

HOW TO

An AI research agent for scientists with high standards

What is scienceOS

Dermatology collection

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SC

Deep research

Draft a mini review about the relevance of lipidomics analysis in dermatology

The Relevance of Lipidomics Analysis in Dermatological Research

Introduction

Lipidomics, the comprehensive study of lipid profiles, has emerged as a pivotal tool in dermatological research. Lipids, including ceramides, cholesterol, and fatty acids, play essential roles in maintaining skin barrier function and cellular health. Dysregulation of these lipids is linked to various skin disorders, such as atopic dermatitis and psoriasis. Advanced analytical techniques like mass spectrometry, lipidomics enables precise quantification and identification of lipids across different anatomical sites, depths, and individuals. This mini review explores the methodologies and applications of lipidomics, highlighting its transformative potential in understanding and treating skin diseases.

Analytical Methods and Technologies in Skin Lipidomics

Shotgun mass spectrometry is a cornerstone of high-throughput skin lipidomics, enabling the simultaneous analysis of numerous **sebaceous and stratum corneum lipids**. This technique involves direct infusion of lipid extracts into a mass spectrometer without prior chromatographic separation, allowing rapid acquisition of complex lipid profiles. Advanced instruments, such as the QExactive mass spectrometer, are essential for resolving overlapping signals and identifying specific lipid species, including ceramides, cholesterol, and triacylglycerols. [In Sadowski, 2017](#)

The advantages of shotgun lipidomics include broad lipid coverage, absolute quantification, and unprecedented throughput, which is critical for large-scale studies and clinical applications. Recent studies have used this approach to analyze over 268 skin samples, revealing depth-dependent lipid gradients and identifying novel biomarkers for skin conditions. [In Sadowski, 2017](#) p2 ; [In Sadowski, 2017](#) p8 . Additionally, tape-stripping combined with

+

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ABOUT scienceOS



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- TU Dresden & WHU

The team developing scienceOS

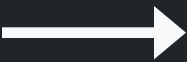
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Simplicity

Agility

Vision



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global challenges.

The guiding principles of scienceOS

USER PROBLEMS

USE CASE

- 1** Scientific answers
slide 5
- 2** Explore citations
slide 14
- 3** Compare papers
slide 20
- 4** Drafting texts
slide 26

PROBLEM

- „I am starting a new R&D project and need to quickly gain an overview about the field.“*
- „There are too many publications. I need to find the best and most relevant papers.“*
- „I need to compare the results from several papers and assess their validity.“*
- „A grant application deadline is approaching. I still need to write the introduction!“*

scienceOS

- Ask research questions and **follow-ups** to dive into detail.
- Create citation networks and **analyze** how papers are cited.
- Upload** research papers to quickly chat with them.
- Generate** answers based on your literature collection.

How scienceOS supports your research

HOW TO

Access to the knowledge of mankind

1 Example

100 sources

Citation network

What are the implications of these findings for dermatological research?

Can you elaborate on the methodologies used in these studies?

Are there any recent advancements in mass spectrometry techniques for lipid analysis?

SC

Create diagram

Tape Stripping

Collects Stratum Corneum Samples

Mass Spectrometry

Quantifies Lipid Classes

Skin Lipid Analysis

Used in Disease Monitoring

Atopic Dermatitis

Used in Aging Studies

Age-Related Lipid Changes

Identifies Biomarkers

Diabetes

What are the benefits of using Mermaid Markdown for visual representations?

Can you explain the significance of highlighting nodes in diagrams?

How does tape stripping work?

📄 ⭐ ↺ ✎

Ask anything

+

✎

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Ask a question.

1

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SC

Which non-invasive methods allow for quantification of different lipid classes in the skin?



Several non-invasive methods are available for quantifying different lipid classes in the skin:

1. **Tape Stripping Combined with Mass Spectrometry:** Tape stripping collects stratum corneum samples, which can be analyzed using high-throughput shotgun mass spectrometry to quantify up to 16 lipid classes, including sebaceous and stratum corneum lipids [Sadowski, 2017](#).
2. **Cyanoacrylate Stripping and Thin-Layer Chromatography:** Cyanoacrylate stripping collects skin surface lipids, which are then separated and quantified using high-performance thin-layer chromatography and densitometric methods [Röpke, 1996](#).
3. **Raman Microspectroscopy:** This technique provides in vivo analysis of lipid content, conformation, and organization in the stratum corneum, offering insights into lipid-protein ratios and skin barrier function [Verzeaux, 2018](#).
4. **Short-Wave Infrared (SWIR) Spectroscopy:** SWIR spectroscopy, combined with tape stripping, enables depth profiling of lipids and water in the stratum corneum, with high sensitivity and specificity compared to other methods [Ezerskaia, 2018](#).
5. **Skin Surface Lipid RNA Analysis:** Lipids collected from skin surface can also be analyzed for RNA content, providing molecular insights into lipid synthesis and skin conditions [Shima, 2022](#).

These methods vary in their focus, from lipid quantification to molecular profiling, and are suitable for different research and clinical applications.

100 sources

Citation network

What are the advantages of each method mentioned?

Are there any limitations to these techniques?

Can these methods be used for diagnosing skin conditions?

Expand this answer



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Click on **citation markers** for source details.

2

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Sadowski, 2017

Source Network Citations PDF

Large-scale human skin lipidomics by quantitative, high-throughput shotgun mass spectrometry
2017, Tomasz Sadowski, C. Klose, M. Gerl, Anna Wójcik-Maciejewicz, R. Herzog, K. Simons, A. Reich, M. A. Surma
Scientific Reports
doi 10.1038/srep43761 28266621 PDF

TLDR A quantitative high-throughput shotgun mass spectrometry-based platform for lipid analysis of tape-stripped SC skin samples is developed and validated and sebaceous lipids are found to constitute an abundant component of the SC lipidome as they diffuse into the topmost SC layers forming a gradient.

ABSTRACT
The lipid composition of human skin is essential for its function; however the simultaneous quantification of a wide range of stratum corneum (SC) and sebaceous lipids is not trivial. We developed and validated a quantitative high-throughput shotgun mass spectrometry-based platform for lipid analysis of tape-stripped SC skin samples. It features coverage of 16 lipid classes; total quantification to the level of individual lipid molecules; high reproducibility and high-throughput capabilities. With this method we conducted a large lipidomic survey of 268 human SC samples, where we investigated the relationship between sampling depth and lipid composition, lipidome variability in samples from 14 different sampling sites on the human body and finally, we assessed the impact of age and sex on lipidome variability in 104 healthy subjects. We found sebaceous lipids to constitute an abundant component of the SC lipidome as they diffuse into the topmost SC layers forming a gradient. Lipidomic variability with respect to sampling depth, site and subject is considerable, and mainly accredited to sebaceous lipids, while stratum corneum lipids vary less. This stresses the importance of sampling design and the role of sebaceous lipids in skin studies.

64 citations | SJR 1.5 Q1

Organize Add to library

non-invasive approach for lipid assessment [Furuichi, 2010](#).

6. Non-Invasive Transcriptomics:

- RNA analysis from skin surface lipids (SSL-R) can provide insights into lipid synthesis-related gene expression, offering an indirect method to study lipid metabolism in the skin [Inoue, 2021](#).

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HOW TO

Create a **table** to compile information.

3



SC

Create a table with further papers that made use of mass spectrometry-based quantification of skin lipids.



Here is a table summarizing studies that utilized mass spectrometry for quantification of skin lipids:

Study	Methodology	Key Findings	Link
Sadowski, 2017	High-throughput shotgun mass spectrometry	Quantified 16 lipid classes in stratum corneum samples; analyzed lipid variability by sampling depth, site, age, and sex	Sadowski, 2017
Kendall, 2018	Various mass spectrometry approaches	Explored targeted and untargeted lipidomics, including imaging techniques for anatomical lipid distribution	Kendall, 2018
Li, 2016	Lipidomics profiling	Investigated lipid alterations in inflammatory skin diseases like atopic dermatitis and psoriasis	Li, 2016
Sjövall, 2018	Time-of-flight secondary ion mass spectrometry (ToF-SIMS)	Imaged spatial distribution of lipids and topically applied compounds in skin layers	Sjövall, 2018
Michael-Jubeli, 2011	High-temperature gas chromatography-mass spectrometry	Profiled skin surface lipids, identifying over 200 compounds in a single run	Michael-Jubeli, 2011
Li, 2022	UPLC-QTOF-MS	Identified sphingolipids as potential biomarkers for type 2 diabetes through skin lipid analysis	Li, 2022
Chen, 2023	UPLC-QTOF-MS	Explored lipid differences in hand skin surface among females of different ages	Chen, 2023
Yang, 2021	UPLC-QTOF-MS	Analyzed lipid alterations in pregnant women, revealing weakened skin barrier function	Yang, 2021
Mitchell, 2015	MALDI-MS imaging	Studied lipid distribution in living skin equivalents during development and maturation	Mitchell, 2015

These studies highlight the versatility of mass spectrometry techniques in analyzing skin lipids for various applications, including disease monitoring, aging, and physiological changes.

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a **diagram**.

4

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100 sources

Citation network

What are the implications of these findings for dermatological research?

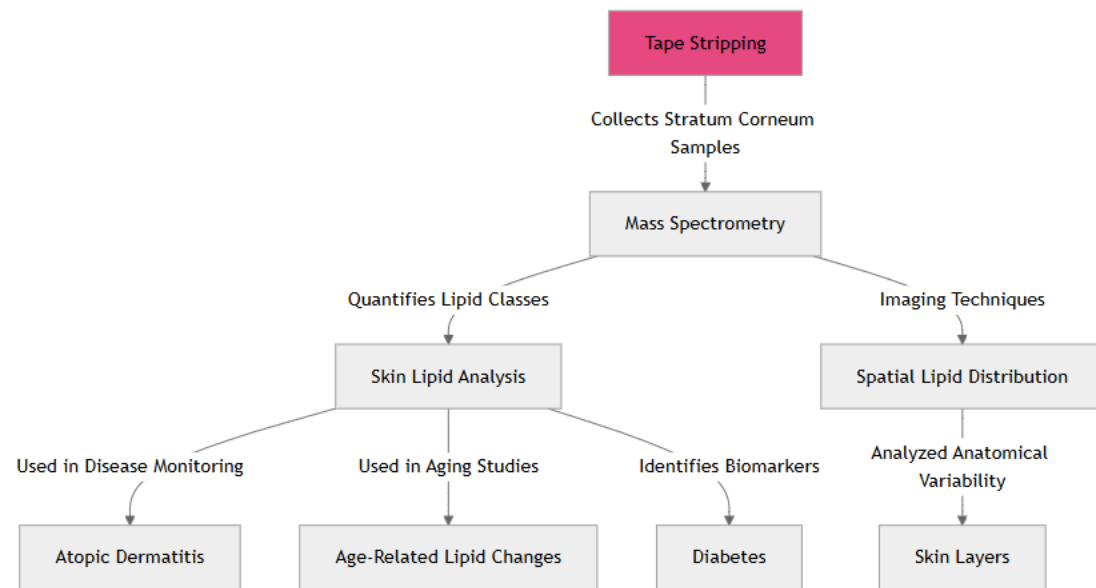
Can you elaborate on the methodologies used in these studies?

Are there any recent advancements in mass spectrometry techniques for lipid analysis?

Expand this answer

SC

Create diagram



What are the benefits of using Mermaid Markdown for visual representations?

Can you explain the significance of highlighting nodes in diagrams?

How does tape stripping contribute to skin lipid analysis?



Ask anything



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HOW TO


Selecting the
‘Deep research’
mode will provide
a detailed report.

5



Generate deep research reports based on hundreds of sources

SC

 Deep research

Provide a comprehensive overview about mass spectrometry-based lipid analysis in dermatology research.



Mass Spectrometry-Based Lipid Analysis in Dermatology Research

Introduction


Mass spectrometry-based lipid analysis has become a cornerstone in dermatology research, offering unparalleled insights into the complex lipid compositions of skin. Lipids play critical roles in maintaining the epidermal barrier, regulating hydration, and modulating inflammation, making their study essential for understanding skin health and disease. Advances in lipidomics, driven by techniques like electrospray ionization (ESI) and matrix-assisted laser desorption ionization (MALDI), have enabled precise quantification and spatial mapping of lipids. This report explores the transformative impact of these methodologies on dermatological research, highlighting their potential to uncover biomarkers, elucidate disease mechanisms, and inform therapeutic strategies.

Mass Spectrometry Techniques for Lipid Analysis

Electrospray ionization (ESI) has revolutionized lipidomics by enabling highly sensitive and precise quantification of lipid species. ESI operates by ionizing lipids directly from biological extracts, allowing for the analysis of complex lipid mixtures without extensive sample preparation. Advances in ESI have improved ionization efficiency and reduced matrix effects, particularly through the use of internal standards and chemical modifiers, which enhance the accuracy of lipid quantification ([Yang, 2011](#) ; [Wang, 2017](#)). Direct infusion methods, combined with tandem mass spectrometry, further streamline lipid profiling, enabling rapid and comprehensive analysis of lipid compositions ([Brügger, 2014](#)).

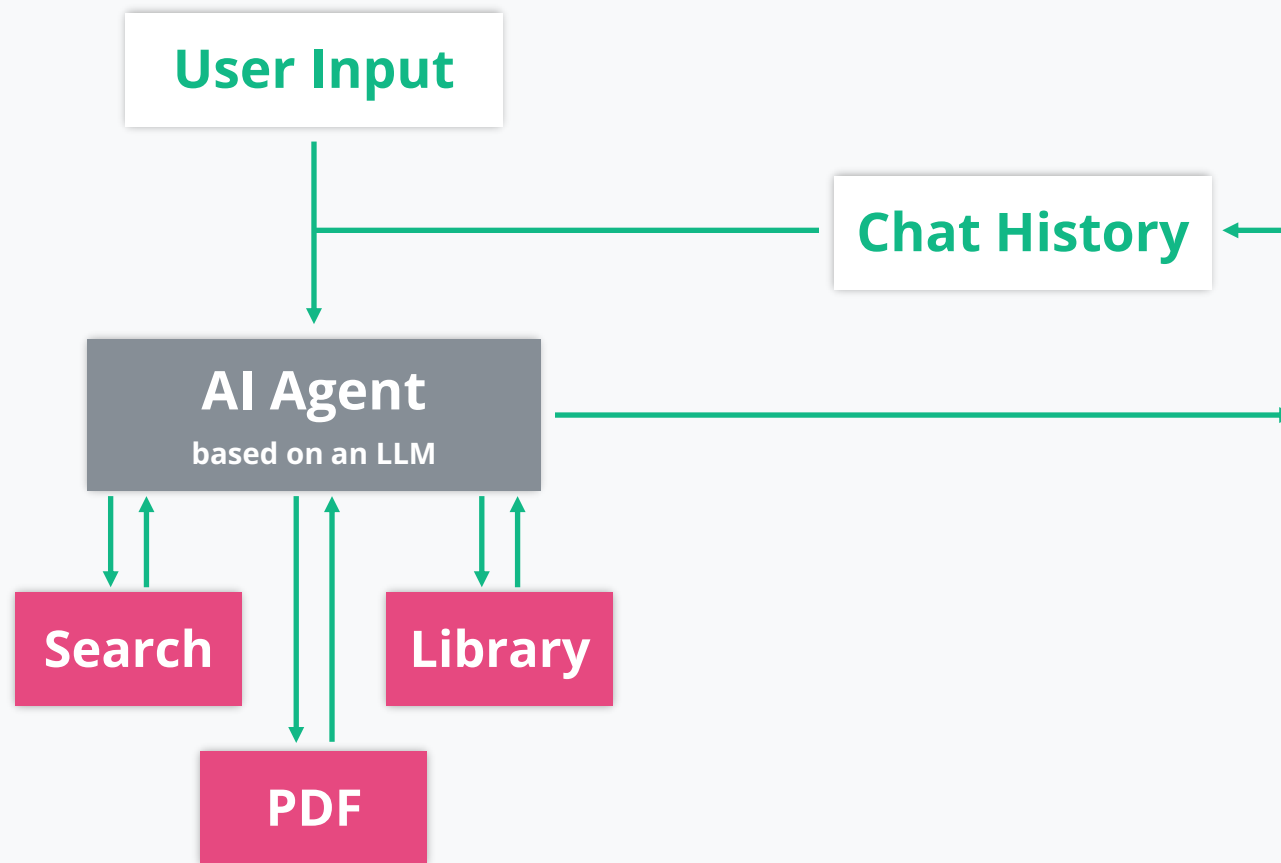
Matrix-assisted laser desorption ionization (MALDI) complements ESI by providing spatial resolution of lipid distributions in tissues. MALDI imaging mass spectrometry (IMS) has been instrumental in dermatology research, revealing lipid



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HOW DOES IT WORK



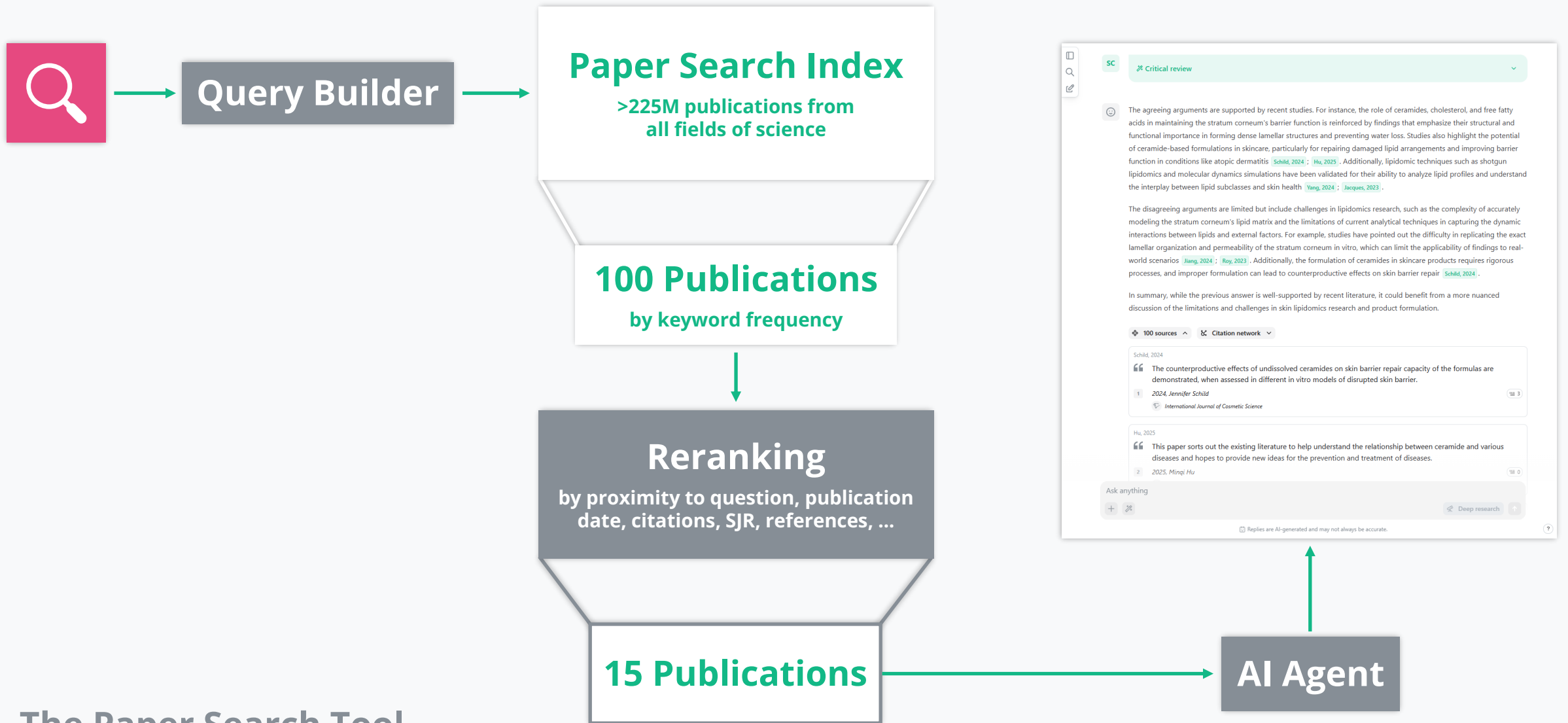
The screenshot displays the scienceOS AI research agent interface. At the top, a green header bar indicates the current topic: **SC Critical review**. The main content area shows a detailed analysis of ceramides, discussing their role in maintaining the stratum corneum's barrier function and the challenges in lipidomics research. The text is supported by recent studies, with citations like [Schild, 2024](#), [Hu, 2025](#), [Yang, 2024](#), and [Jacques, 2023](#).

Below the text, a section titled **100 sources** and **Citation network** provides a list of references. The first reference is by [Schild, 2024](#), titled "The counterproductive effects of undissolved ceramides on skin barrier repair capacity of the formulas are demonstrated, when assessed in different in vitro models of disrupted skin barrier." The second reference is by [Hu, 2025](#), titled "This paper sorts out the existing literature to help understand the relationship between ceramide and various diseases and hopes to provide new ideas for the prevention and treatment of diseases."

At the bottom, there is a search bar with the placeholder text "Ask anything" and a "Deep research" button. A disclaimer at the very bottom states: "Replies are AI-generated and may not always be accurate."

The scienceOS AI research agent

HOW DOES IT WORK



The Paper Search Tool

HOW TO

Explore networks of related papers

2 Example

4. **Short-wave infrared (SWIR) Spectroscopy:** SWIR spectroscopy, combined with... of lipids and water in the stratum corneum, with high sensitivity and specificity. [Ezerskaia, 2018](#).

5. **Skin Surface Lipid RNA Analysis:** Lipids collected from skin surface can also be... molecular insights into lipid synthesis and skin conditions. [Shima, 2022](#).

These methods vary in their focus, from lipid quantification to molecular profiling, and clinical applications.

100 sources Citation network

What are the advantages of each method mentioned? Are there any limitations to the methods mentioned?

Can these methods be used for diagnosing skin conditions? Expand this answer

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Then, click on the
button **Citation
network**.

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❖ 100 sources

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What are the advantages of each method mentioned?

Are there any limitations to these techniques?

Can these methods be used for diagnosing skin conditions?

🔗 Expand this answer



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or **foundational**
papers in the
citation network.

2

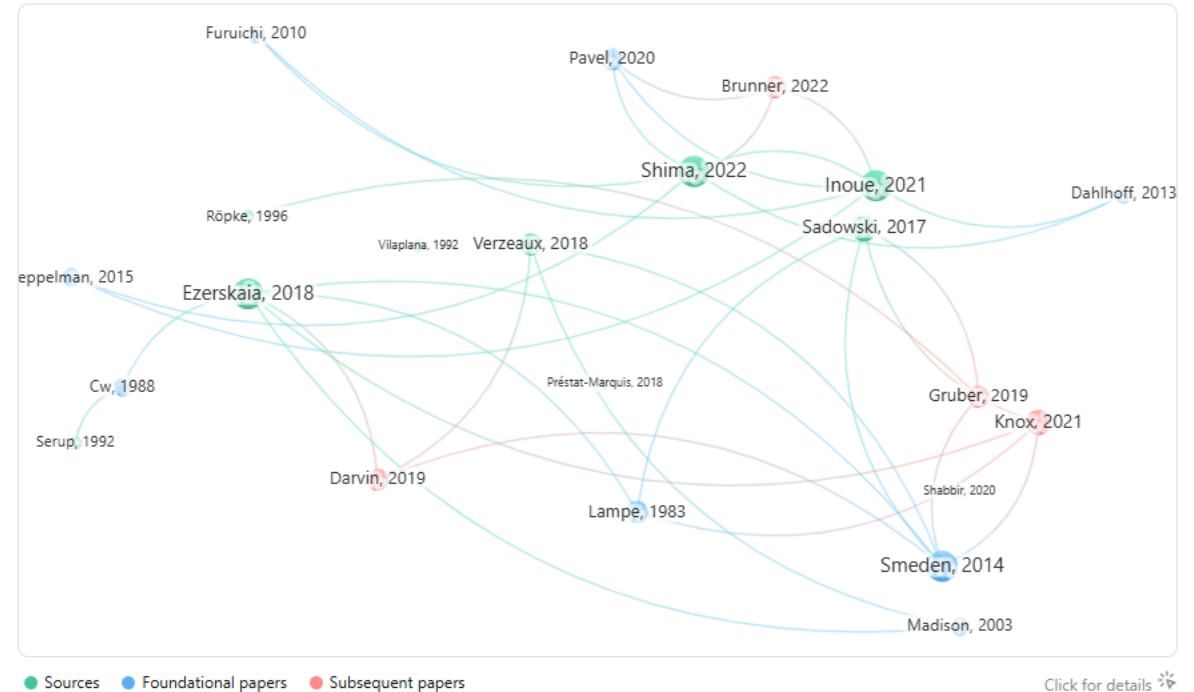
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100 sources Citation network



What are the advantages of each method mentioned?

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Can these methods be used for diagnosing skin conditions?

Expand this answer



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3



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...

6 selected

Large-scale human skin lipidomics by quantitative, high-throughput shotgun mass spectrometry

2017, Tomasz Sadowski, C. Klose, M. Gerl, Anna Wójcik-Maciejewicz, R. Herzog, K. Simons, A. Reich, M. A. Surma

Scientific Reports

Remove from collection(s)

Remove from library

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Human epidermal stem cell differentiation is modulated by specific lipid subspecies

2020, Matteo Vietri Rudan, Ajay Mishra, C. Klose, U. Eggert, F. Watt

Proceedings of the National Academy of Sciences of the United States of America

Dermatology Lipidomics

25 | 5.0

Changes in levels of omega-O-acylceramides and related processing enzymes of sun-exposed and sun-protected facial stratum corneum in differently pigmented ethnic groups

2022, A. Rawlings, R. Schoop, C. Klose, J. Monneuse, B. Summers, R. Voegeli

International Journal of Cosmetic Science

Lipidomics Dermatology

9

Distribution of Domains Formed by Lateral Packing of Intercellular Lipid in the Stratum Corneum.

2023, Hiroki Ohnari, E. Naru, O. Sakata, Y. Obata

Chemical & pharmaceutical bulletin

Dermatology Lipidomics

8

Alteration of barrier properties, stratum corneum ceramides and microbiome composition in response to lotion application on cosmetic dry skin

2022, Barry Murphy, S. Grimshaw, M. Hoptroff, Sarah Paterson, David Arnold, Andrew Cawley, Suzanne E. Adams, F. Falciani, T. D...

Scientific Reports

Lipidomics Dermatology

28 | 1.0

Stratum Corneum Lipids in Non-Lesional Atopic and Healthy Skin following Moisturizer Application: A Randomized Clinical Experiment

2024, M. G. Ahlström, R. Bjerre, M. G. Ahlström, L. Skov, J. D. Johansen

Life

Lipidomics Dermatology

1 | 0.8

Verwaltung und Verwaltungsreformen in Europa

2013, Sabine Kuhlmann, H. Wollmann

Verwaltung und Verwaltungsreformen in Europa.pdf

OV-1

48

Verantwortungsvolle Steuerung und Leitung öffentlicher Unternehmen

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4

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rafts in nonionic detergents like Triton X-100, followed by density gradient centrifugation. While this method identifies cholesterol- and sphingolipid-rich domains, it often disrupts native membrane structures, leading to artifacts that may not reflect the true organization of the membrane.

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technique
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Y

nce for lipid
raft, 2013 .
g to results
nanoscale

Alternative models challenge the classical raft concept by proposing mechanisms such as lipid-protein interactions, annular lipid shells, and mesoscale domains. These models emphasize the role of active cellular processes and cytoskeletal interactions in membrane organization, rather than passive lipid-driven segregation [Mayor, 2004]. For instance, studies show that sphingolipid domains depend on cytoskeletal support rather than cholesterol interactions, contradicting key aspects of the raft hypothesis [Kraft, 2017]. Additionally, dynamic nanoclusters regulated by actin cytoskeleton have been proposed as a more accurate representation of membrane compartmentalization [Plowman, 2005].

These findings suggest that plasma membrane organization is more complex and dynamic than the lipid raft hypothesis alone can explain, necessitating a broader framework to integrate emerging evidence.

↓

Advances in Analytical Techniques and Recent Discoveries

Ask anything

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?

Brown, 2006

Source Network Citations PDF

Lipid rafts, detergent-resistant membranes, and raft targeting signals.

● Sources ● Foundational papers ● Subsequent papers

Click for details ↗

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Citations tab to
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5

Brown, 2006

Source Network **Citations** PDF

Lipid rafts, detergent-resistant membranes, and raft targeting signals.

✓ **Supporting**

Several citations support the findings of Brown (2006), emphasizing the importance of lipid rafts in cellular signaling, protein localization, and membrane dynamics. These studies validate the role of palmitoylation and other post-translational modifications in targeting proteins to lipid rafts [Bhattacharyya, 2013](#) , [Hornemann, 2015](#) , [Sanders, 2014](#) , [Young, 2012](#) . Additionally, they confirm the utility of DRMs as a tool for studying lipid raft-associated proteins, despite their limitations [Domingues, 2010](#) , [Nikolaev, 2017](#) , [Rieke, 2011](#) , [Xu, 2012](#) , [Zadavec, 2010](#) . These citations highlight the paper's contribution to understanding the biochemical and functional properties of lipid rafts.

🕒 **Mentioning**

The cited paper by Deborah A. Brown (2006) is frequently mentioned in discussions about lipid rafts and detergent-resistant membranes (DRMs). It is referenced as a foundational work in understanding the biochemical properties and functional roles of lipid rafts, particularly their resistance to detergents and their association with cholesterol and sphingolipids [Agarwal, 2018](#) , [Bhaskar, 2009](#) , [Botto, 2010](#) , [Chan, 2010](#) , [Cresawn, 2007](#) , [Delint-Ramírez, 2015](#) , [Rajamanickam, 2016](#) , [Sanders, 2014](#) , [Storch, 2007](#) , [Yu, 2007](#) . The paper is often cited in research contexts involving signal transduction, protein trafficking, and membrane organization, highlighting its relevance across various biological processes.

🔍 **Contrasting**

Several citations contrast with Brown (2006), questioning the equivalence of DRMs to native lipid rafts and highlighting methodological artifacts associated with detergent-based isolation techniques. These studies argue that DRMs may not accurately represent the in vivo organization of lipid rafts and caution against overinterpreting results derived from DRM analysis [Asano, 2009](#) , [Bauwens, 2013](#) , [Lingwood, 2010](#) , [Scholz, 2021](#) , [Sprenger, 2010](#) , [Tanner, 2011](#) , [Urbanus, 2012](#) , [Rozentsvet, 2023](#) , [Langowski, 2012](#) , [Heberle, 2017](#) . These critiques highlight ongoing debates about the validity of DRM-based approaches and the dynamic nature of lipid rafts in

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SCIENTIFIC REPORTS

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Summary

Introduction

The study focuses on the skin's stratum corneum (SC), the outermost layer, which is composed of corneocytes embedded in a lipid matrix primarily consisting of ceramides and free fatty acids (FFA). Other lipid classes, such as triacylglycerols (TAG), diacylglycerols (DAG), and esters (CE), are also present. Skin lipid composition varies with age, gender, ethnicity, and environmental factors. Alterations in lipid profiles are linked to dermatological and systemic diseases.

Methods

Lipidomics Techniques

Early studies used thin-layer chromatography to identify ceramide subclasses. A more recent approach, liquid chromatography-mass spectrometry (LC-MS), enabled the identification of 12 ceramide subclasses. Shotgun mass spectrometry, a more recent approach, allows for the identification of ceramide head groups and acyl chains.

Sadowski.pdf

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SCIENTIFIC REPORTS

Large-scale human skin lipidomics by quantitative, high-throughput shotgun mass spectrometry

😊

Thank you for uploading the paper **Large-scale human skin lipidomics by quantitative, high-throughput shotgun mass spectrometry** by **Tomasz Sadowski et al.** (2017), published in Scientific Reports, 10.1038/srep43761 [Sadowski, 2017](#) . I will always answer by reading the uploaded paper, unless you specifically ask me otherwise.

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Thank you for uploading the paper **Large-scale human skin lipidomics by quantitative, high-throughput shotgun mass spectrometry** by **Tomasz Sadowski et al.** (2017), published in Scientific Reports, 10.1038/srep43761 [Sadowski, 2017](#) . I will always answer by reading the uploaded paper, unless you specifically ask me otherwise.

PDF Summary ^

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Summary

Introduction

The study focuses on the skin's stratum corneum (SC), the outermost layer, which is critical for its barrier function. The SC is composed of corneocytes embedded in a lipid matrix primarily consisting of ceramides (Cer), cholesterol (Chol), and free fatty acids (FFA). Other lipid classes, such as triacylglycerols (TAG), diacylglycerols (DAG), and cholesterol esters (CE), are also present. Skin lipid composition varies with age, gender, ethnicity, and environmental factors, and alterations in lipid profiles are linked to dermatological and systemic diseases [Sadowski, 2017](#) [p1](#) .

Methods

Lipidomics Techniques

Early studies used thin-layer chromatography to identify ceramide subclasses. Advances in liquid chromatography-mass spectrometry (LC-MS) enabled the identification of 12 ceramide subclasses based on combinations of sphingoid bases and acyl chains. Shotgun mass spectrometry, a more recent approach, allows high-throughput analysis but lacks

Sadowski.pdf

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Thank you for uploading the paper **Large-scale human skin lipidomics by quantitative, high-throughput shotgun mass spectrometry** by Tomasz Sadowski et al. (2017), published in Scientific Reports, 10.1038/srep43761 [in Sadowski, 2017](#). I will always answer by reading the uploaded paper, unless you specifically ask me otherwise.

PDF Summary

PDF to Slides

SC

Write a brief description of the study design.

The study by Sadowski et al. utilized a **quantitative, high-throughput shotgun mass spectrometry-based platform** to analyze human skin lipidomics. The design involved:

- Sampling Method:** Skin samples were collected using tape-stripping, a non-invasive method allowing control over sampling depth and reproducibility. Samples were taken from 104 subjects, including 65 females and 39 males, across 14 body sites and different depths of the stratum corneum (SC) [in Sadowski, 2017](#) [p2](#).
- Lipid Analysis:** Lipids were extracted using methanol and analyzed via shotgun mass spectrometry, enabling absolute quantification of 16 lipid classes, including ceramides, cholesterol, and sebaceous lipids. Internal standards ensured accuracy [in Sadowski, 2017](#) [p3](#).
- Study Objectives:** The research investigated lipidome variability with respect to sampling depth, body site, and inter-individual differences based on age and sex. Statistical analyses, including principal component analysis, were used to assess lipid profiles [in Sadowski, 2017](#) [p5](#).

This design enabled the largest SC lipidomic study to date, providing insights into lipid composition variability and its physiological implications.

1 source

Citation network

Sadowski.pdf

Ask anything



Deep research

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< 1 2 3 ... 11 >

Lipid extraction. Lipid extraction of tape-stripping samples containing one stripping disc each and scrape biopsy samples alike was carried out in 2 mL polypropylene tubes where 900 μ L of methanol including internal standards was added to each sample. The samples were shaken at 1400 rpm at 4°C for one hour. Thereafter, extracts were transferred to a multi-well plate and dried in a speed vacuum concentrator. Dried extracts were re-suspended in an acquisition mixture of 7.5 mM ammonium acetate in chloroform:methanol:propan-2-ol (1:2:4, V:V:V). For cholesterol, the dried extract was acetylated²⁰, then dried again and re-suspended in the above acquisition mixture. All liquid handling steps were performed using Hamilton Robotics STARlet robotic platform with Anti Droplet Control for pipetting of organic solvents.

MS data acquisition. Samples were analyzed by direct infusion with a QExactive mass spectrometer (Thermo Scientific) equipped with a TriVersa NanoMate ion source (Advion Biosciences) in a single acquisition for both positive and negative ion modes with a resolving power of $R_{m/z=200} = 280000$ for MS and $R_{m/z=200} = 17500$ for MS/MS. MS/MS fragmentation was performed at normalized collision energy of 35% and was triggered by an inclusion list encompassing corresponding MS mass ranges¹⁶. Both MS and MS/MS data were combined to monitor CE, DAG and TAG ions as ammonium adducts and all ceramide sub-classes as acetate adducts. Precursor ions and confirmatory MS/MS fragments as reported previously^{10,13,14} are summarized in Supplementary Table 1. Cholesterol was identified in a separate acquisition as cholesterol-acetate after a derivatization procedure²⁰.

Lipid identification and quantification. The resolving power used allows for identification of lipids based on precursor masses²¹. Combining MS/MS fragmentation data with the high resolution MS precursor data followed by isotopic correction (type I and II according to the strategy described previously^{16,22}), permitted structural elucidation of lipid molecular species. It increased the identification specificity, but also made it possible to unambiguously distinguish all 12 ceramide sub-classes, including NP/AdS and NH/AS pairs.

Internal standards used in this study were chosen not to be natively present in skin samples. Per sample 42 pmol of EOS D9 68:3:2 (18:1:2, 32:0:0, 18:2:0), 14 pmol NS D3 36:1:2 (18:1:2, 18:0:0), 50 pmol DAG D5 34:0:0 (17:0:0, 17:0:0), 100 pmol CE 20:0:0, 1000 pmol cholesterol D6 and 100 pmol TAG D5 51:0:0 (17:0:0, 17:1:0, 17:0:0) were delivered as internal standards. Quantification was conducted via normalization of the isotopically corrected intensity of the monoisotopic peak of each native species to the isotopically corrected intensity of the monoisotopic peak of the internal standard. The quantities of lipid molecular species were calculated from ratios between their respective characteristic MS/MS fragments, as described previously¹⁶. Non-hydroxy and alpha-hydroxy ceramide sub-classes were normalized to deuterated NS, whereas omega-hydroxy ceramides were normalized to deuterated EOS. Quantitative lipidomic data of the study can be found in Supplementary Table 2.

Data analysis and post-processing. Data were analyzed with in-house developed lipid identification software based on LipidXplorer^{23,24}. Only lipid identifications with measured mass deviations below 3 ppm from the theoretical mass for MS and 8 ppm for MS/MS peaks in scans where lock mass was available, and 5 and 12, respectively, where it was not; signal-to-noise ratio greater than 5; and an amount at least 5-fold higher than in corresponding blank samples were considered as positive hits, yielding 862 unique lipids across all samples from all experiments. Further, unless stated otherwise, only lipids present in at least two replicates and above 2 pmol per sample were included in subsequent data analysis, resulting in 509 unique lipids. Data visualization, linear regression (linear least squares method), and correlation (two-tailed Pearson and Spearman correlation) calculations were performed on Prism6.0h software (GraphPad Software, Inc.). Where it does not lower figure clarity, individual data points are shown²⁵.

Statistical models were trained with the R Environment for Statistical Computing (R version 3.3.2 (2016-10-31)), by the caret package (version 6.0-73)²⁶, which in turn uses the randomForest package (version 4.6-12)²⁷. For statistical modeling only lipids present in at least 50% of samples per cohort were used. If a lipid was present in one cohort, it was also included for other cohorts, even if its occurrence rate was lower. During model training with 5 times repeated 10 times cross validation, the resampled data were preprocessed by centering and scaling, missing values were imputed with the median, and near zero variance predictors were removed.

Results

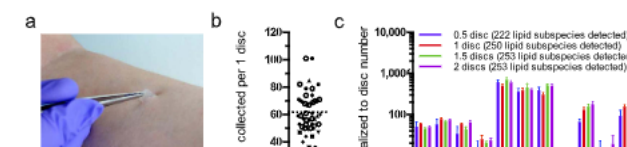
High throughput-compatible skin sampling and sample processing. In order to take advantage of the quick spectra acquisition capabilities of shotgun mass spectrometry, the sampling procedure and all other sample-handling steps were optimized for speed, throughput and convenience utilizing automation whenever possible. Automation of procedures also benefits in higher reproducibility²⁸.

Tape-stripping was used as it was simultaneously the most convenient and non-invasive sampling method (Fig. 1a). It also had the additional advantage of allowing for control over the sampling depth (by collecting the appropriate stratum corneum layer by sequential stripping) and collecting comparable sample amounts. As surface furrows might affect the amount of material collected²⁹, we gravimetrically determined the reproducibility of sample amount collected via tape-stripping of the second layer with one stripping disc to be $62 \pm 14 \mu$ g (mean \pm s.d.) (Fig. 1b). Extraction of lipids with commonly used organic solvents from a polymeric tape with adhesive (i.e. stripping disc) was complicated because established methods utilizing chloroform^{30,31} or methyl *tert*-butyl ether²² interfered with tape constituents, physically dissolving them. We found, however, that methanol extraction successfully used for skin lipidomics in previous studies¹¹ allowed for efficient extraction of skin lipids

SCIENTIFIC REPORTS | 7:43761 | DOI: 10.1038/srep43761

3

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Comparing the results of papers

SC

Create a table to compare the results for all twelve ceramide subclasses. Sort the subclasses by alphabet.



The results for the twelve ceramide subclasses from both studies are summarized below. The table is sorted alphabetically by subclass name.

Ceramide Subclass	Observations from Ahlström et al. (2024)	Observations from Sadowski et al. (2017)
AdS	No significant difference observed between AD and controls Ahlström, 2024 p4 .	Included in analysis; no specific results highlighted Sadowski, 2017 p5 .
AH	No significant difference observed between AD and controls Ahlström, 2024 p4 .	Included in analysis; no specific results highlighted Sadowski, 2017 p5 .
AP	No significant difference observed between AD and controls Ahlström, 2024 p4 .	Included in analysis; no specific results highlighted Sadowski, 2017 p5 .
AS	Higher levels in AD compared to controls ($p = 0.011$) Ahlström, 2024 p4 .	Included in analysis; no specific results highlighted Sadowski, 2017 p5 .
EOdS	No significant difference observed between AD and controls Ahlström, 2024 p4 .	Low abundance in samples; detected in deeper layers Sadowski, 2017 p4 .
EOH	No significant difference observed between AD and controls Ahlström, 2024 p4 .	Increased with sampling depth Sadowski, 2017 p5 .
EOS	Higher relative abundance in controls compared to AD ($p = 0.024$) Ahlström, 2024 p4 .	Increased with sampling depth Sadowski, 2017 p5 .
EOP	No significant difference observed between AD and controls Ahlström, 2024 p4 .	Included in analysis; no specific results highlighted Sadowski, 2017 p5 .
NH	Higher levels in AD compared to controls ($p = 0.01$)	Included in analysis; no specific results highlighted

Sadowski.pdf Ahlstroem.pdf

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Is this in line with other papers?



I will review the findings from other studies to determine whether they align with the results of Ahlström et al. (2024) and Sadowski et al. (2017). Please hold on.

The findings from Ahlström et al. (2024) and Sadowski et al. (2017) align with broader trends observed in other studies on ceramide subclasses in atopic dermatitis (AD) and healthy skin. Key points include:

1. Altered Ceramide Profiles in AD:

- Ahlström et al. reported higher levels of ceramide subclasses such as NS and NH in AD, consistent with studies showing altered ceramide profiles in AD due to immune-driven effects and skin barrier dysfunction [Tonicic, 2020](#) , [Imokawa, 2021](#) .
- Decreased levels of ceramide EOS in AD, as noted by Ahlström et al., are also supported by findings of reduced ultra-long-chain ceramides in AD, which are critical for skin barrier integrity [Bakar, 2024](#) , [Kondo, 2024](#) .

2. Impact of Inflammation and Cytokines:

- Studies highlight the role of Th2 cytokines in modifying ceramide profiles, particularly reducing ceramide EOS and altering ceramide NS composition, which mirrors the trends observed in Ahlström et al. [Bakar, 2024](#) , [Chu, 2023](#) .

3. Variability Across Studies:

- While Sadowski et al. focused on healthy skin variability, other studies emphasize the disease-specific changes in ceramide subclasses, such as increased unsaturated ceramides in AD [Kondo, 2024](#) .

Overall, the findings from both papers are consistent with the literature, emphasizing the importance of ceramide composition in skin health and AD pathogenesis. Let me know if you'd like further details on specific studies!

100 sources

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Can you elaborate on the role of Th2 cytokines in ceramide profile alterations?

What are the implications of altered ceramide profiles for AD treatment?

Sadowski.pdf

Ahlstroem.pdf

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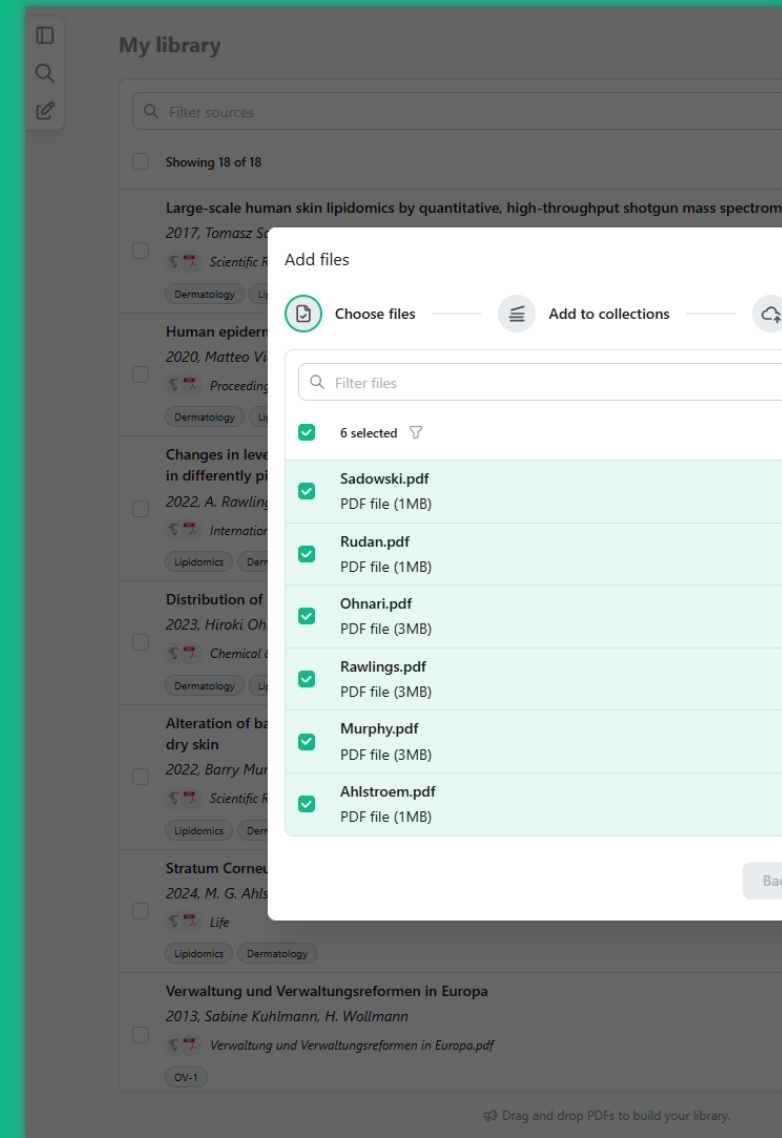
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4 Example

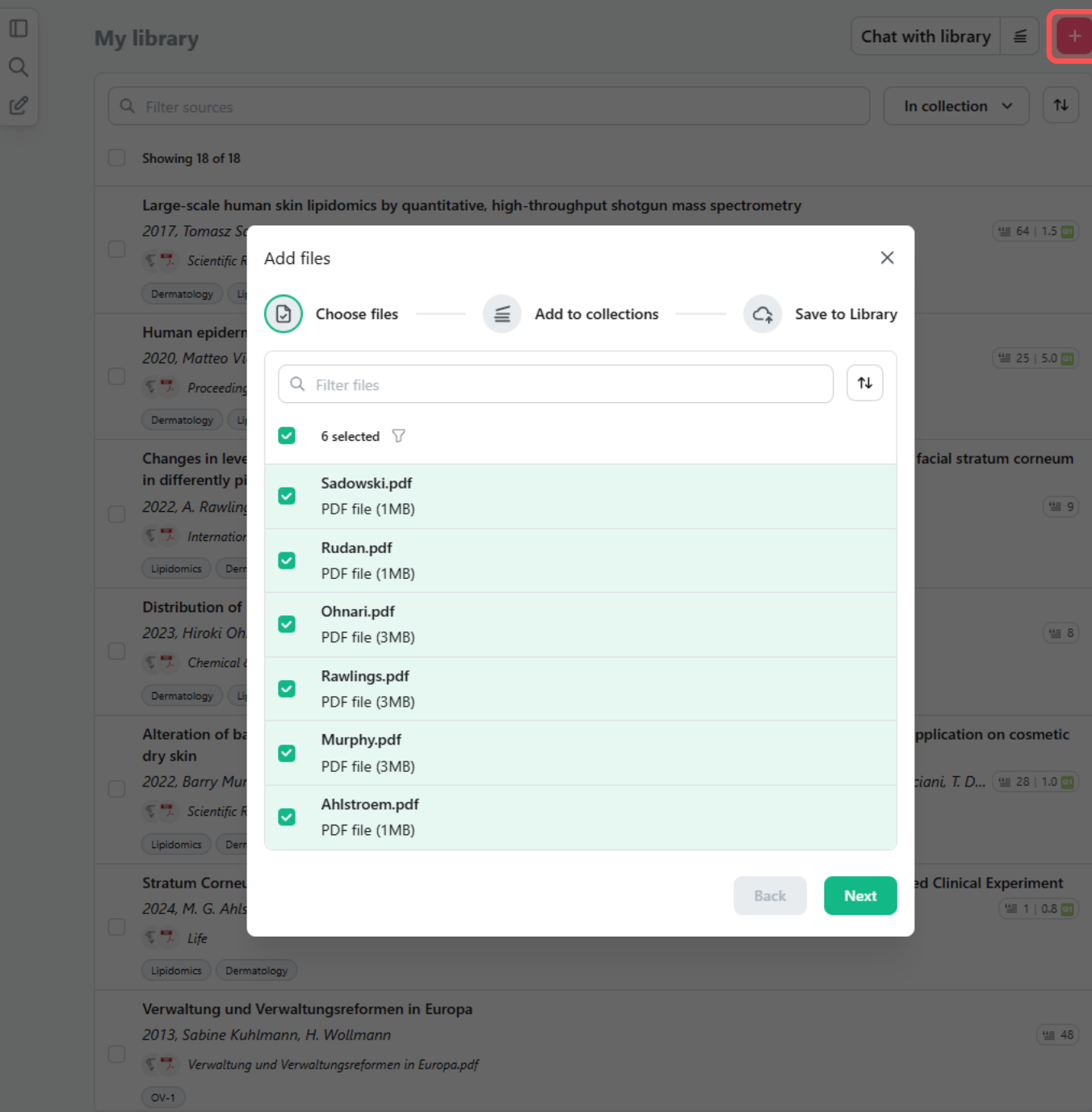


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Large-scale human skin lipidomics by quantitative, high-throughput shotgun mass spectrometry
2017, Tomasz Sadowski, C. Klose, M. Gerl, Anna Wójcik-Maciejewicz, R. Herzog, K. Simons, A. Reich, M. A. Surma
Scientific Reports
Dermatology Lipidomics

64 | 1.5

✓

Human epidermal stem cell differentiation is modulated by specific lipid subspecies
2020, Matteo Vietri Rudan, Ajay Mishra, C. Klose, U. Eggert, F. Watt
Proceedings of the National Academy of Sciences of the United States of America
Dermatology Lipidomics

25 | 5.0

✓

Changes in levels of omega-O-acylceramides and related processing enzymes of sun-exposed and sun-protected facial stratum corneum in differently pigmented ethnic groups
2022, A. Rawlings, R. Schoop, C. Klose, J. Monneuse, B. Summers, R. Voegeli
International Journal of Cosmetic Science
Lipidomics Dermatology

9

✓

Distribution of Domains Formed by Lateral Packing of Intercellular Lipid in the Stratum Corneum.
2023, Hiroki Ohnari, E. Naru, O. Sakata, Y. Obata
Chemical & pharmaceutical bulletin
Dermatology Lipidomics

8

✓

Alteration of barrier properties, stratum corneum ceramides and microbiome composition in response to lotion application on cosmetic dry skin
2022, Barry Murphy, S. Grimshaw, M. Hoptroff, Sarah Paterson, David Arnold, Andrew Cawley, Suzanne E. Adams, F. Falciani, T. D...
Scientific Reports
Lipidomics Dermatology

28 | 1.0

✓

Stratum Corneum Lipids in Non-Lesional Atopic and Healthy Skin following Moisturizer Application: A Randomized Clinical Experiment
2024, M. G. Ahlström, R. Bjerre, M. G. Ahlström, L. Skov, J. D. Johansen
Life
Lipidomics Dermatology

1 | 0.8

Verwaltung und Verwaltungsreformen in Europa
2013, Sabine Kuhlmann, H. Wollmann
Verwaltung und Verwaltungsreformen in Europa.pdf
OV-1

48

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Writing a grant application

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Take a deep dive into my dermatology collection. Then, draft the introduction for a grant application about the relevance of lipidomics methodology development for dermatological research and product development.



Draft Introduction for Grant Application

The stratum corneum (SC), the outermost layer of human skin, plays a critical role in maintaining barrier function, hydration, and protection against environmental insults. This functionality is largely governed by its lipid composition, which includes ceramides, cholesterol, and free fatty acids organized into lamellar structures. Dysregulation of these lipids is implicated in various dermatological conditions, such as atopic dermatitis, xerosis, and impaired barrier function, highlighting the need for advanced methodologies to study lipid dynamics [Sadowski, 2017](#) [p8](#) , [Murphy, 2022](#) [p2](#) .

Recent advances in lipidomics, particularly shotgun mass spectrometry, have enabled high-throughput, quantitative analysis of lipid species, offering unprecedented insights into their roles in skin physiology and pathology. For example, lipidomic profiling has revealed site-specific and age-related variations in lipid composition, as well as the regulatory potential of individual lipid subspecies in keratinocyte differentiation [Rudan, 2020](#) [p3](#) , [Sadowski, 2017](#) [p6](#) . Furthermore, lipidomics has demonstrated the impact of topical treatments on lipid profiles, suggesting therapeutic avenues for restoring skin barrier integrity [Ahlström, 2024](#) [p7](#) .

This grant proposal aims to advance lipidomics methodologies tailored for dermatological research, focusing on their application in understanding skin diseases and optimizing cosmetic and pharmaceutical product development. By integrating cutting-edge lipidomics with dermatological science, this initiative seeks to uncover novel biomarkers and therapeutic targets, ultimately enhancing skin health and treatment efficacy.

4 sources

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What are the current limitations of lipidomics in dermatological research?

Can you elaborate on the therapeutic applications of lipidomics findings?

How does lipidomics compare to other methodologies in studying skin physiology?

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SC

🔗 Critical review



The agreeing arguments are supported by recent studies. For instance, the role of ceramides, cholesterol, and free fatty acids in maintaining the stratum corneum's barrier function is reinforced by findings that emphasize their structural and functional importance in forming dense lamellar structures and preventing water loss. Studies also highlight the potential of ceramide-based formulations in skincare, particularly for repairing damaged lipid arrangements and improving barrier function in conditions like atopic dermatitis [Schild, 2024](#) ; [Hu, 2025](#) . Additionally, lipidomic techniques such as shotgun lipidomics and molecular dynamics simulations have been validated for their ability to analyze lipid profiles and understand the interplay between lipid subclasses and skin health [Yang, 2024](#) ; [Jacques, 2023](#) .

The disagreeing arguments are limited but include challenges in lipidomics research, such as the complexity of accurately modeling the stratum corneum's lipid matrix and the limitations of current analytical techniques in capturing the dynamic interactions between lipids and external factors. For example, studies have pointed out the difficulty in replicating the exact lamellar organization and permeability of the stratum corneum in vitro, which can limit the applicability of findings to real-world scenarios [Jiang, 2024](#) ; [Roy, 2023](#) . Additionally, the formulation of ceramides in skincare products requires rigorous processes, and improper formulation can lead to counterproductive effects on skin barrier repair [Schild, 2024](#) .

In summary, while the previous answer is well-supported by recent literature, it could benefit from a more nuanced discussion of the limitations and challenges in skin lipidomics research and product formulation.

❖ 100 sources ^

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Schild, 2024



The counterproductive effects of undissolved ceramides on skin barrier repair capacity of the formulas are demonstrated, when assessed in different in vitro models of disrupted skin barrier.

1

2024, Jennifer Schild



International Journal of Cosmetic Science

3

Hu, 2025



This paper sorts out the existing literature to help understand the relationship between ceramide and various diseases and hopes to provide new ideas for the prevention and treatment of diseases.

2

2025, Minqi Hu

0

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Draft a mini review about the relevance of lipidomics analysis in dermatological research.



The Relevance of Lipidomics Analysis in Dermatological Research

Introduction

Lipidomics, the comprehensive study of lipid profiles, has emerged as a pivotal tool in dermatological research. Skin lipids, including ceramides, cholesterol, and fatty acids, play essential roles in maintaining barrier function and overall skin health. Dysregulation of these lipids is linked to various skin disorders, such as atopic dermatitis and xerosis. By leveraging advanced analytical techniques like mass spectrometry, lipidomics enables precise characterization of lipid variability across anatomical sites, depths, and individuals. This mini review explores the methodologies, biological insights, and clinical applications of lipidomics, highlighting its transformative potential in understanding skin physiology and pathology.

Analytical Methods and Technologies in Skin Lipidomics

Shotgun mass spectrometry is a cornerstone of high-throughput skin lipidomics, enabling comprehensive analysis of sebaceous and stratum corneum lipids. This technique involves direct infusion of lipid extracts into a mass spectrometer without prior chromatographic separation, allowing rapid acquisition of complex spectra. High-resolution instruments, such as the QExactive mass spectrometer, are essential for resolving overlapping signals and ensuring accurate identification of lipid species, including ceramides, cholesterol, and triacylglycerols [Sadowski, 2017](#) p3 ; [Ohnari, 2023](#) p2 .

The advantages of shotgun lipidomics include broad lipid coverage, absolute quantification using internal standards, and unprecedented throughput, which is critical for large-scale studies and clinical applications. For example, this method has been used to analyze over 268 skin samples, revealing depth-dependent lipid gradients and inter-individual variability [Sadowski, 2017](#) p2 ; [Sadowski, 2017](#) p8 . Additionally, tape-stripping combined with shotgun lipidomics provides a non-



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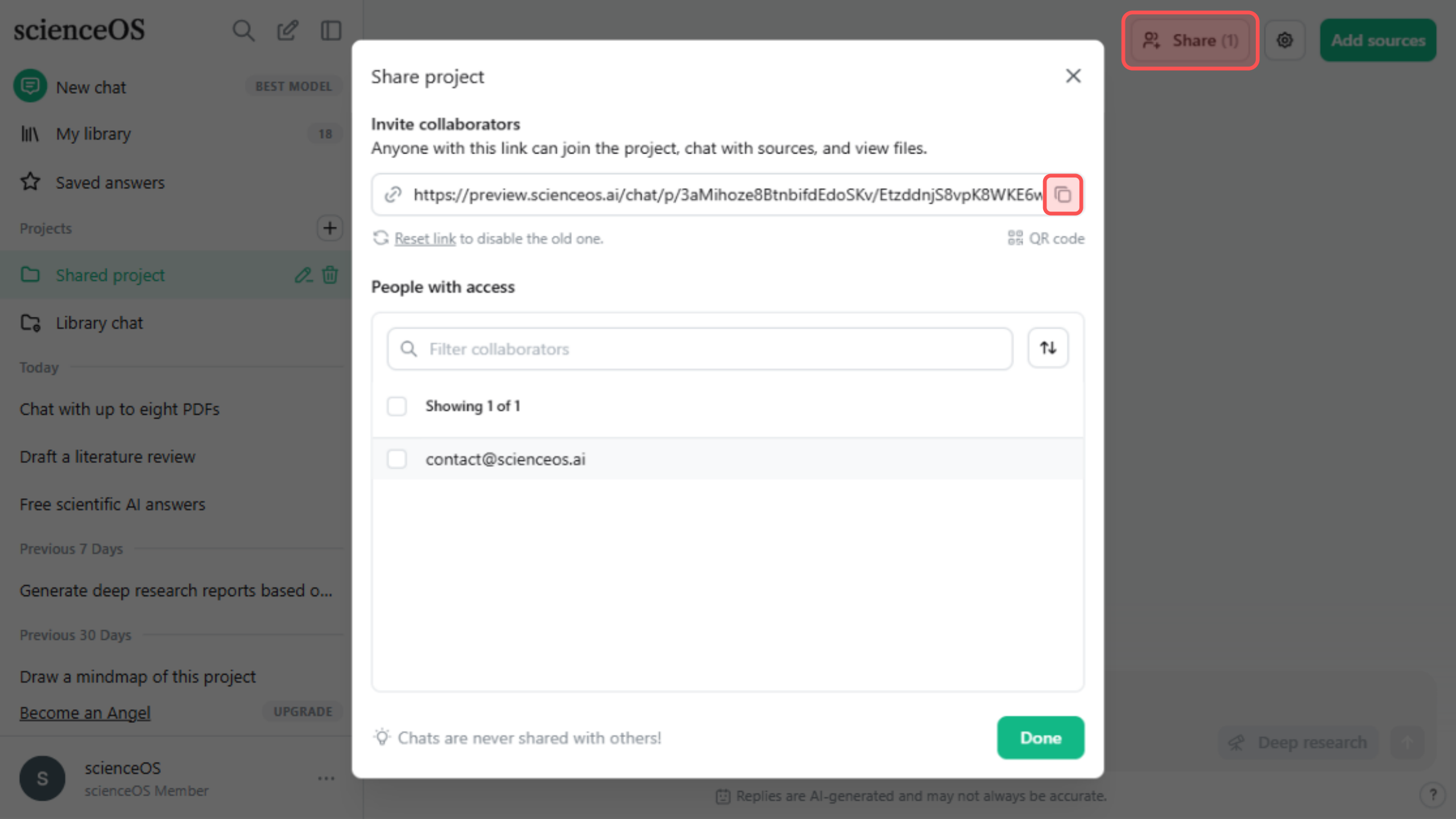
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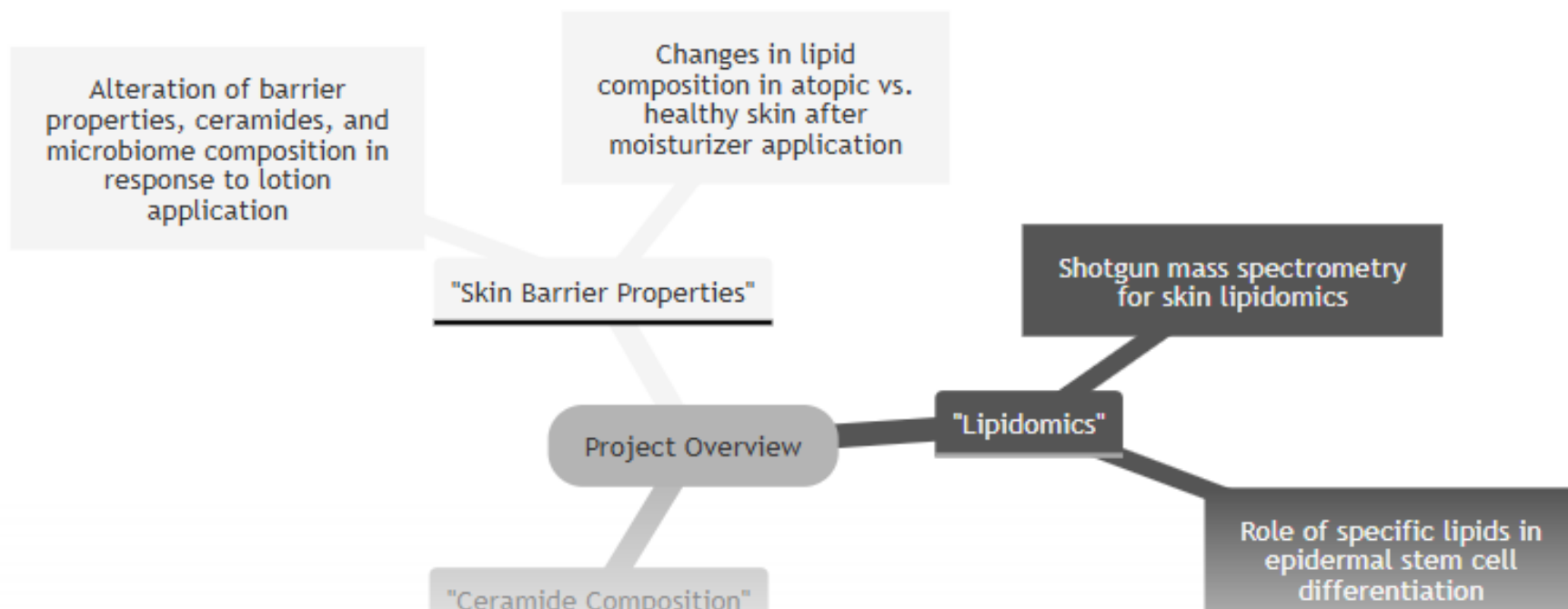
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