membrane, adding different molecules to mimic the real-life complexity of membranes.

All these components, created on separate software, are then combined into a single model of the system on a visualisation software where the components can be translated, rotated, or modified in other ways.

"I can tell the simulation program that I want to build a system where the AMP is close enough to the membrane for us to see if the AMP infiltrates the membrane and how. I can add water and ions to accurately recreate the skin's environment."

Dr Valeria Losasso, Computational Scientist, STFC Scientific Computing

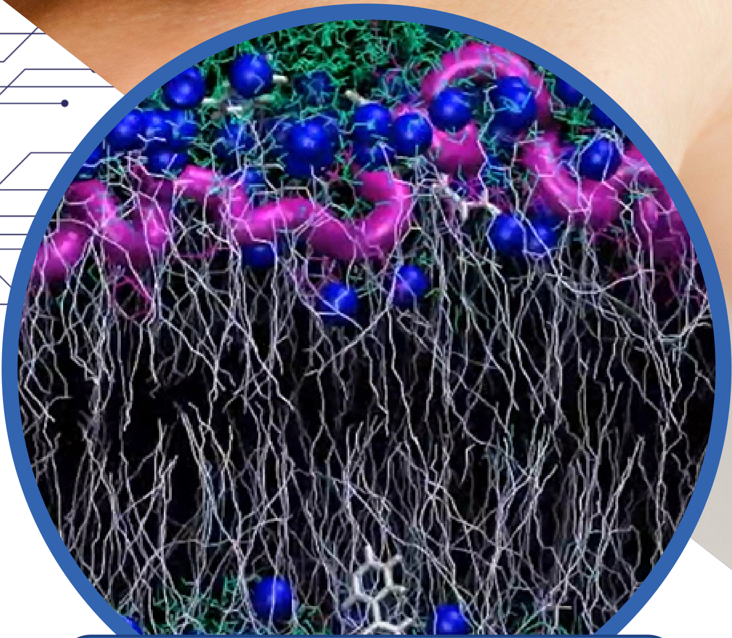
Once the structure of the model is properly set up, the components need to be ‘brought to life’. The scientists need the model components to behave in a way that accurately reflects their real-life counterparts.

When the model is as dynamic and realistic as possible, the simulation is run on high-performance computers to observe how the niacinamide and AMP interact with each other and with the bacterial membrane.

The study identified two key interaction mechanisms for how niacinamide physically enhances AMP activity.

> **“In both mechanisms, the AMPs arrange themselves to form pores that create an opening for the contents of the bacterial cell to leak out. This leakage or ‘bursting’ causes the cell to die.”**
>
> **Dr Valeria Losasso, Computational Scientist, STFC Scientific Computing**

The first mechanism involves niacinamide interacting directly with AMP by forming the same bonds that are found between water molecules. This makes it easier for AMPs to insert into the bacterial membrane, disrupting it.



A simulation of AMP (purple) infiltrating the bacterial membrane, helped by niacinamide (white molecule).

The second mechanism relies on niacinamide interacting with the bacterial membrane on its own. This interaction disrupts the bacterial membrane ahead of AMP’s insertion, making it easier for AMP to infiltrate the membrane.

Benefits of this research

This study has enabled scientists and industry to better understand the interaction between niacinamide molecules and AMPs, and the mechanisms they use to attack harmful bacterial cells that can affect our skin.

This is already leading to a new generation of improved skin hygiene products and cosmetics that can boost the skin’s natural defences.

It is also opening up opportunities for the design and use of other small molecules in both skincare development and health-related applications.

Written and designed by Rui Wen Lim, Science Communication Industrial Placement Student, STFC Scientific Computing Communications and Impact Team