HOW TO

The AI research agent for scientists with high standards

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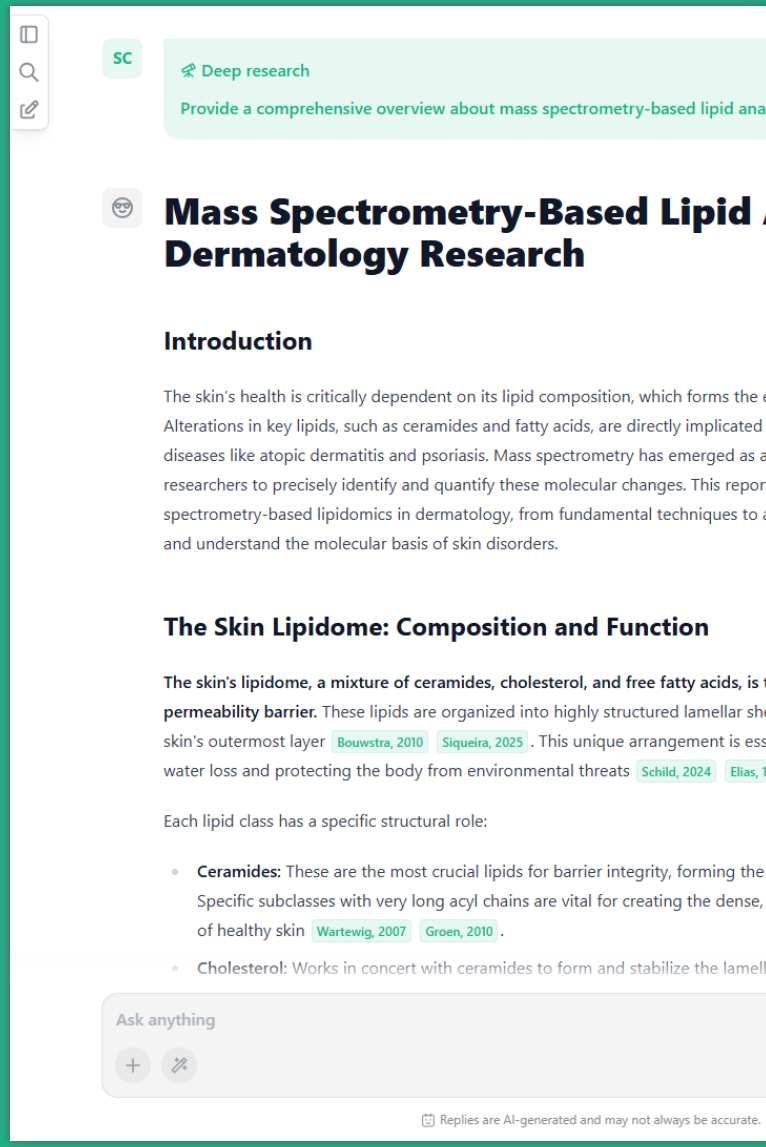

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Where scientists can swiftly tackle global challenges.

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USER PROBLEMS

USE CASE	PROBLEM	scienceOS
1 Scientific answers slide 4	*„I am starting a new R&D project and need to quickly gain an overview about the field.“*	Ask research questions and **follow-ups** to dive into detail.
2 Explore citations slide 15	*„There are too many publications. I need to find the best and most relevant papers.“*	Create citation networks and **analyze** how papers are cited.
3 Compare papers slide 19	*„I need to compare the results from several papers and assess their validity.“*	**Upload** research papers to quickly chat with them.
4 Drafting texts slide 25	*„A grant application deadline is approaching. I still need to write the introduction!“*	**Generate** answers based on your literature collection.

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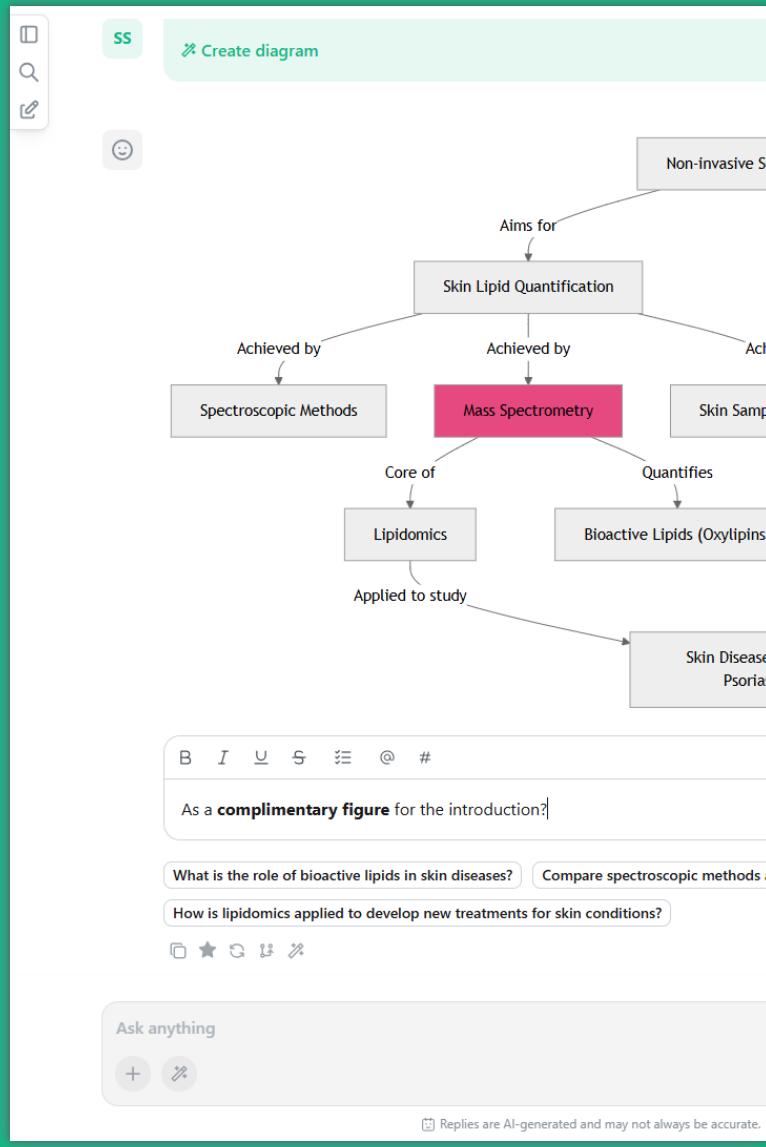

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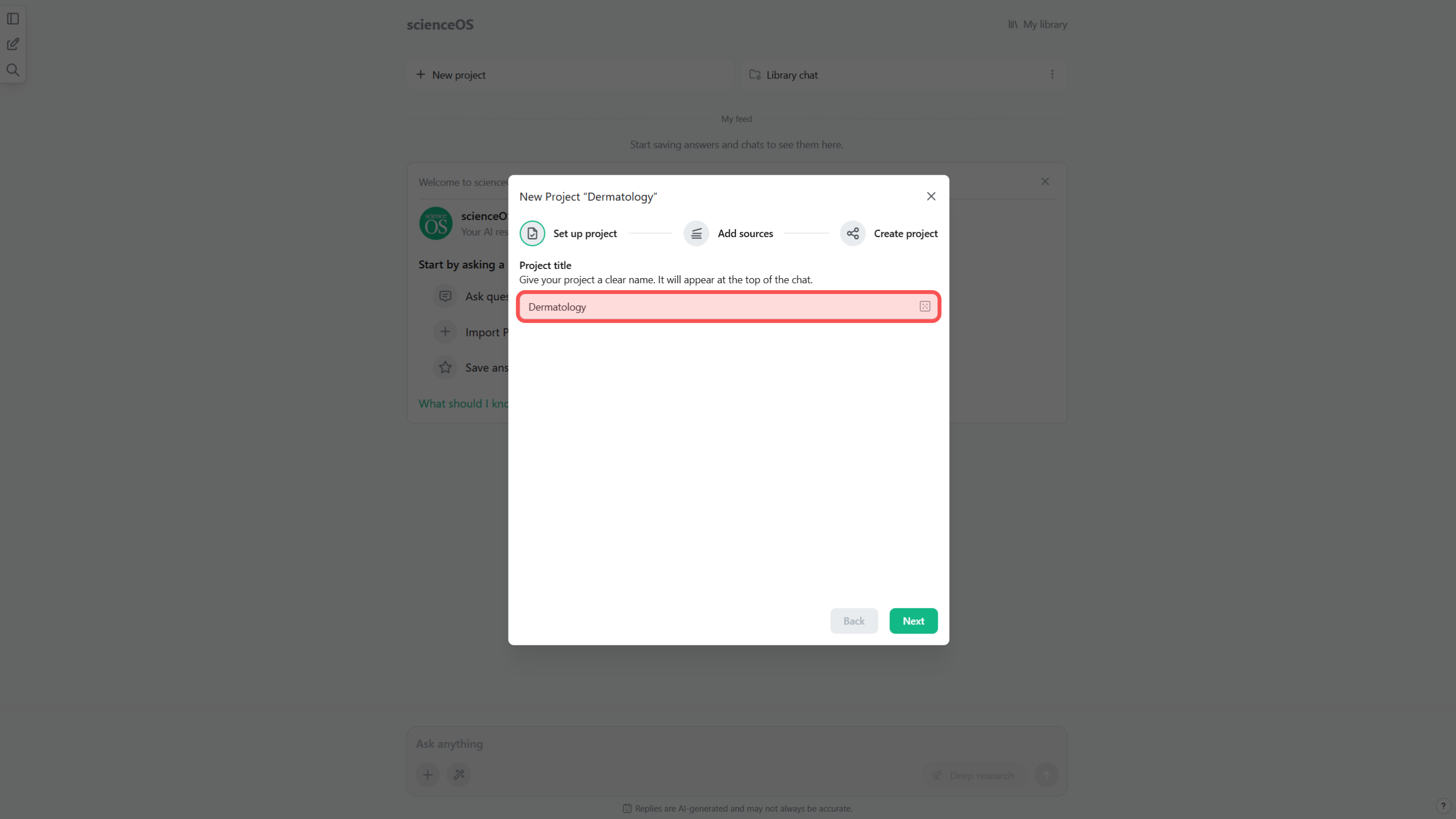
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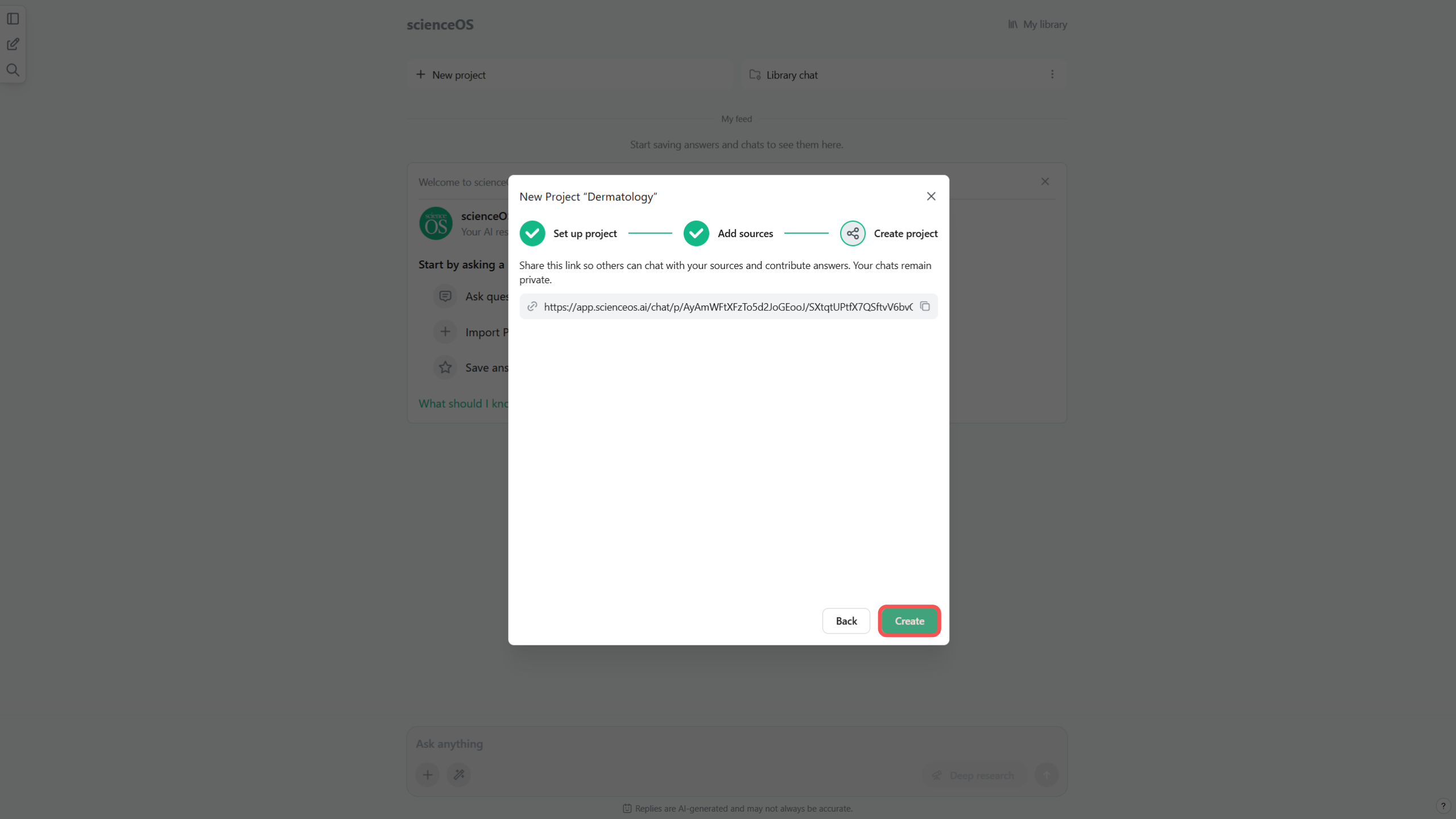
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Add a note...

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

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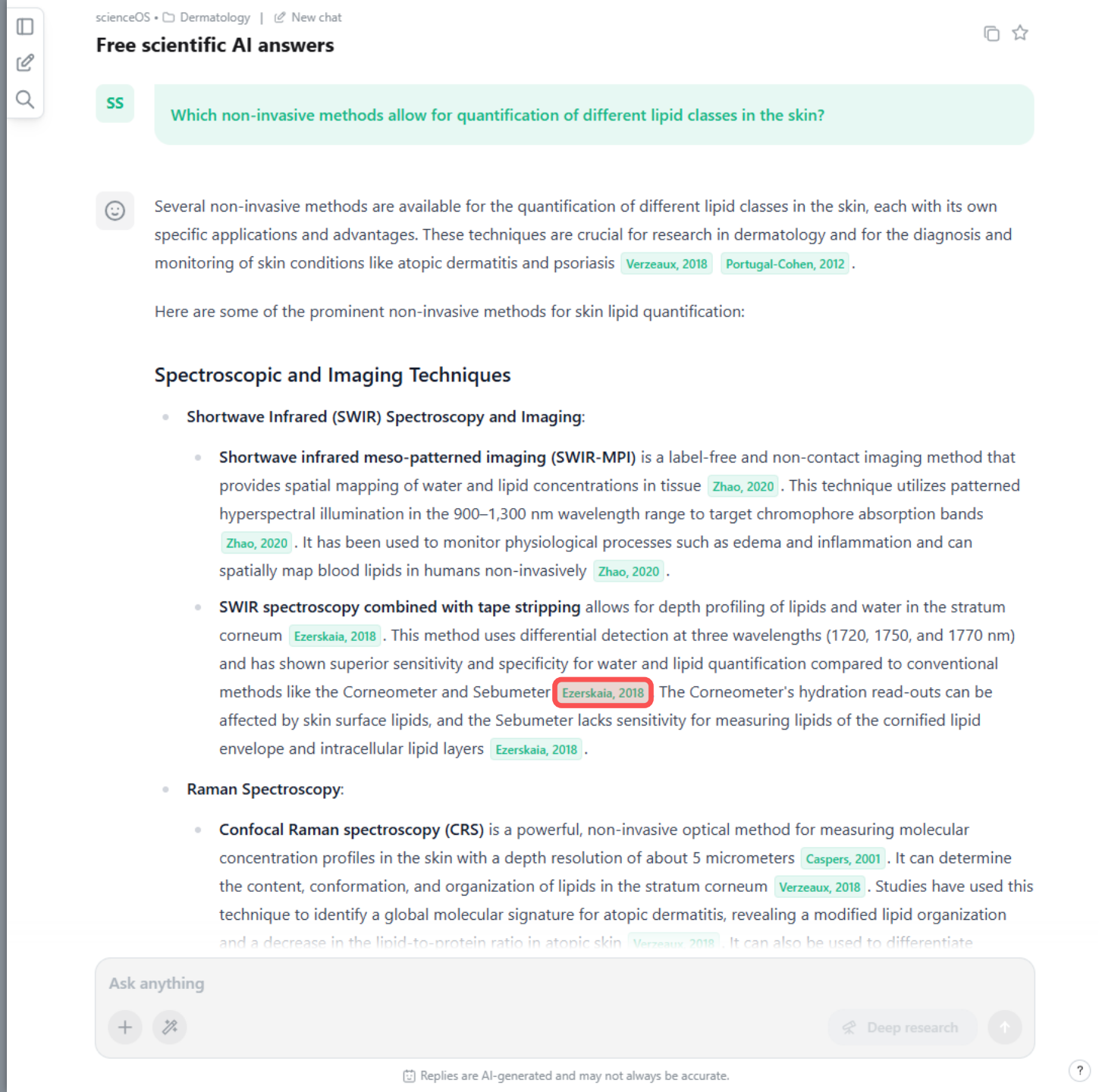

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Click on **citation markers** for source details.

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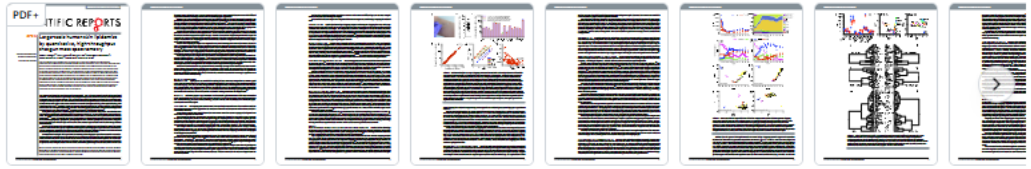
Sadowski, 2017

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

10.1038/srep43761 28266621 CC BY



TL;DR — 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.

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.

Dermatology Grant Lipidomics Skin

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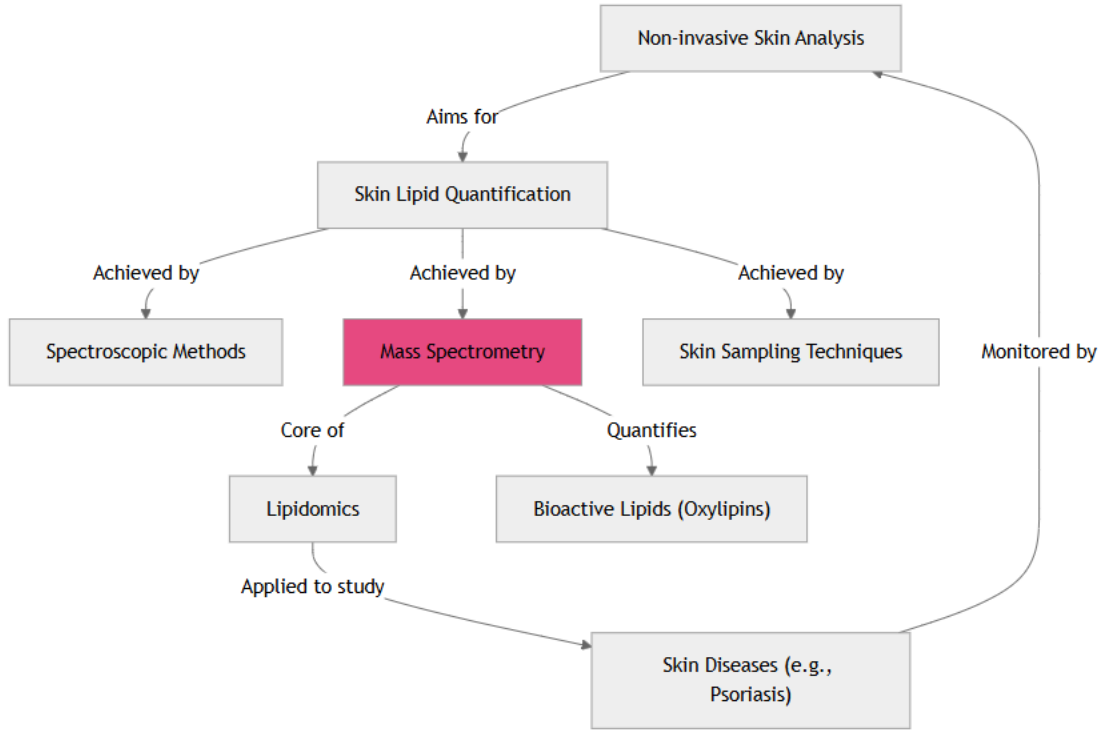

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What is the role of bioactive lipids in skin diseases?

Compare spectroscopic methods and mass spectrometry for skin analysis.

How is lipidomics applied to develop new treatments for skin conditions?

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

Mass Spectrometry-Based Lipid Analysis in Dermatology Research

Introduction

The skin’s health is critically dependent on its lipid composition, which forms the essential epidermal permeability barrier. Alterations in key lipids, such as ceramides and fatty acids, are directly implicated in the pathogenesis of inflammatory skin diseases like atopic dermatitis and psoriasis. Mass spectrometry has emerged as a pivotal analytical technology, enabling researchers to precisely identify and quantify these molecular changes. This report explores the application of mass spectrometry-based lipidomics in dermatology, from fundamental techniques to advanced spatial imaging, to diagnose and understand the molecular basis of skin disorders.

The Skin Lipidome: Composition and Function

The skin's lipidome, a mixture of ceramides, cholesterol, and free fatty acids, is the primary architect of the epidermal permeability barrier. These lipids are organized into highly structured lamellar sheets within the stratum corneum, the skin's outermost layer Bouwstra, 2010 Siqueira, 2025 . This unique arrangement is essential for preventing transepidermal water loss and protecting the body from environmental threats Schild, 2024 Elias, 1992 .

Each lipid class has a specific structural role:

- **Ceramides:** These are the most crucial lipids for barrier integrity, forming the backbone of the lamellar structures. Specific subclasses with very long acyl chains are vital for creating the dense, impermeable organization characteristic of healthy skin Wartewig, 2007 Groen, 2010 .
- **Cholesterol:** Works in concert with ceramides to form and stabilize the lamellar phases Bouwstra, 2001 .

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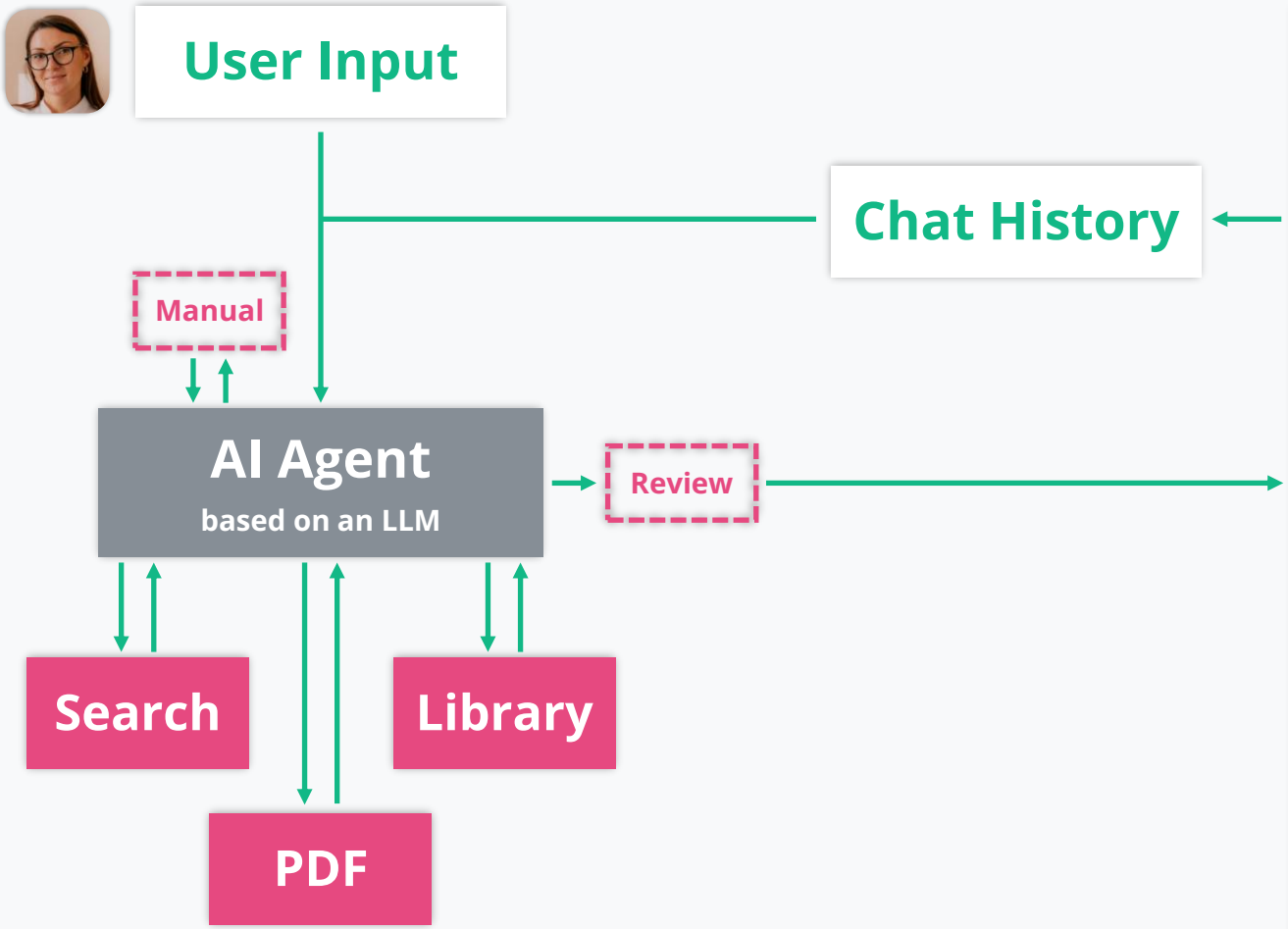

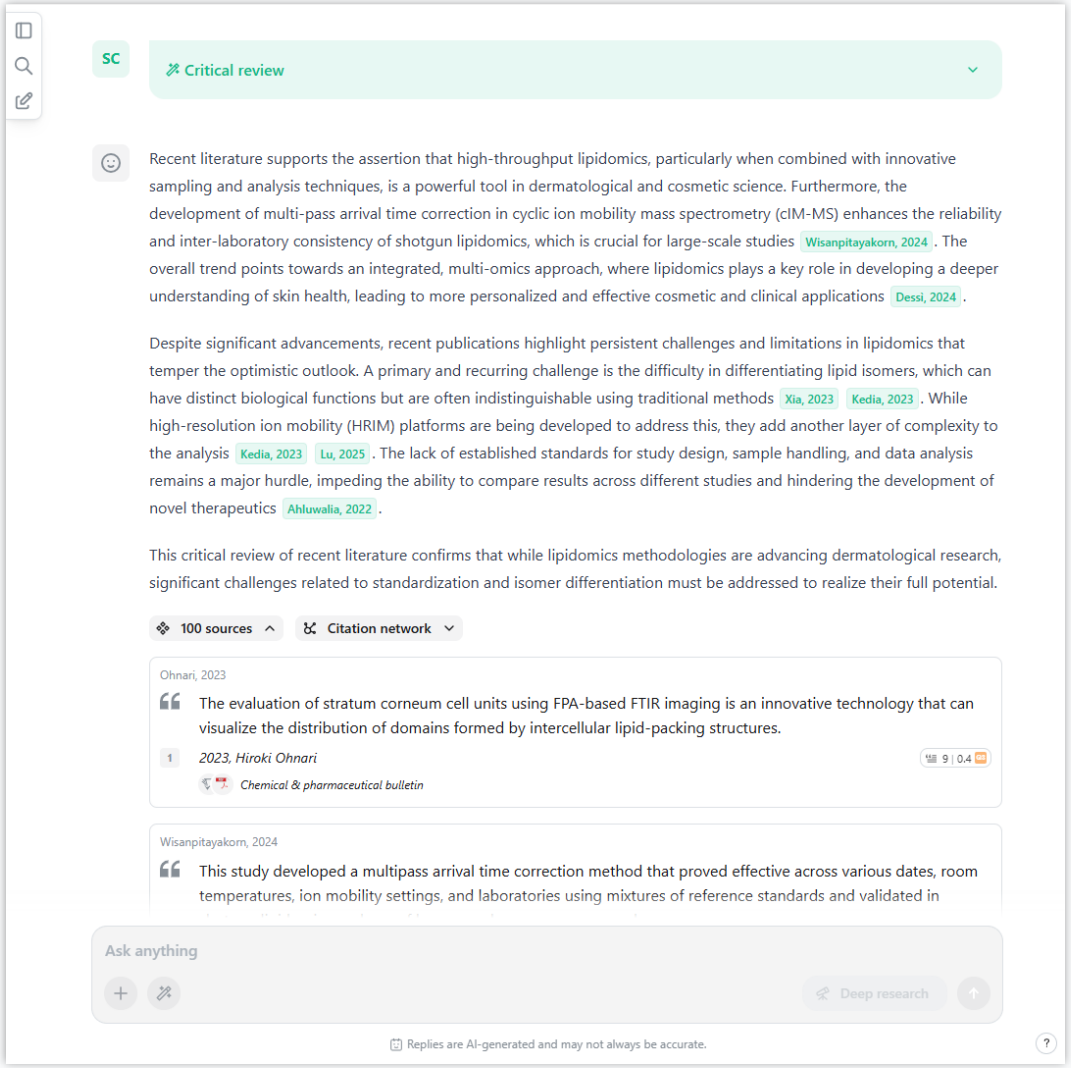

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Explore networks of related papers

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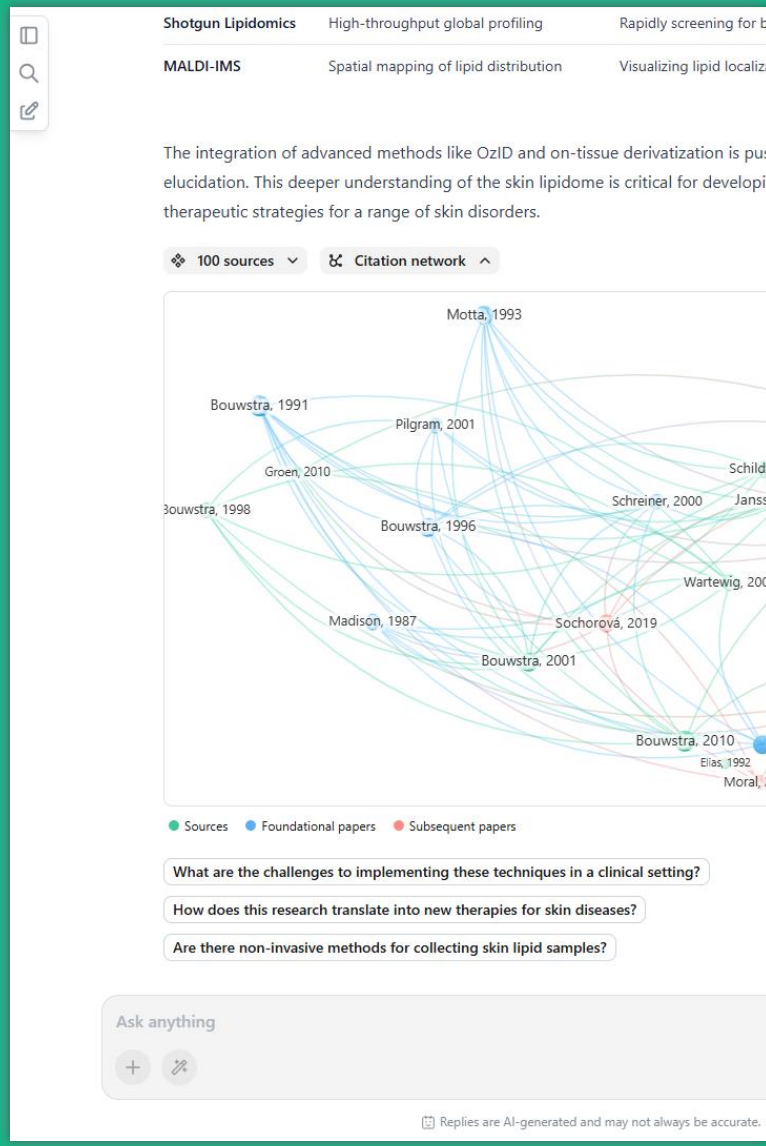

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- **Ozone-Induced Dissociation (OzID):** A gas-phase reaction within the mass spectrometer that cleaves lipids at C=C bonds, revealing their exact locations and uncovering previously hidden lipid diversity Menzel, 2022 Ross, 2023 .
- **Covalent Adduct Chemical Ionization (CACI):** A method used for the comprehensive characterization of complex sebum lipids, including fatty acids and squalene Qi, 2025 Wang, 2024 .

Conclusion

Mass spectrometry-based lipidomics has become indispensable in dermatology, providing unparalleled insight into the molecular basis of skin health and disease. By enabling the precise identification and quantification of lipids, these techniques have directly linked alterations in ceramides and fatty acids to the impaired barrier function seen in atopic dermatitis and psoriasis. The strategic application of different MS methodologies allows researchers to move from broad, hypothesis-generating discovery to detailed spatial and structural analysis.

Technique	Primary Strength	Key Application in Dermatology
LC-MS	Separation of isomers; high sensitivity	Quantifying specific ceramides and other low-abundance lipids.
Shotgun Lipidomics	High-throughput global profiling	Rapidly screening for broad changes in the skin lipidome.
MALDI-IMS	Spatial mapping of lipid distribution	Visualizing lipid localization in skin structures and lesions.

The integration of advanced methods like OzID and on-tissue derivatization is pushing the field toward complete structural elucidation. This deeper understanding of the skin lipidome is critical for developing targeted diagnostics and novel therapeutic strategies for a range of skin disorders.

100 sources | Citation network

What are the challenges to implementing these techniques in a clinical setting?

How does this research translate into new therapies for skin diseases?

Are there non-invasive methods for collecting skin lipid samples?

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Shotgun Lipidomics	High-throughput global profiling	Rapidly screening for broad changes in the skin lipidome.
MALDI-IMS	Spatial mapping of lipid distribution	Visualizing lipid localization in skin structures and lesions.

The integration of advanced methods like OzID and on-tissue derivatization is pushing the field toward complete structural elucidation. This deeper understanding of the skin lipidome is critical for developing targeted diagnostics and novel therapeutic strategies for a range of skin disorders.

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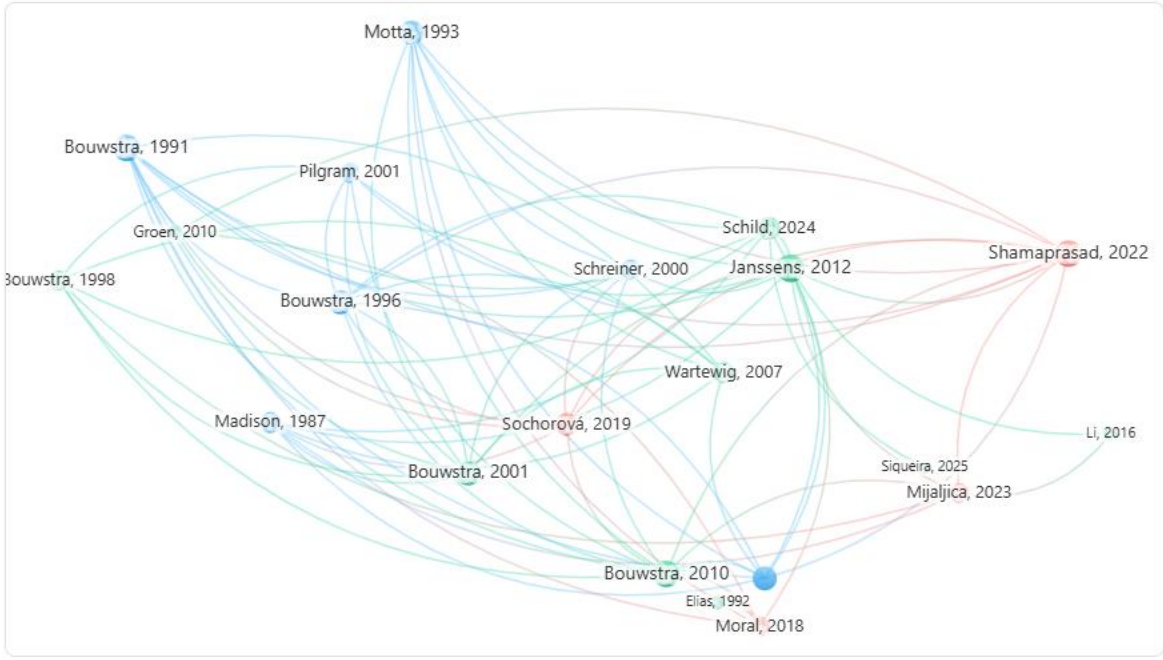

Sources Foundational papers Subsequent papers Click for details

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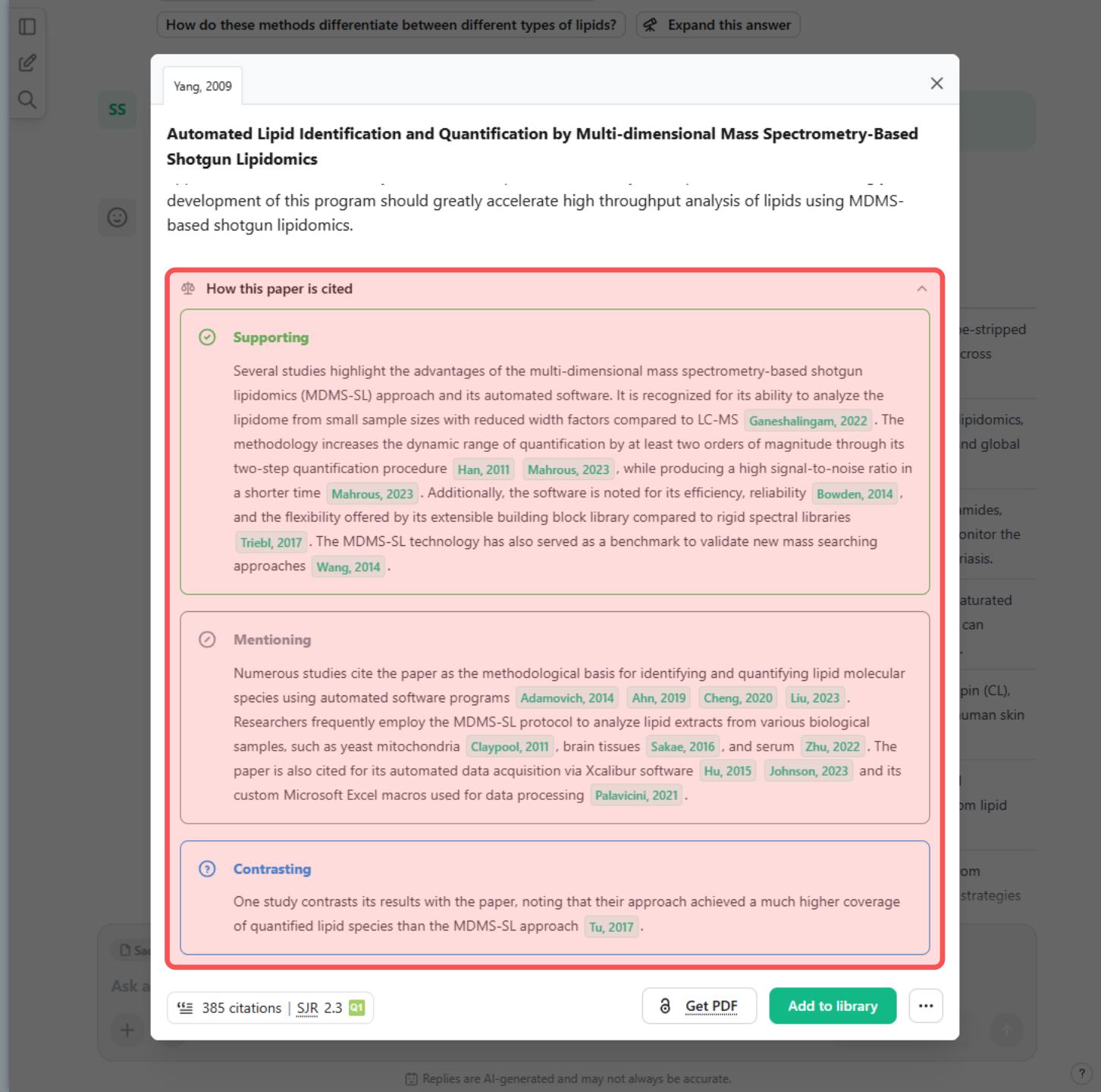

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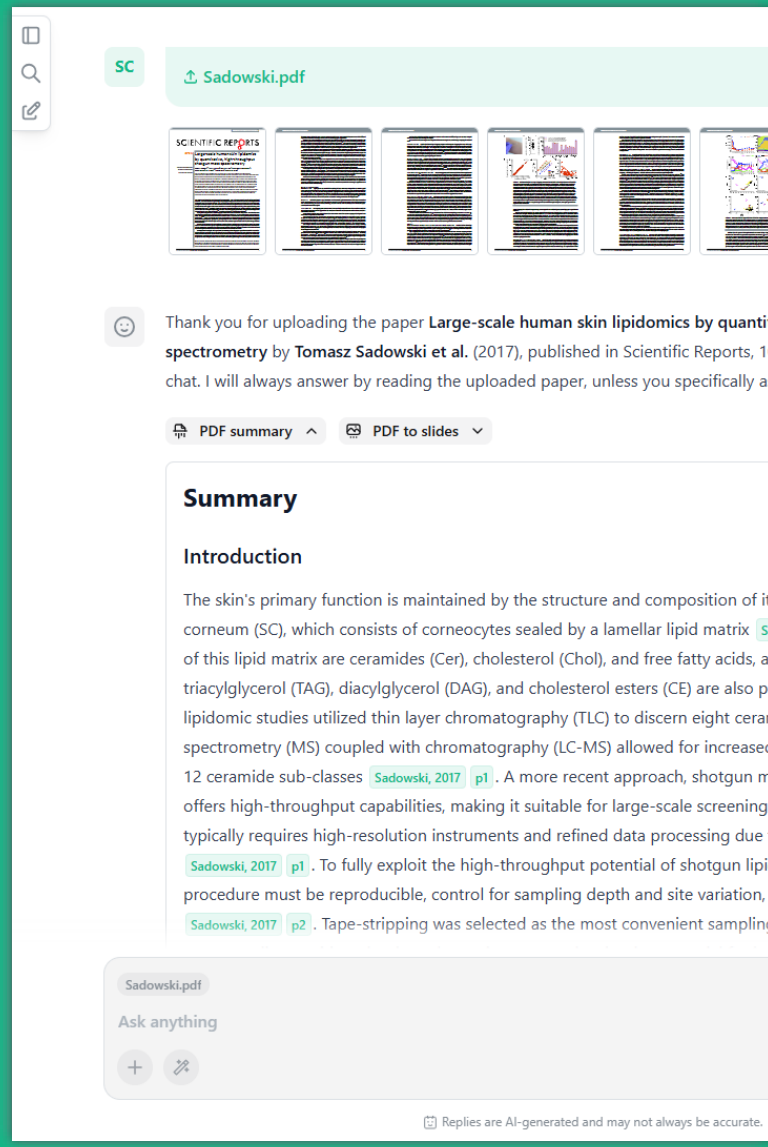

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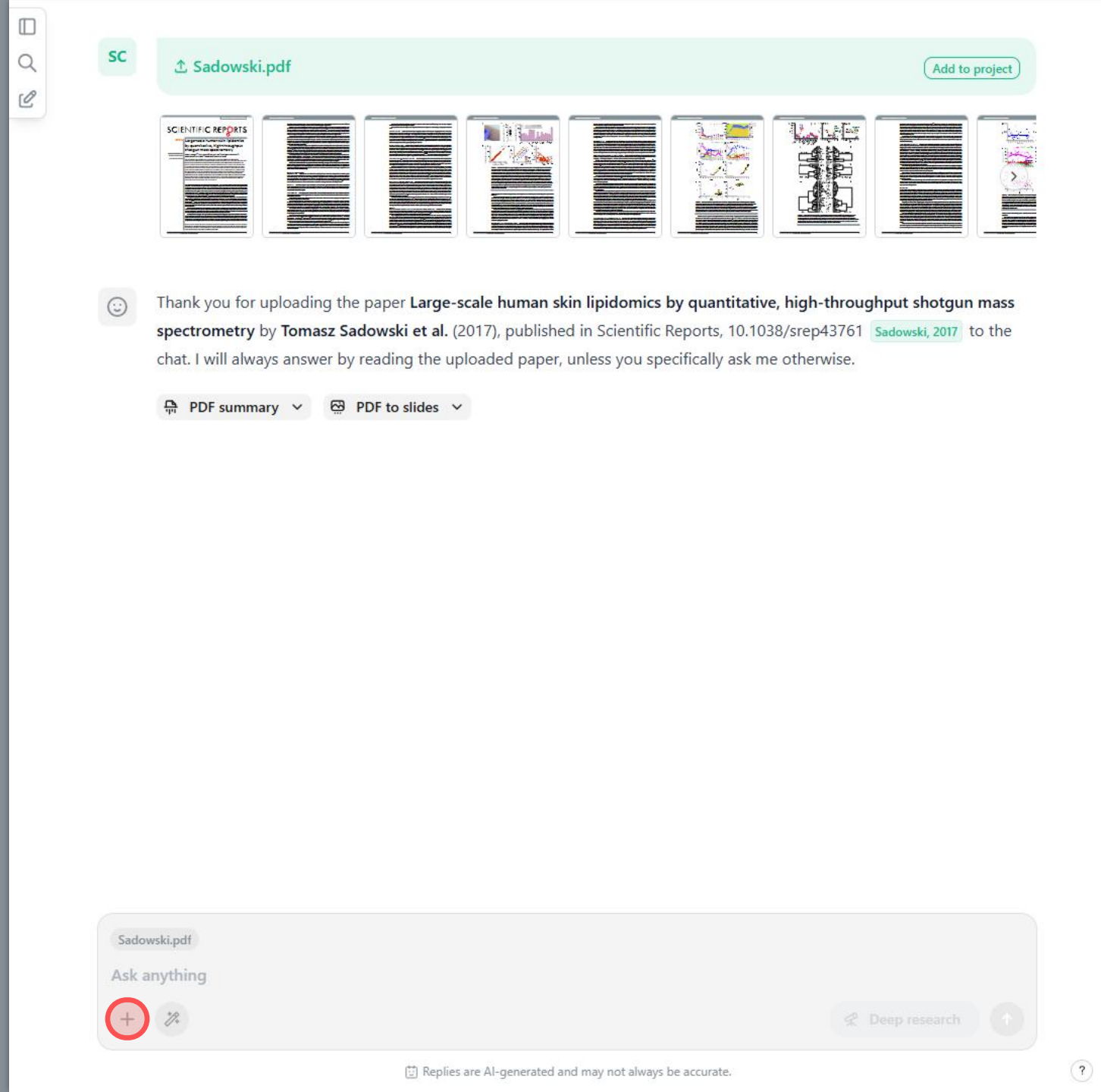

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2

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SC

Sadowski.pdf

Add to project

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 to the chat. I will always answer by reading the uploaded paper, unless you specifically ask me otherwise.

PDF summary | PDF to slides

Summary

Introduction

The skin's primary function is maintained by the structure and composition of its outermost layer, the stratum corneum (SC), which consists of corneocytes sealed by a lamellar lipid matrix Sadowski, 2017 p1. The main constituents of this lipid matrix are ceramides (Cer), cholesterol (Chol), and free fatty acids, although other classes like triacylglycerol (TAG), diacylglycerol (DAG), and cholesterol esters (CE) are also present Sadowski, 2017 p1. Historically, lipidomic studies utilized thin layer chromatography (TLC) to discern eight ceramide sub-classes, but modern mass spectrometry (MS) coupled with chromatography (LC-MS) allowed for increased sensitivity and the differentiation of 12 ceramide sub-classes Sadowski, 2017 p1. A more recent approach, shotgun mass spectrometry (direct infusion), offers high-throughput capabilities, making it suitable for large-scale screening and clinical applications, although it typically requires high-resolution instruments and refined data processing due to complex spectra Sadowski, 2017 p1 Sadowski, 2017 p1. To fully exploit the high-throughput potential of shotgun lipidomics for skin analysis, the sampling procedure must be reproducible, control for sampling depth and site variation, and avoid introducing contaminants Sadowski, 2017 p2. Tape-stripping was selected as the most convenient sampling method because it allows control

Sadowski.pdf

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SC

Show me the data how age impacts skin lipid composition.

The analysis revealed the following key findings regarding the effect of age:

- **Total Lipid Amount**: For females, there was a significant negative correlation between age and the total amount of lipids, meaning older females had fewer lipids on their skin surface Sadowski, 2017 p8 . This correlation was not observed in males p8 .
- **Sebaceous Lipids**: With increasing age, the relative amounts of triacylglycerols (TAG) and diacylglycerols (DAG), which are major components of sebum, decreased Sadowski, 2017 p8 . This effect was more pronounced in females p8 . This is consistent with previous findings that sebum production decreases with age p8 .
- **Cholesterol**: As the fraction of sebaceous lipids decreased with age, the relative amount of cholesterol increased Sadowski, 2017 p8 , p8 .
- **Ceramides and Cholesterol Esters**: The relative levels of ceramides and cholesterol esters remained constant across different ages Sadowski, 2017 p8 .

The figure below from the study illustrates the changes in the relative amounts of different lipid groups with age for both males and females Sadowski, 2017 p9

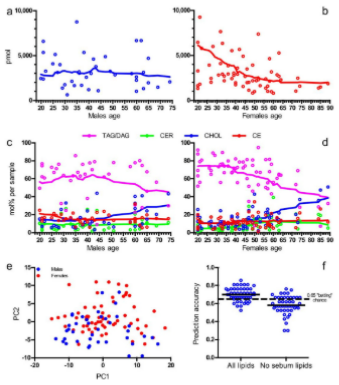

Figure 4c and 4d from Sadowski et al. (2017): Profiles of lipid groups of (c) males and (d) females of different age. Lines

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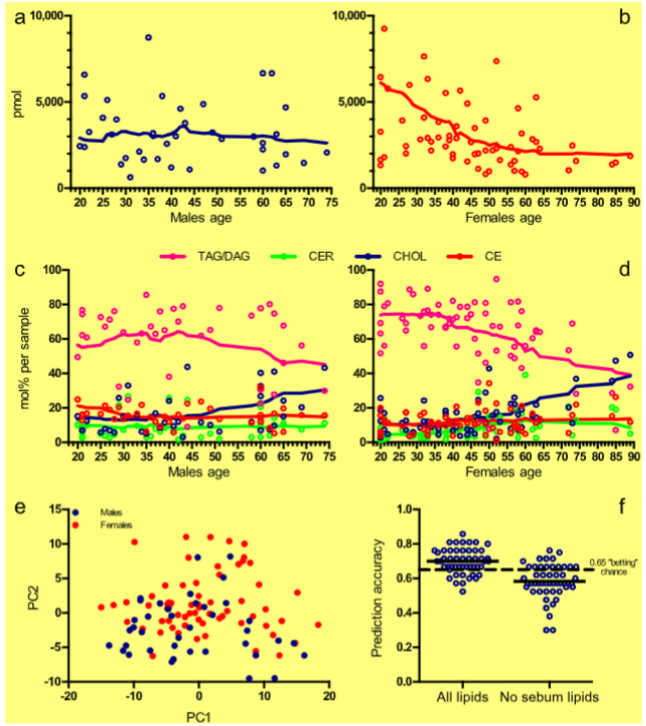

Figure 4. Inter-individual variation. (**a**,**b**) Amounts of lipids measured of (**a**) males and (**b**) females of different age (here the two most extreme pmol values are not shown to improve clarity). Lines represent 0-order polynomial smoothing function with 8 neighbours averaged. (**c**,**d**) Profiles of lipid groups of (**c**) males and (**d**) females of different age. Lines represent 0-order polynomial smoothing function with 8 neighbours averaged. (**e**) Principal component analysis of males and females of different age lipidomes with lipid sub-species as input. (**f**) Sex prediction accuracy (test error) of random forest classification with all lipid data and data excluding sebum lipids. Points show individual results of a 5 times repeated 10 times cross validation with horizontal lines representing their mean. The dashed line is the 0.65 Null Error Rate, the prediction error was based on always choosing the majority class.

among females then among males. However male and female samples could not be distinguished by their lipidomes.

This study raises important issues for future comparative skin lipidomic study design. Firstly, our study demonstrates the importance of the choice of sampling site and sampling depth. Depending on the objective of the study, these parameters along with age of the subjects must be controlled because their influence on measured lipidomes is dominant. Secondly, lipidome variability precludes the establishment of a general skin lipidome baseline, and comparisons should rather be made between adjacent sampling sites of the same subject. Therefore, in intervention studies topical drugs or agents should be applied to one skin site, while preferentially an adjacent, untreated site should be chosen as a negative control. These sites would then be tape-stripped and their lipidomes analyzed.

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SC

Create a table to compare the results of both papers regarding the twelve ceramide subclasses. Sort them by alphabet.

Here is a comparison of the results from the two studies regarding the twelve ceramide subclasses.

Ceramide Subclass	Sadowski et al. (2017) Findings	Ahlström et al. (2024) Findings
AdS (Alphahydroxy-dehydrosphingosine)	One of the less abundant ceramide subclasses Sadowski, 2017 p4 .	No significant difference was found in the amount of AdS between non-lesional atopic dermatitis (AD) skin and healthy control skin Ahlström, 2024 p4 .
AH (Alphahydroxy-6-hydroxysphingosine)	One of the less abundant ceramide subclasses Sadowski, 2017 p4 .	No significant difference was observed in AH levels between AD and healthy skin Ahlström, 2024 p4 .
AP (Alphahydroxy-phytosphingosine)	A moderately abundant ceramide subclass Sadowski, 2017 p4 .	No significant difference was found in AP levels between AD and healthy skin Ahlström, 2024 p4 .
AS (Alphahydroxy-sphingosine)	One of the less abundant ceramide subclasses Sadowski, 2017 p4 .	The amount of AS was significantly higher in the non-lesional skin of AD patients compared to healthy controls (p = 0.011) Ahlström, 2024 p4 .
EOdS (Omegahydroxy-dehydrosphingosine)	One of the least abundant ceramide subclasses, sometimes falling below the limit of detection in smaller sample amounts Sadowski, 2017 p4 .	No significant difference was seen in EOdS levels between AD and healthy skin Ahlström, 2024 p4 . It was a very low component of the EO CER subgroup (2.4%) Ahlström, 2024 p4 .
EOH (Omegahydroxy-6-hydroxy-sphingosine)	One of the less abundant ceramide subclasses Sadowski, 2017 p4 .	No significant difference was found in EOH levels between AD and healthy skin Ahlström, 2024 p4 . It was a major component of the EO CER subgroup (39.3%) Ahlström, 2024 p4 .
EOP (Omegahydroxy-phytosphingosine)	A moderately abundant ceramide subclass Sadowski, 2017 p4 .	No significant difference was observed in EOP levels between AD and healthy skin Ahlström, 2024 p4 . It was a minor component of the EO CER subgroup (6.1%) Ahlström, 2024 p4 .
EOS (Omegahydroxy-	A moderately abundant ceramide	No significant difference was found in total EOS levels between AD

Sadowski.pdf Ahlstroem.pdf

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Is this in line with what other papers report?

The findings from Sadowski et al. (2017) and Ahlström et al. (2024) present a nuanced picture that aligns with some aspects of the literature but also highlights the complexity and sometimes conflicting results in this area of research.

Ahlström et al. (2024) found that the amounts of ceramide subclasses NS, AS, NdS, and NH were significantly higher in the non-lesional skin of patients with atopic dermatitis (AD) compared to healthy controls Ahlström, 2024 p4. This specific observation is supported by other studies. For instance, a study on pediatric AD patients also found that CER[AS] and CER[NS] were elevated and correlated with disease severity Shen, 2018. Similarly, another study noted that the ratios of several ceramide subclasses, including [NH]/[NS] and [NdS]/[AS], were significantly different in the non-lesional skin of AD patients compared to healthy controls Yokose, 2020.

However, this increase in specific ceramide subclasses contrasts with a large body of research indicating that AD is generally characterized by a **deficiency in total ceramides** Imokawa, 1991 Imokawa, 2021. Specifically, studies have frequently reported significantly lower levels of ceramide 1 (EOS) and ceramide 3 (NP) in AD skin Nardo, 1998 Macheleidt, 2002. This overall deficiency is considered a primary factor in the impaired skin barrier function and dry skin seen in AD patients Imokawa, 1991 Nardo, 1998.

The discrepancy in findings can be attributed to several factors:

- **Lesional vs. Non-Lesional Skin**: The changes in lipid composition can be different in visibly inflamed (lesional) skin compared to normal-appearing (non-lesional) skin. Some studies report that ceramide changes are most pronounced in lesional skin, while others find that the non-lesional skin of AD patients already shows significant alterations Imokawa, 1991 Toncic, 2020. One study even concluded that the ceramide profiles of uninvolved skin in AD were comparable to healthy skin Farwanah, 2005.
- **Specific Ceramide Chain Lengths**: Total amounts of a ceramide subclass may not tell the whole story. Ahlström et al. (2024) noted that while total EOS levels were not different, there was a significant reduction in *long-chain* EOS ceramides in the AD group Ahlström, 2024 p1. This aligns with other research emphasizing a "hydrocarbon chain length deficiency" as a key feature of atopic skin Macheleidt, 2002.

Sadowski.pdf Ahlstroem.pdf

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Drafting texts based on your own literature

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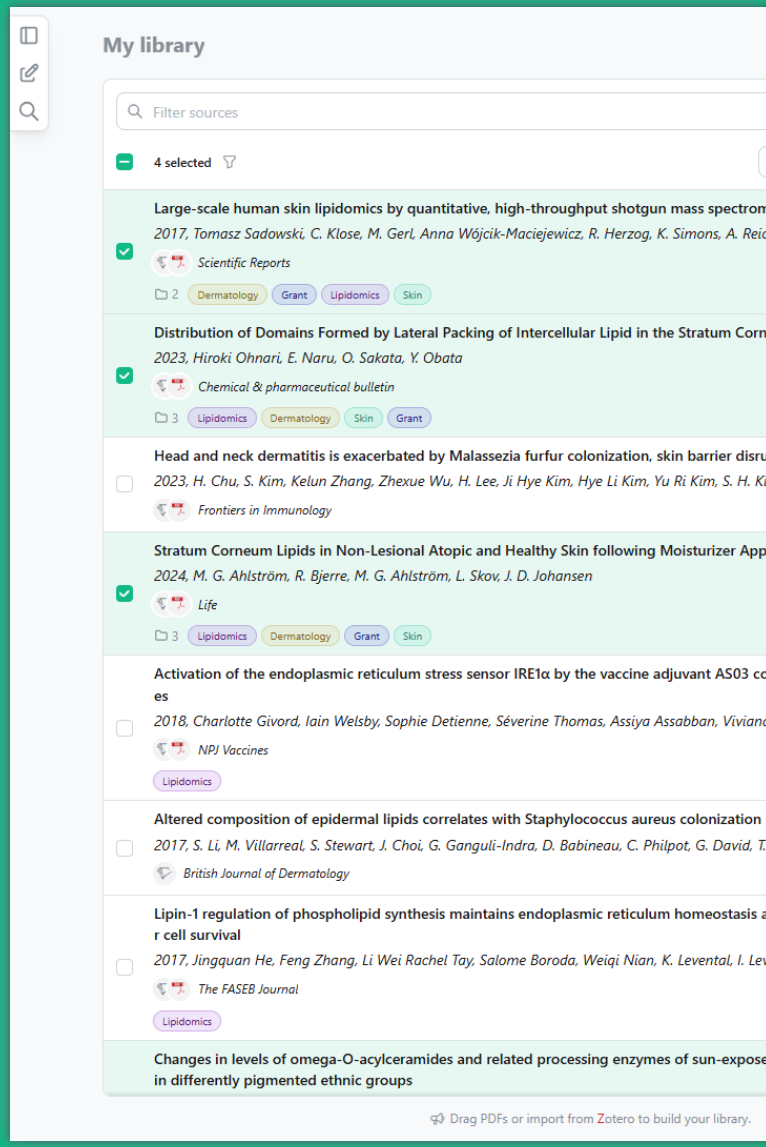

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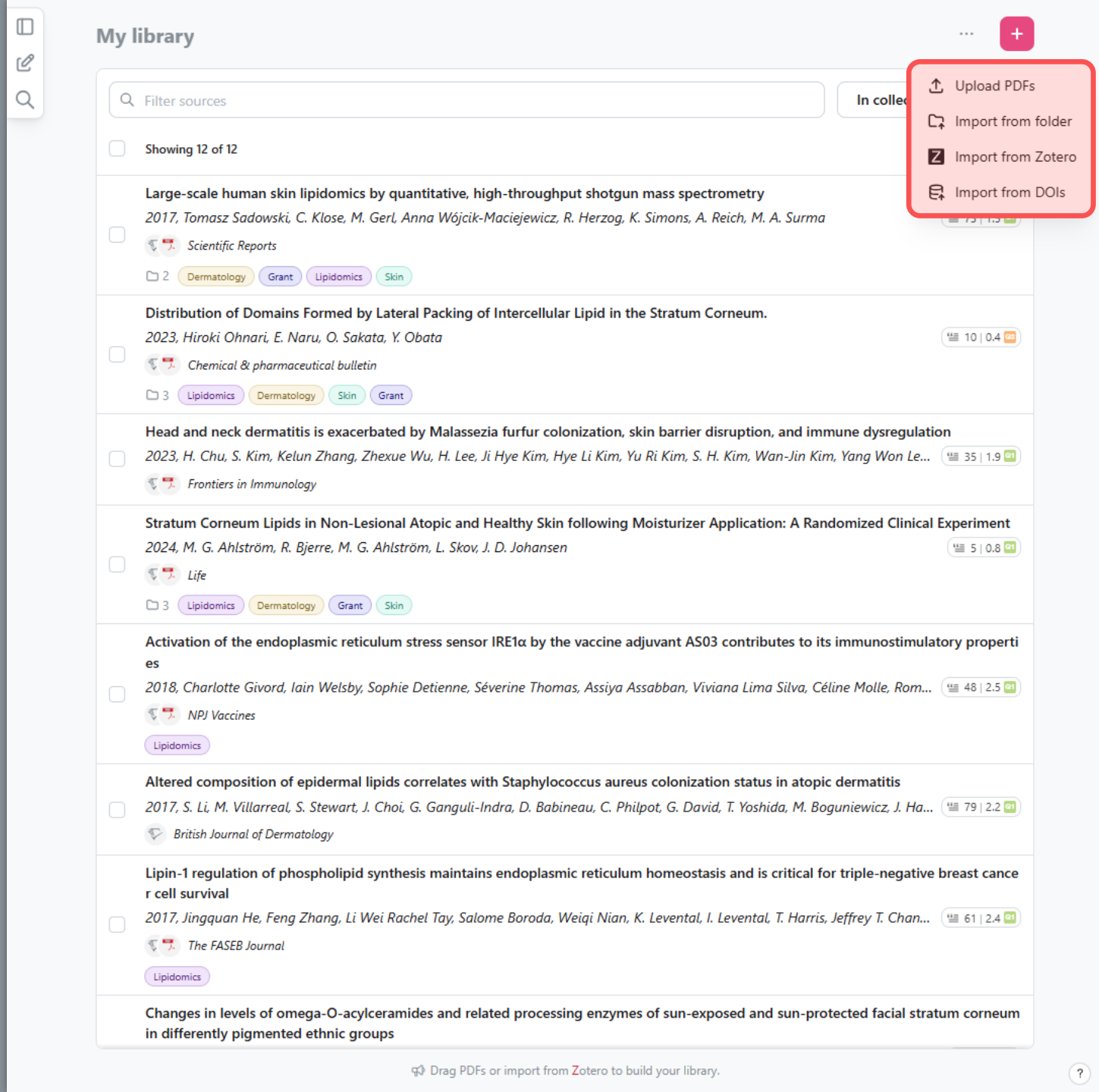

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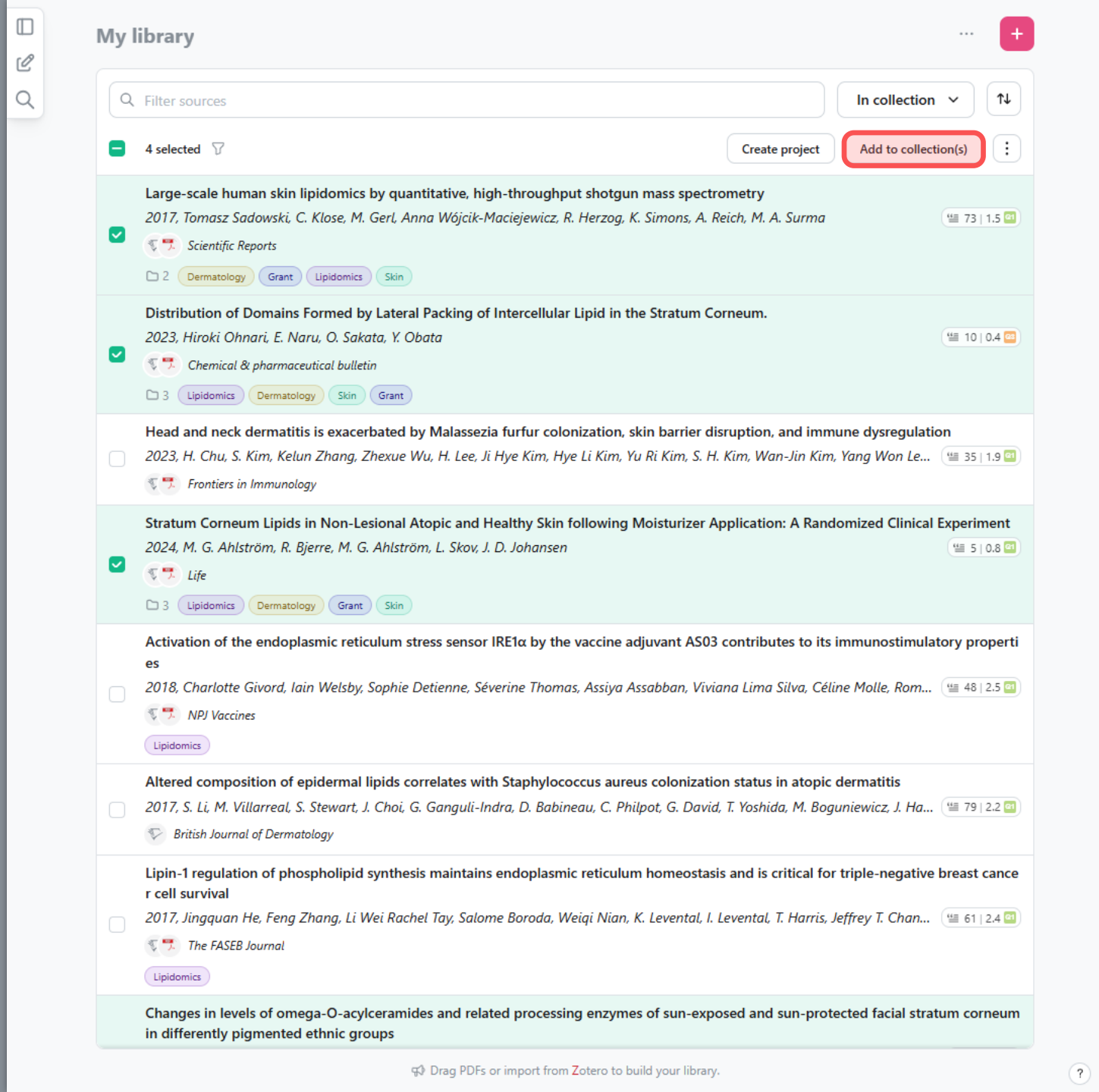

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Add a note...

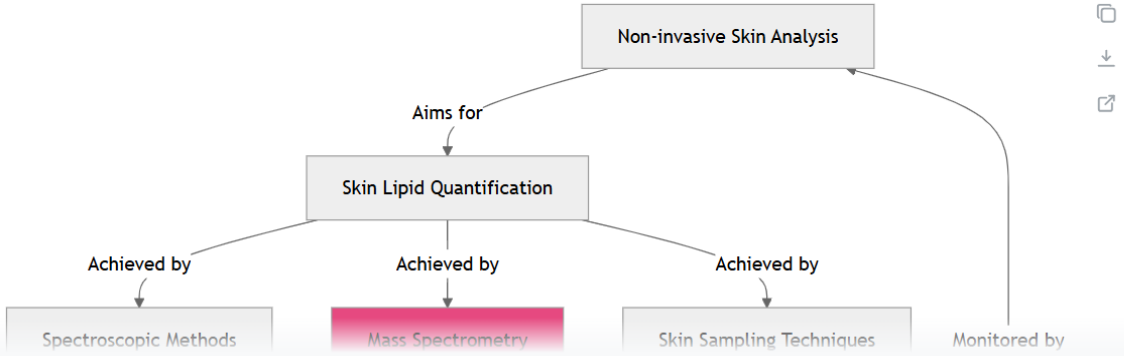
Saved chat in Dermatology

You
about 1 month ago

As a **complimentary figure** for the introduction?

Free scientific AI answers

Create diagram



Ask this project

Deep research

Replies are AI-generated and may not always be accurate.

In project "Dermatology"

Includes 230 million research papers.

Filter

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Achieved by
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Spectroscopic Methods
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Skin Sampling Techniques

Ask this project

Deep research

Replies are AI-generated and may not always be accurate.

Add sources

You have added 6 sources from your library.

All listed sources in my library

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Suggestions (1 selected)

- [ ] Lipidomics
- [x] Dermatology
- [ ] Skin
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- [x] 230 million research papers

Save

HOW TO

Add sources from your library to projects and chat with them.

3

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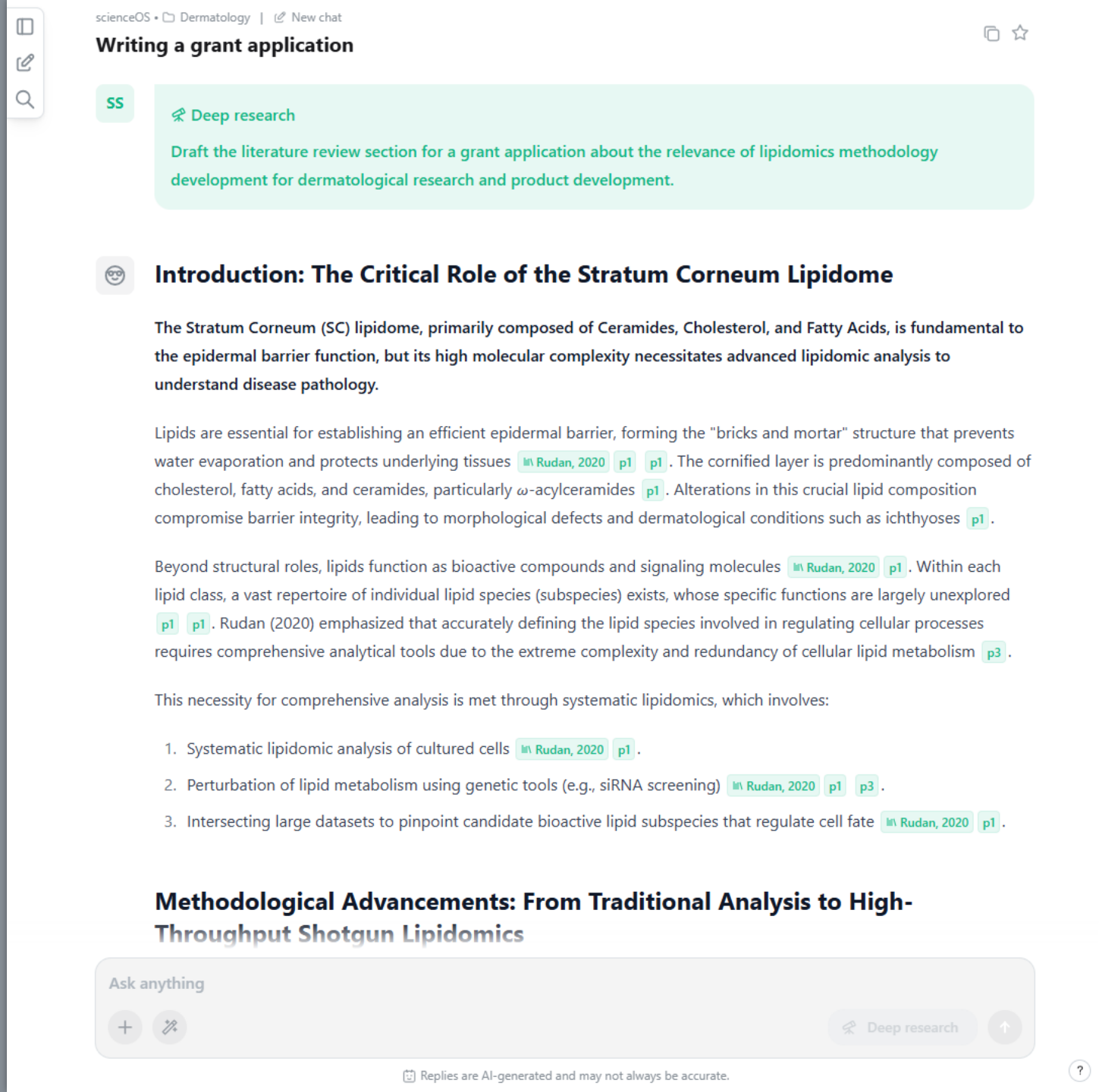

HOW TO

Review yourself: combine library answers with data from 230M papers.

4

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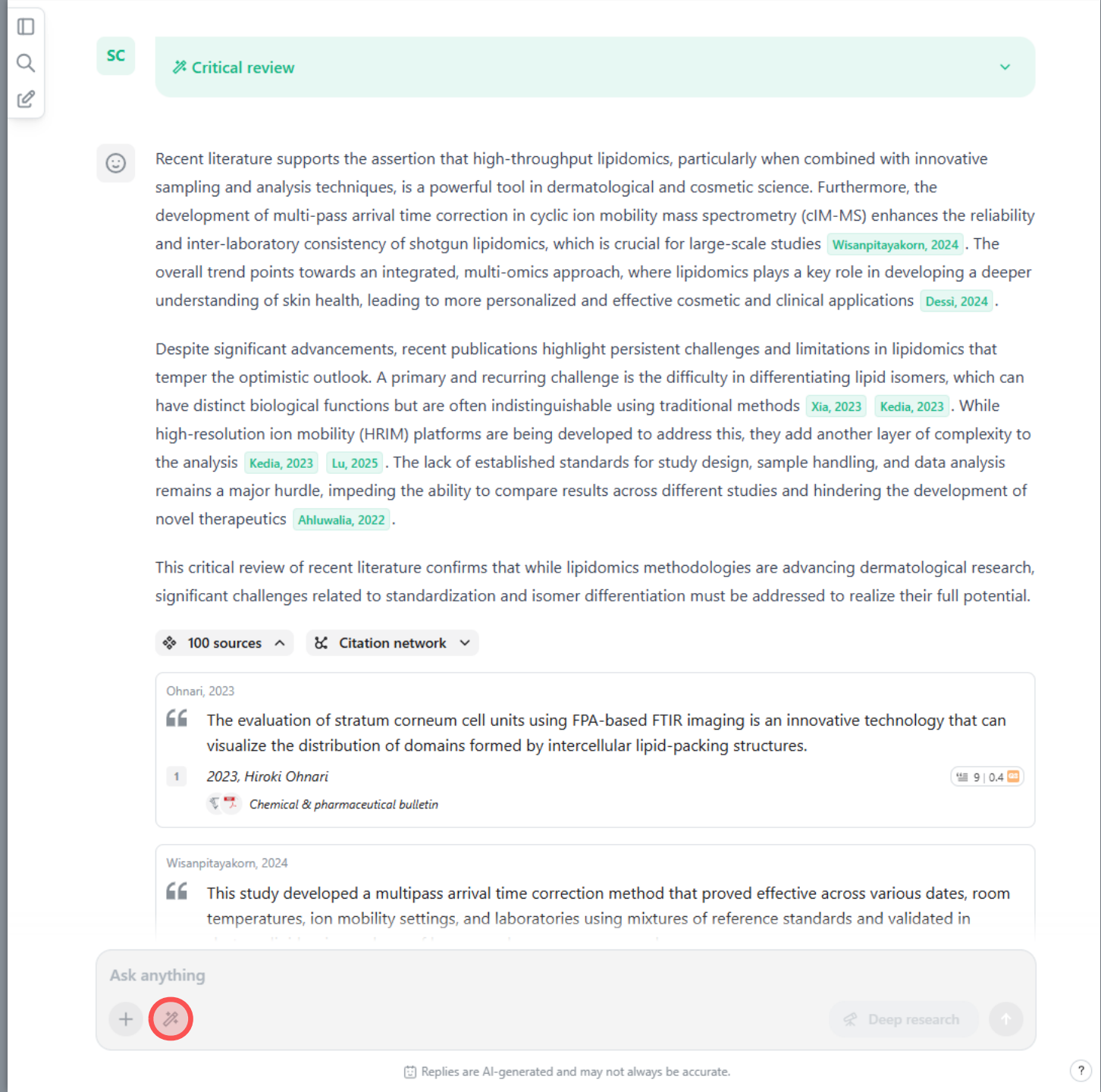

CONCLUSION

1 Get **scientific** answers.

Use the AI science chat and ‚Deep research' to quickly gain an overview about a new research area.

2 Find **related** papers.

Create citation networks and analyze how a paper has been cited.

3 **Evaluate** research papers.

Upload up to eight research papers per chat. Ask questions to them and compare results.

4 Work with your **papers**.

Import up to 4000 PDFs to your library. Draft texts and critically review yourself.

The last 30 min in 4 bullet points

Free

Access our small model and work with scienceOS for free.

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Use our free small model

- Four queries per chat
- PDF chat (text only)
- Chat with your full library
- Create citation networks

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Access our best model and all other tools of scienceOS.

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- Unlimited queries per chat
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- Access to deep research
- Run consensus analyses
- PDF bulk import (100 files)

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A fair price for a powerful tool

USER PROBLEMS

USE CASE	PROBLEM
1 Design workflows slide 4	*„I am not sure how to do s… scienceOS.“*
2 Extract data slide 8	*„I need to extract the same… from 100 or more papers.“*
3 Verify citations slide 16	*„All citation claims in my m… be bulletproof before subm…*
4 Work together slide 25	*„We are a team of reseache… stay synced with each other…*

Advanced webinar: click here!

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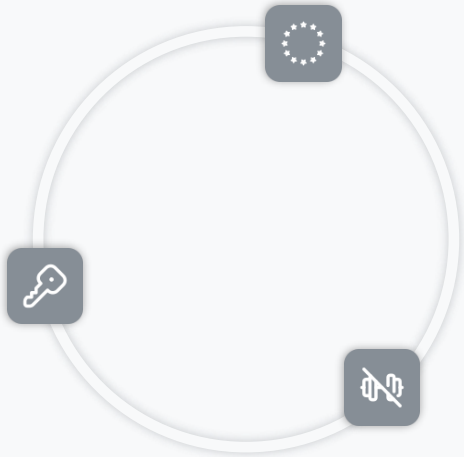
DATA SECURITY



1 We are **European**.

All our AI and machine learning models, as well as your chats, your uploaded files, and your user data are located on servers within the European Union.

2 We **do not train** on your data.

Neither your inputs (prompts, uploaded files, etc.) nor outputs (text answers, image files, etc.) are used to train scienceOS AI models.

3 We keep your data **secure**.

When you upload files, they are encrypted and accessible only to you. Other users may only access your files once you proactively share them. You control your data.

A science platform with robust data protection