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3D MOLECULAR MAPS OF THE HUMAN SKIN SURFACE

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Abstract: Here we explored the topographical body distribution of skin molecules and bacteria by spatial mapping of mass spectrometry (MS) and microbial DNA sequence data. The 3D topographical maps were constructed from samples collected at ~400 distinct body sites, from each of two volunteers, using a specific workflow (Figure 1). To better interpret the MS data, molecular networking was applied to MS/MS spectra. Compounds are grouped based on their MS/MS similarity serving as a proxy for structural similarity and visualized in Cytoscape. The generated maps revealed that the spatially localized chemical and microbial diversity on the skin are not only defined by microbes or skin cells and their interactions, but also by daily routines, including our hygiene habits, and use of beauty products. Our results highlighted that the chemical make-up of the outermost layer of the skin is highly individualized as the chemistry is defined by a person's lifestyle. A spatial bacterial and metabolite skin map thus provides insight into the molecular interrelations of humans and our microbiota, and reflects current and past individual behavior. These maps lay a foundation for further studies of the spatially-defined interactions of human skin, microbiota and external environmental factors, with a potential for monitoring variations of skin chemicals and microbes and their influence on human health and susceptibility to disease [1].
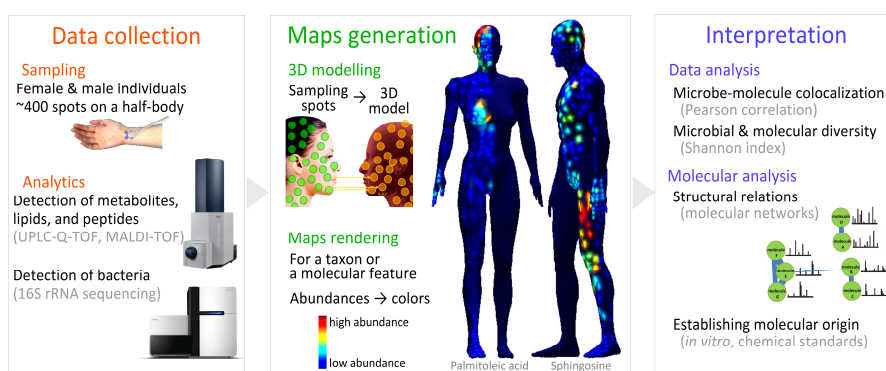
Figure 1. General Workflow for Construction of High-Spatial Resolution 3D Models. The data analysis involved integrative analysis of heterogeneous big data followed up by structural biochemical analysis of molecular features of interest.

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