

# Leveraging Artificial Intelligence to Uncover Natural, Soothing Peptides for Personal Care

Moussou P PhD<sup>1</sup>, Ludwig P PhD<sup>2</sup>, Chan WK<sup>2</sup>, Foster N<sup>3</sup>, André-Frei V PhD<sup>1</sup>, Kalem C<sup>1</sup>

1 BASF Beauty Care Solutions France, Lyon, France

2 BASF Corporation, NY, United States

3 Nuritas, Dublin, Ireland

## Background

Consumers across all ages are health conscious and want to preserve their skin health by a proactive and protective approach. Unfortunately, low-grade silent inflammation, or inflammaging, is on the rise, due to our exposure to an increasing variety of external agents that our bodies are not accustomed to. This silent inflammation underlies alteration of skin and scalp<sup>1</sup> with irritations and discomfort. In nature, there are thousands of raw materials, consisting of trillion of natural molecules. Some of these molecules, in particular peptides, can be beneficial for a healthy beauty, fighting against the damages on skin resulting from this silent inflammation. In the past, peptides were too vast in numbers to screen, but today thanks to Artificial Intelligence, it is now possible to explore the information coming from huge volume of data to discover some hidden connections, and thus to identify natural anti-inflammaging peptides faster and more accurately than with traditional methods.

## Objective

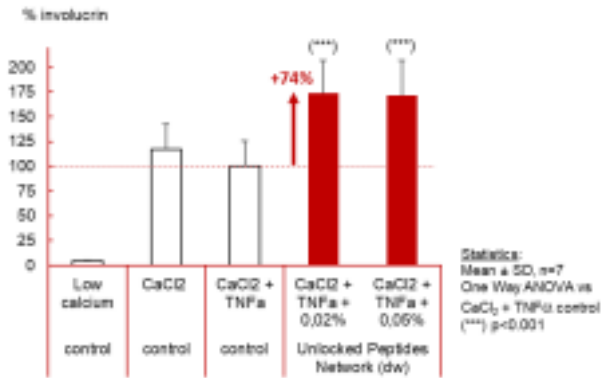
The aim of this study was to discover new natural anti-inflammaging peptides with the help of Artificial Intelligence (AI), and to create a solution based on safe natural peptides from a vegetal food source, to naturally keep skin healthy.

## Methodology

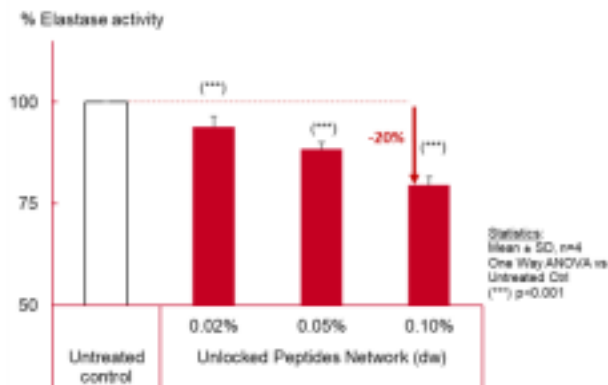
The discovery approach combined predictions generated by machine learning with *in vitro* tests to evaluate trillions of potential peptides. Using several data entries (unstructured and structured literature, public structured proteomic and metabolomic databases, peptide library, and phenotypic data from cell assays), a predicted architecture was built *via* deep learning models to identify and unlock anti inflammaging peptides from vegetal food proteins. The anti-inflammaging activity of the unlocked peptides solution was assessed through *in vitro* assays, on involucrin synthesis on TNFalpha-treated epidermal keratinocytes (NHEK)<sup>2</sup> and on human neutrophil elastase inhibition<sup>3</sup>. Two clinical studies were conducted: a shampoo, placebo-controlled double-blind study on 44 volunteers having a sensitive and irritated scalp, and a body wash consumer study with assessment of elicited emotions.

## Results

From this AI approach a natural solution characterized by 4 specific peptides, from 12 to 17 amino acids, was discovered in rice proteins. A controlled enzymatic hydrolysis process was developed to unlock these peptides from rice (*Oryza sativa*) proteins and produce the Unlocked Peptides Network. *In vitro* assays demonstrated their stimulating effect on involucrin synthesis in TNFalpha-treated NHEK and elastase inhibition (Fig 1 and 2).



**Figure 1:** Effect of the Unlocked Peptides Network (dry weight) on involucrin expression in TNF $\alpha$  treated keratinocytes

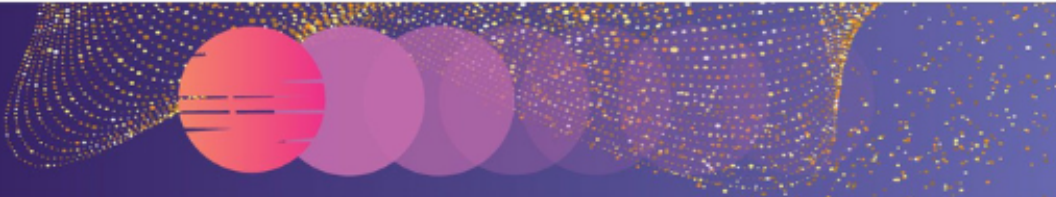


**Figure 2:** Effect of the Unlocked Peptides Network (dry weight) on elastase inhibition

*In vivo*, the peptide solution improved the scalp health with a reduction of scalp redness and pH, significantly versus the placebo shampoo. In the body wash consumer study, a significant majority of the panelists felt a less itchy, irritated and more comfortable skin, and the product use was associated with positive emotions: confidence, excitement, content.



**Figure 3:** Illustrative pictures of the scalp on 2 volunteers demonstrating the reduction of redness and scales by a shampoo containing 2% of the Unlocked Peptides Network



**Conclusion**

From vast amount of molecular diversity of peptides, Artificial Intelligence technology enabled to discover an anti-inflammaging peptides solution characterized by 4 peptides. *In vitro* and *in vivo* testing has proven that this natural peptide network improved the scalp and skin equilibrium and comfort and elicited positive emotions in rinse-off applications. It responds to the demand of consumers who want to feel better with their hair, scalp and skin and would like to expand their cleansing experience with more associated positive feelings.

Artificial intelligence is one of the key drivers of the new industrial revolution. It changes the way we work and interact with data and technology and provides, by in silico prediction and machine learning, the power to obtain accurate and efficient solutions for innovative bioactive cosmetic ingredients. It enables us to discover new generation of natural plant-based peptides to answer to the consumers demand of simple and safe products for clean beauty with scientifically proven claims.

**References**

1. Zhuang Y & Lyga J. *Drug targets*. **13**: 153-161 (2014)
2. Kim BE, Howell MD, Guttman E, Gilleaudeau PM, Cardinale IR, Boguniewicz M, Krueger JG, Leung DYM. *J Invest Dermatol*. **131**: 1272-1279 (2011)
3. Antonicelli F & Hornebeck W. In *Inflammation, Advancing Age and Nutrition: Research and Clinical Interventions*. Chapter **21**: 255-265 (2013)