ABSTRACT

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Podium Title (Session B): *Natural Anti-Inflammaging Peptides for Hair, Scalp and Body Care Designed through Artificial Intelligence.*

Background information (Short introduction)

There are thousands of plants, consisting of trillion of molecules. Some of these molecules can be beneficial for a healthy beauty, in particular peptides to fight against low-grade inflammation, or inflammaging, which underlies alteration of skin and scalp with irritations and discomfort. In the past peptides were too vast in numbers to screen. With Artificial Intelligence, this is now possible to identify natural anti-inflammaging peptides faster and more accurately than with traditional metho

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 meet the trend of clean beauty.

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 proteomics and metabolomics databases, peptides 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 predicted peptides solution was assessed through in vitro assays, on involucrin synthesis on TNFalpha-treated epidermal keratinocytes (NHEK) and on human neutrophil elastase inhibition. Two clinical studies were conducted: a shampoo, placebo-controlled double-blind study with 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 vitro assays demonstrated their stimulating effect on TNFalpha-treated NHEK and elastase inhibition.

In vivo, the peptides solution improved the scalp balance 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.

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.

Why is this important to the industry?

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.

Podium Title (Session G): *A new 3D-autologous iPSC-derived model to mimic hair bulb structure and multiple crosstalk*

Background information (Short introduction)

Human hair follicles are complex skin appendages dependent on multiple crosstalks between ectodermal and mesodermal cells which are essential to control hair growth, quality and pigmentation.

Current animal models and in vitro 2D-cultures cannot completely reflect in vivo mechanisms. In addition, the availability of human hair samples is limited due to ongoing advances in surgery practice. Then, there is a need for a 3D-model restoring these cellular interactions to study the hair follicle.

Objective

For this reason, we developed an in vitro 3D-hair bulb model based on three different hair cell types: outer root sheath keratinocytes (producing hair shaft), melanocytes (pigmentation) and dermal papilla cells (DP) (controlling hair homeostasis), all coming from an identical donor and resolving the hair sample limitation.

Methodology

We focused on developing an in vitro 3D-autologous hair bulb derived from induced pluripotent stem cells (iPSCs). Via iPSC technology, somatic cells are transferred into pluripotent state. With an appropriate protocol, it is possible to differentiate iPSC into any cell types and then by combining them to establish autologous micro-organs. Here, some iPSCs were differentiated into keratinocytes stem cells through a non-neuroectodermal induction. After an initiation in

neural crest cells, other iPSCs were differentiated in DP cells and melanocytes via specific protocols. These three iPSC-derived cell types were then combined into a bulb-like spheroid.

Results

Differentiation protocols were optimized by evaluating the expression of specific markers. The iPSC-derived hair bulb-keratinocytes expressed markers with a similar gene/protein profile compared to their in vivo equivalent (K14-15-33a-86, p63, MSX2, DLX2).

We also confirmed the melanocyte functionality by observing the transfer of melanin into keratinocytes (melanin production, expressions of PMEL17, c-KIT, SOX10, TYR, TRP1-2, melanin transfer into HaCaT). iPSC-derived DP also showed a specific profile (Versican, CD44 - 73, Vimentin, Corin, IGF1, NOG) and demonstrated their hair functionality.

Conclusion

We observed this model has a structure close to the in vivo hair bulb (core of DP surrounded by multi-layered hair bulb-keratinocytes and functional melanocytes) stable during at least 2 weeks.

With this new 3D model based on iPSCs, we reached to obtain an in vitro autologous hair bulb, with in vivo-like hair bulb structure and restored multiple crosstalks.

Why is this important to the industry?

A 3D-model restoring these cellular interactions is of high demand to study the hair follicle and validate new drugs. Moreover, the autologous aspect and the iPSC origin provide a highly reproducible and adjustable model suitable for high throughput screening, specific ethnical investigation or hair follicle development exploration.

Philip Ludwig is the Technical Account Manager for Personal Care actives in North America. Mr. Ludwig works with BASF R&D and customers to provide new skin care actives. From exciting botanicals to novel microbial ferments to synthetic chemistries, Mr. Ludwig utilizes the strength of BASF’s science to provide efficacious solutions for customers. Mr. Ludwig has written multiple patents and over a dozen research articles relating to new personal care ingredients. He has been a featured speaker at over a dozen industry events and seminars. In his previous role, his last three products have won five international awards at PCHi and In-Cosmetics for being either a best new ingredient or most innovative.