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Development and application of Time-of-flight secondary ion mass spectrometry (ToF-SIMS) for skin permeation studies

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ABSTRACT

The skin accounts for approximately 16% of human body weight, with a surface area of approximately 2 m^2 in adults. It provides a physical barrier to the environment, maintains homeostasis by limiting the loss of water, electrolytes, and heat, and protects against microorganisms, toxic agents, and ultraviolet radiation. The outermost layer of the skin, the stratum corneum, serves as a first line of defense against volatile organic compounds, heavy metals, and other hazardous substances. Hence, understanding the skin uptake of environmental chemicals and particles is crucial for assessing the risks associated with pollution and for developing strategies to mitigate these risks. Moreover, elucidating the mechanisms of skin penetration by different pollutants and chemicals can contribute to the development of protective skincare products and other preventive measures.

Lipids in the skin are one of the main protective components and are crucial components of the stratum corneum where they play a significant role in the skin's barrier function. They fill the spaces between corneocytes and create a hydrophobic barrier that prevents the easy passage of substances, including chemicals and particles from the environment. The study of skin uptake and lipids changes in skin is of great interest in understanding underlying mechanisms of exposure to chemicals and environmental agents.

Mass spectrometry imaging (MSI) is a powerful label-free technique to study the skin composition as well as the link between lipid changes and the permeation of different chemicals. One of the most common MSI techniques is time of flight secondary ion mass spectrometry (ToF-SIMS), which provides ultra-high spatial resolution due the use of the focused ion beam to eject and ionize molecules in the sample surface.

The papers in this thesis describe the application of ToF-SIMS to investigate human skin tissue samples to reveal the permeation of metals and chemicals through the skin layers, as well as to study lipid changes caused by the uptake of these substances. Different sample preparation methods and different human skin samples and models have been examined to provide the best possible results. The method is now ready to be applied in testing pharmaceuticals, cosmetics, occupational skin hazards, and skin allergens independently or as a complementary approach to answer more complicated scientific questions.

Keywords: *Mass spectrometry imaging, ToF-SIMS, lipids, skin, human skin models, toxicology, allergen, permeation studies, contact allergy, sunscreen, skin lipids, lipid change.*