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Original Research Article

PREDICTION OF FRAGRANT COMPOUNDS USED IN SKIN CARE PRODUCTS CAUSING SKIN SENSITIVITY USING IN SILICO METHODS

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Abstract:

Personal care products are directly applied to the surface of the human body frequently and relatively in large quantities which may affect the skin unpleasantly. Fragrant components are widely used in skincare products for their sensory appeal, but they are also a common cause of skin irritation and allergic reactions. This study uses Bioinformatic tools such as docking and prediction methods such as QSAR (Quantitative Structure Activity Relationship) to examine the molecular and chemical activity of fragrant compounds like linalool, eugenol, citronellol, etc with Epidermal Growth Factor (EGF) & Cytokines present in the skin that can contribute to skin sensitivity. This modelling methodology has been specifically created to maintain quality in cruelty free products.

Keywords: *Fragrant components, Docking, QSAR (Quantitative Structure Activity Relationship), Skin sensitivity.*

Introduction:

Personal care products, particularly skincare formulations, are widely used in daily routines, often applied in substantial amounts directly onto the skin. While these products aim to enhance skin health and aesthetics, certain ingredients can lead to adverse effects, including irritation and allergic reactions. Among these, fragrant compounds are a primary concern, as they are frequently associated with contact dermatitis and skin sensitivity. Despite their desirable sensory attributes, many fragrances have been identified as potential allergens, prompting the need for systematic evaluation of their safety in skincare formulations.

Traditional methods for assessing the skin sensitivity potential of chemical compounds rely on animal testing and in vitro assays, both of which have ethical, economic, and practical limitations. In recent years, in silico approaches, such as molecular docking and Quantitative Structure-Activity Relationship (QSAR) modelling, have emerged as powerful tools for predicting biological interactions and toxicity risks without the need for animal testing. These computational techniques allow researchers to analyze the molecular interactions between fragrance compounds and key skin proteins, such as Epidermal Growth Factor (EGF) and cytokines, which play critical roles in skin barrier function and inflammatory responses.

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This study aims to employ bioinformatics and predictive modelling techniques to investigate the potential of common fragrance compounds—such as linalool, eugenol, and citronellol—to induce skin sensitivity. By evaluating their molecular interactions with skin-related proteins, this research seeks to contribute to the development of safer, cruelty-free skincare formulations. The findings of this study will provide valuable insights for the cosmetic industry and regulatory bodies, promoting the formulation of skin-friendly personal care products while minimizing adverse reactions.

Methodolgy:

This study employs computational bioinformatics (CB) docking software to analyze the interaction between fragrant compounds and key skin proteins involved in sensitivity responses. The methodology consists of the following steps:

1. Selection of Fragrant Compounds:

A set of widely used fragrant compounds in skincare products, including linalool, eugenol, and citronellol, were chosen based on their prevalence in formulations and reported skin sensitization potential. The chemical structures of these compounds were retrieved from publicly available databases such as PubChem and ChEMBL.

2. Target Protein Selection and Preparation:

Key skin proteins associated with skin sensitivity and inflammatory responses were selected as docking targets. These include:

- Epidermal Growth Factor (EGF) – involved in skin barrier function and regeneration
- Keratin – a structural fibrous protein found in the skin, hair, and nails, playing a crucial role in providing strength and protection.

The three-dimensional (3D) structures of these proteins were obtained from the Protein Data Bank (PDB). Missing residues, water molecules, and non-essential ligands were removed to prepare the proteins for docking.

3. Molecular Docking Analysis Using CB Docking Software:

- Software Selection: The CB Docking software was used due to its efficiency in identifying ligand-binding sites and predicting binding affinities.
- Binding Site Identification: CB Docking automatically detected potential binding pockets within the EGF and cytokine structures, determining the most favourable sites for ligand interactions.
- Docking Simulation: Each fragrance compound was docked against the selected skin proteins to analyze molecular interactions.
- Scoring and Ranking: The binding affinities were quantified using scoring functions provided by the docking software, ranking the compounds based on their potential to interact with and affect skin proteins.

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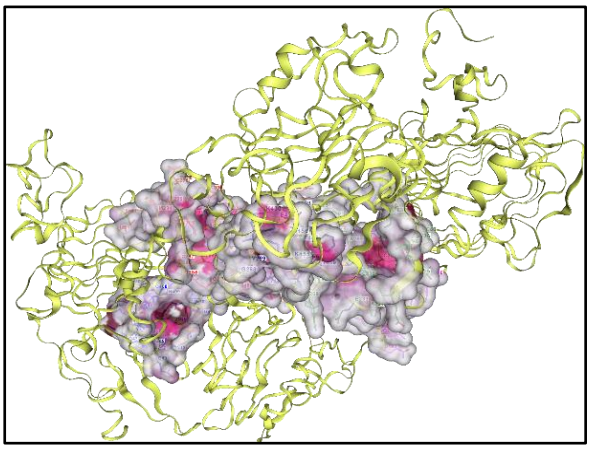
Results and Discussion:



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C2	1593	48, 42, 57	21, 17, 19
C3	1458	73, 78, 42	11, 16, 17
C4	1420	94, 67, 42	16, 17, 19
C5	1269	100, 49, 40	24, 13, 11

Fig 1 & 1.1 Eugenol and epidermal growth factor

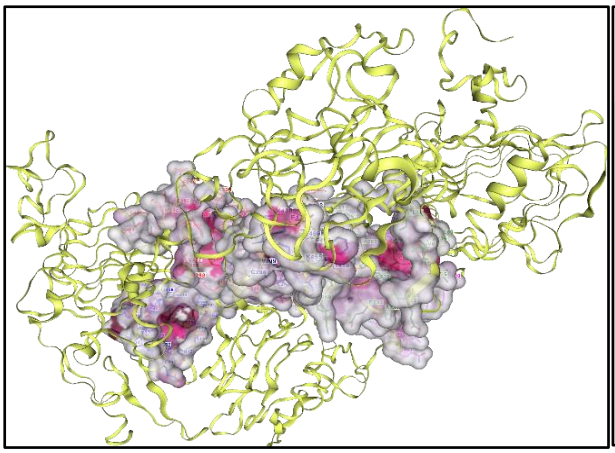

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Fig.2 & 2.1 Linalool and Epidermal Growth Factor

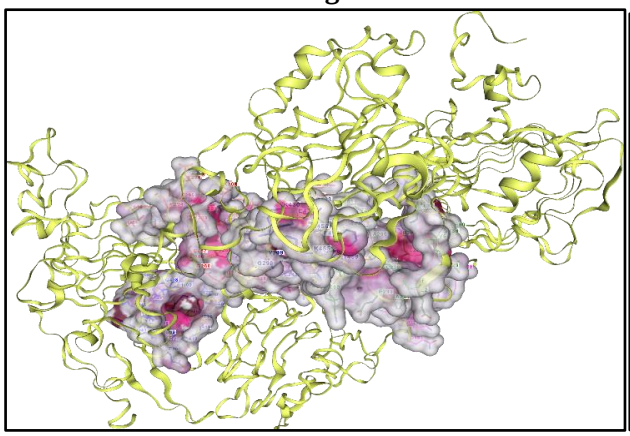

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Fig.3 & 3.1. Citronellol and Epidermal Growth Factor

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This in silico study of fragrant compounds used in skincare products provides valuable insights into their potential to induce skin sensitivity through molecular interactions with key skin proteins such as Epidermal Growth Factor (EGF) and keratin. The docking results demonstrate that compounds like eugenol, linalool, and citronellol exhibit binding affinities to similar binding cavities on these proteins, suggesting that they may exert comparable effects on skin barrier function and inflammatory responses. These findings highlight the importance of computational methods in predicting allergenic potential and can contribute to the development of safer, cruelty-free cosmetic formulations.

Conclusion:

Future studies could utilize advanced molecular docking software such as AutoDock4 to validate the observed binding interactions with more precision. The gathered CB Dock results will serve as a preliminary analysis, and performing docking using AutoDock4 will confirm these findings, providing the best conformation and binding affinity of the ligand to the protein. Furthermore, a reference skin-sensitive protein, such as those associated with dermatitis, can be used to compare the docking results. If the ligand binds similarly to both EGF and the reference protein, this would provide further evidence of the compound's potential to cause skin sensitivity. On these findings, we can determine which compounds are causative agents for such skin sensitivity.

Additionally, integrating QSAR modelling and molecular dynamics simulations would further enhance the predictive accuracy of these methods, offering a comprehensive framework for assessing skin sensitivity risks. Visual representation of the protein could be achieved using ChimeraX software, while Avogadro software can be employed to visualize the ligand structures.

The table below contains compounds, that are some of the most commonly found fragrant components in today's skincare products and could be predicted in future studies as potential causative agents of skin sensitivity based on their molecular interactions.

Skin protein	**Fragrant Compounds**			
Epidermal growth factor	Linalool	Farnesol	Benzyl Benzoate	Amyl Cinnamal
Keratin	Limonene	Cinnamal	Isoeugenol	Methyl eugenol
Albumin	Eugenol	Coumarin	Benzyl alcohol	Atranol
Elastin	Citral	Benzyl Salicylate	Tree Moss Extract	Chloroatranol
	Geraniol	Oakmoss extract	Anisyl Alcohol	Tolu Balsam

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