SCC78

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Speaker Abstracts

Session G: AI Beauty Revolution

SCC 78TH ANNUAL SCIENTIFIC MEETING & SHOWCASE
DECEMBER 11-13, 2024 | LOS ANGELES, CA

Precision Prebiotics - Skin Microbiome Modulation for Cosmetic Benefits

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ABSTRACT

Traditionally, cosmetic products have relied on chemistry-based approaches to provide skin benefits. However, there is a changing landscape of personal care products, particularly in relation to how they interact with our bodies. This research aims to demonstrate the effectiveness of a novel methodology in developing prebiotics for modulating the skin microbiome. Prebiotics designed to target skin microbiomes associated with dandruff and axillary malodor, and thereby resolve those conditions, were used to demonstrate the validity of the methodology. For instance, application of a prebiotic-enriched deodorant significantly mitigated underarm odor, corroborated by microbial population shifts. Similarly, a prebiotic-formulated shampoo demonstrated a notable reduction in scalp maladies, with a clinical trial confirming an 86% improvement in flakiness and 100% reduction in redness among participants. These findings not only affirm the viability of targeting the skin microbiome for cosmetic benefits but also mark a promising departure towards sustainable, biologically harmonious personal care innovations.

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Screening Antioxidant Ingredients Using Machine Learning and Physics-based Modeling

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ABSTRACT

Antioxidants are an important ingredient for cosmetic products to alleviate oxidative stress. While high-throughput screening for new antioxidant candidates still remains challenging experimentally. And the data-driven machine learning models would require the input of a reliable dataset. Here we present an efficient computational approach that combines the physics-based and machine learning tools to address this issue, and this approach only uses molecular structures as inputs.

We used molecular quantum mechanical (QM) calculation and machine learning to predict the antioxidant activity through hydrogen atom transfer (HAT) mechanism. We first constructed a library of flavonoid structures and then calculated the hydrogen dissociation energies of the hydroxyl group in solvents using QM. The machine learning model was trained and validated using the hydrogen dissociation energies from QM calculations. We can easily screen thousands of molecules, and this physics-based and machine learning combined approach can be used for other properties.

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Transferring Knowledge from Synthetic to Natural Compounds: A Deep Learning Approach

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ABSTRACT

In recent years, deep learning (DL) models have demonstrated significant potential in predicting chemical-target interactions (CTIs), thereby accelerating the discovery of new ingredients. This study delves into the application of transfer learning to utilize DL models trained on synthetic compounds for predicting interactions involving natural products. Using the advanced FusionDTA model, we analyzed a dataset consisting of 5,214 natural compounds, 257,377 synthetic compounds, and 3,409 protein targets from the ChEMBL dataset. Model performance was assessed using metrics such as mean square error (MSE), root mean square error (RMSE), and Spearman correlation coefficient on a holdout set of unseen natural products. The results revealed that models trained solely on synthetic compounds exhibited poor generalization to natural compounds (MSE 1.663, RMSE 1.283, Spearman 0.31). Notably, employing transfer learning - pretraining on synthetic compounds and fine-tuning on natural compounds - yielded significantly improved performance (MSE 1.015, RMSE 0.991, Spearman 0.53). These findings underscore the efficacy of transfer learning in enhancing DL model accuracy for natural product research and expediting the ingredient discovery process.

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A Platform Integrating Biological Assays, Proteomic Analyses, Network Pharmacology, Machine Learning, and Target Binding Techniques for the Discovery of Skin Protective Natural Products

Dr. Hang Ma

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ABSTRACT

Natural products hold promise for cosmeceutical development, but systematic AI-integrated approaches for their evaluation are lacking. We developed a platform incorporating biological assays (antioxidant, anti-inflammatory), proteomics characterization, machine learning-based analyses, and surface plasmon resonance (SPR)-based binding affinity to evaluate natural products for cosmeceutical applications. The platform provides insights into 1) efficacy assessment of skin protective effects, 2) understanding mechanisms at the proteomic level, 3) rationale for synergistic combinations, 4) large-scale data interpretation via machine learning, and 5) validation of biomarkers for skin protection. In a case study, we evaluated the effects of reactive carbonyl species (RCS) on human keratinocytes and characterized proteomic changes. Screening a natural product library using AI-assisted methods identified several promising candidates, including polyphenols such as cannflavins and gallotannins. Our findings demonstrate that this platform can enhance research and development efforts for effective, science-backed cosmeceuticals.