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Research Article

Bibliometric Mapping and In Silico ADME Profiling of Bioactive Compounds in Germinated Oats with Antidiabetic Potential

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Abstract

Type 2 Diabetes Mellitus (T2DM) is a growing global health burden, where dietary interventions play a crucial role in prevention and management. Oats (*Avena sativa*), known for their β-glucan, phenolic compounds, and GABA content, exhibit glycaemic-regulating effects. Germination enhances the bioactive profile of oats, yet limited studies explore its impact on pharmacological properties relevant to diabetes. An integrative bibliometric and in silico pharmacokinetic analysis was conducted to explore the therapeutic potential of germinated oat compounds in diabetes management. VOSviewer software was used for bibliometric co-occurrence analysis of keywords related to oats, germination, and diabetes. Germination-enhanced compounds- β-glucan, avenanthramides, ferulic acid, and Gamma-Aminobutyric Acid (GABA), were analysed using SwissADME software for solubility, GI absorption, Blood- Brain Barrier (BBB) permeability, drug-likeness, and bioavailability. The bibliometric map revealed a lack of focused research connecting germinated oats and glycaemic control. Among the compounds, ferulic acid showed high oral bioavailability and BBB permeability. Avenanthramides had favourable drug-likeness and absorption. GABA demonstrated good solubility and GI absorption, while β-glucan showed poor oral bioavailability but potential enzyme inhibition activity. Germinated oats are underexplored in the context of diabetes. Ferulic acid and avenanthramides promise as antidiabetic agents, while β-glucan and GABA may support functional food or enzyme-targeted applications.

Keywords: ADME analysis, Bibliometric Analysis, Diabetes, Germinated oats

Abbreviations: T2DM: Type 2 Diabetes Mellitus; GABA: Gamma-Aminobutyric Acid; ADME: Absorption, Distribution, Metabolism, and Excretion; BBB: Blood-Brain Barrier; GI: Gastrointestinal; SMILES: Simplified Molecular Input Line Entry System; CYP: Cytochrome P450 (enzymes); P-gp: P-glycoprotein; TPSA: Topological Polar Surface Area; FA: Ferulic Acid; Log P: Partition Coefficient (logarithm of compound's partition between octanol and water).

Introduction

Functional foods play a crucial role in prevention and management of Type 2 Diabetes Mellitus (T2DM), a growing global health concern [1]. Oats (*Avena sativa*), rich in bioactive compounds offer antioxidant, cholesterol-lowering, and glycaemic-regulating benefits [2-5]. Germination- a traditional process involving grain soaking and sprouting, enhances these bioactive components, improving the nutritional profile and potentially supporting glucose control and oxidative stress reduction in diabetes [6-8]. This study aims to bridge the knowledge gaps of integrated studies on the specific role of germinated oats in diabetes management through two key objectives: first, to conduct a bibliometric analysis to identify thematic trends, research gaps, and emerging focus areas concerning germinated oats and diabetes; and second, to assess the pharmacokinetic

properties and drug-likeness of key bioactive compounds enhanced during oat germination using in silico tools.

Materials and Methods

Bibliometric Analysis

To understand the research landscape surrounding germinated oats and their potential antidiabetic properties, a bibliometric analysis [9,10] was conducted using Scopus, Web of Science and Science Direct databases. The following keywords were used in various combinations: oats, *Avena sativa*, germination, diabetes, glycaemic index, antidiabetic, β-glucan, GABA, and phenolics. The data extracted were exported in .csv format and analysed using VOSviewer software (version 1.6.20).

Selection of Bioactive Compounds

Based on a review of scientific literature, four bioactive compounds were identified as being significantly enhanced in oats post-germination and their reported physiological relevance in glycaemic regulation: β-glucan, avenanthramides, ferulic acid, and gamma-aminobutyric acid (GABA) [11-14].

ADME and Drug-Likeness Evaluation

To assess the pharmacokinetic behaviour and oral drug potential of the selected compounds, an in silico ADME (Absorption, Distribution, Metabolism, and Excretion) analysis was carried out using the SwissADME, a tool for early-stage drug screening and bioavailability assessment [15,16].

The chemical structures and SMILES (Simplified Molecular Input Line Entry System) structure of the four compounds were retrieved from the PubChem database and run on SwissADME for analysis. The following parameters were evaluated (Table 1):

Table 1: Study Parameters for ADME Evaluation of key bioactive compounds.

Parameter	Significance
Molecular Weight	The total mass of a compound's atoms. Ideal range for oral drugs is typically <500 Da. Higher weight may limit absorption and bioavailability. [17]
Topological Polar Surface Area (TPSA)	Indicates polarity of a molecule. TPSA <140 Å^2 is favorable for oral absorption; <90 Å^2 may allow blood-brain barrier (BBB) penetration.[18]
Gastrointestinal (GI) Absorption	Predicts likelihood of compound being absorbed through the intestine. High GI absorption is preferable for oral agents.[19]
Blood-Brain Barrier (BBB) Permeability	Indicates if compound can cross BBB. Important for CNS activity or avoiding unwanted neurological side effects.[20]
Lipinski's Rule of Five	Predicts oral bioavailability based on molecular weight, HBD, HBA, and log P. Violating >1 rule suggests poor absorption.[21]
Veber's Rule	Suggests good bioavailability if TPSA ≤140 Å^2 and ≤10 rotatable bonds. Focuses on flexibility and polarity.[22]
Egan's Rule	Combines log P and TPSA to predict oral bioavailability. Compounds outside defined range may have poor permeability.[23]
Bioavailability Score	Probability (0 to 1) of the compound being orally bioavailable. A score of 0.55 is considered moderate; 1.0 is excellent.
Synthetic Accessibility	Scaled from 1 (easy) to 10 (very difficult). Reflects ease of chemical synthesis. Lower values are preferred for formulation feasibility.
Cytochrome P450 Enzyme Inhibition	Predicts whether compound inhibits key CYP enzymes (CYP1A2, CYP2C9, CYP2C19, CYP2D6, CYP3A4). Inhibitors may lead to drug interactions or toxicity.

Figure 1 presents a schematic overview of the methodology adopted in this study, encompassing bibliometric analysis, compound selection, and ADME/drug-likeness evaluation.

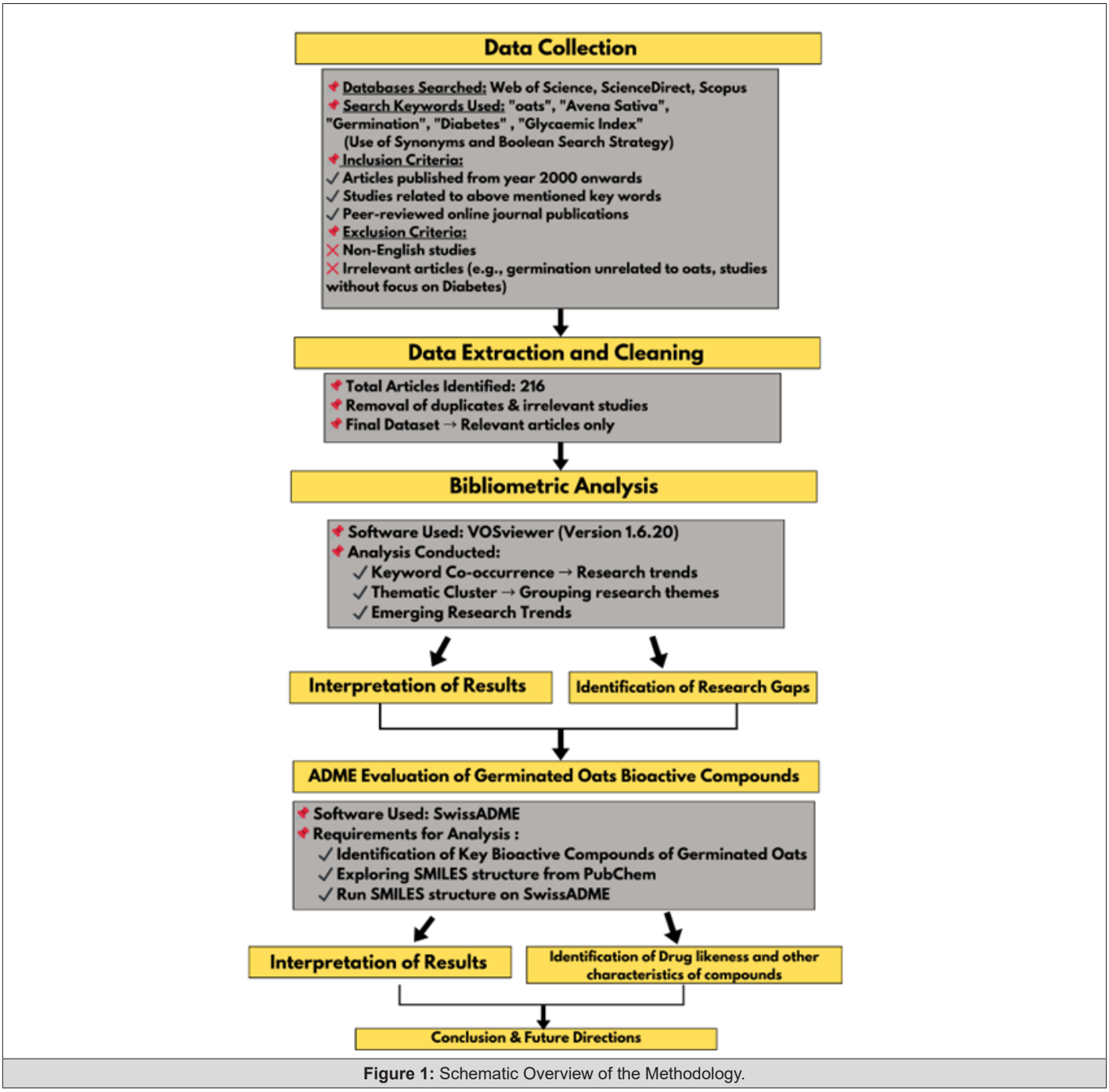

Figure 1: Schematic Overview of the Methodology.

Results

Bibliometric Analysis

The keyword co-occurrence and network structure analysis was conducted using VOSviewer, based on 147 keywords extracted from the selected literature on germinated oats and diabetes. Among these, 38 keywords met the minimum occurrence threshold of two and were included in the final network analysis. In this visualization, each node represented a keyword, with the size of the node corresponding to its frequency in the literature and the thickness of the edges indicating the strength of co-occurrence between terms.

The central and most prominent node in the network was "oats," which was thematically and spatially linked with terms such as "germination," "β-glucan," "dietary fibre," "functional properties," "flour," "systematic review," and "meta-analysis." This indicated that oats have been a major focus of research, particularly with regard to their compositional analysis, processing techniques, and health-related benefits. The strong direct connection between "oats" and "germination" further highlighted that germination has been studied as a key processing method for enhancing the nutritional and functional quality of oats (Figure 2a).

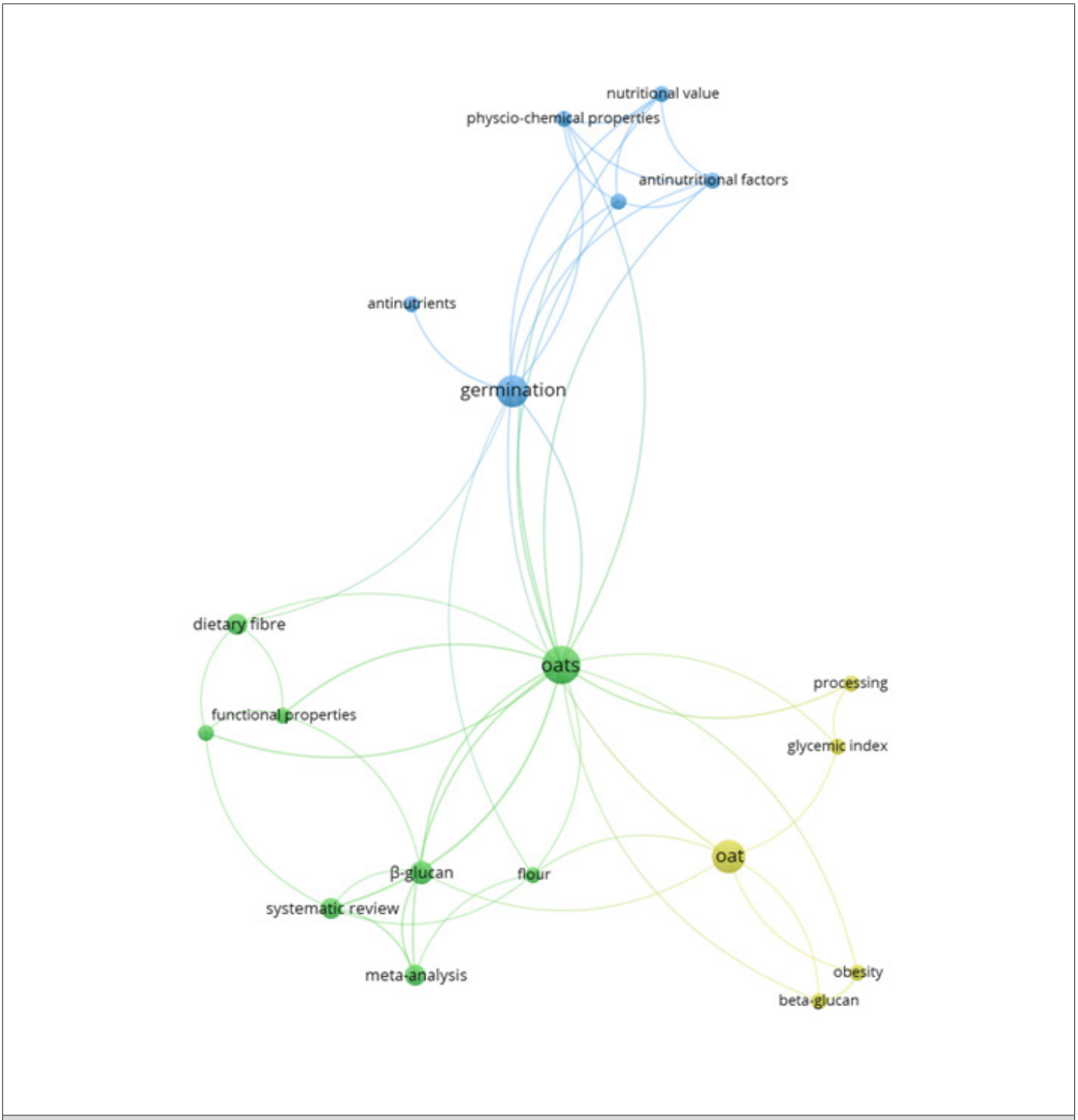
nutritional value
physcio-chemical properties
antinutritional factors
antinutrients
germination
dietary fibre
oats
processing
functional properties
glycemic index
oat
β-glucan
flour
systematic review
meta-analysis
obesity
beta-glucan

Figure 2(a):

The 38 keywords were algorithmically grouped into four distinct thematic clusters, each representing a research theme. Cluster 1 (green) centered around "oats," "β-glucan," "dietary fibre," "functional properties," and related terms, suggesting a dominant focus on compositional analysis and the functional roles of oats in nutrition. Cluster 2 (blue) contained terms such as "germination," "antinutritional factors," "nutritional value," and "physico-chemical properties," indicating a strong research emphasis on the effects of germination on the biochemical and nutritional profiles of oats.

Cluster 3 (yellow) included keywords like "glycaemic index," "obesity," "processing," and "beta-glucan," representing a health outcome-oriented theme. However, within this cluster, the connections between germination and health-related endpoints such as glycaemic index or obesity appeared to be weak or indirect. Cluster 4 (purple) was formed by the isolated node "antihyperglycaemia activity," which did not show meaningful co-occurrence with any of the other major terms, especially "germination" or "oats." This suggested that although the antihyperglycaemic potential of oats is acknowledged in some studies, it is not deeply embedded in the broader research network (Figure 2b).

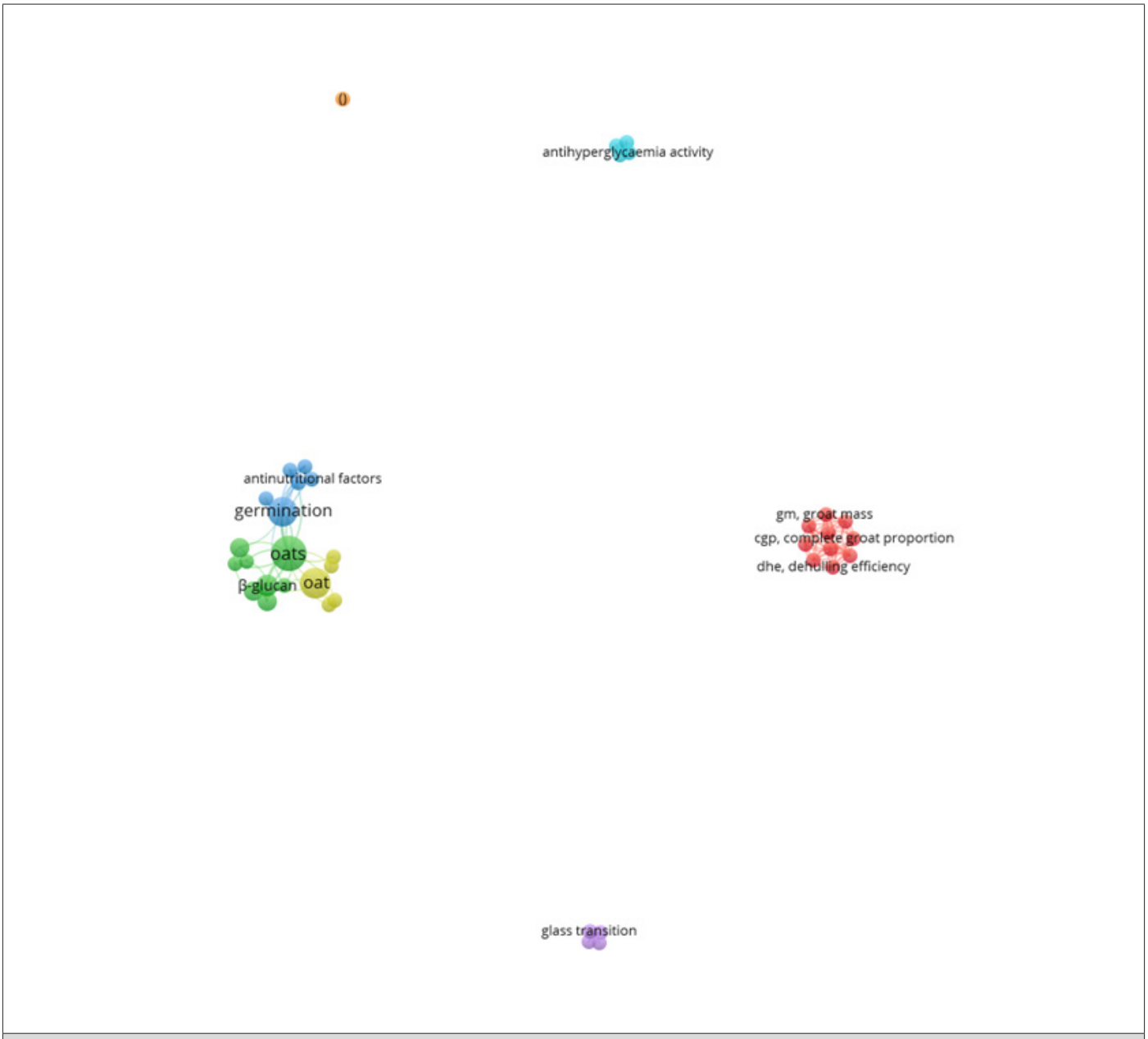

Figure 2(b)

The overlay visualization provided insights into how research themes have evolved over time. Keywords were color-coded based on their average publication year, ranging from blue (older terms) to yellow (recent terms). The analysis showed that terms like "germination," "β-glucan," "glycaemic index," and "obesity" have become more prominent in recent years (2015 onwards), suggesting a growing interest in studying oats from a metabolic health and processing enhancement perspective. On the other hand, terms such as "dietary fibre," "functional properties," and "processing" appeared in green, reflecting their mid-range temporal prominence, while some earlier general terms were shown in blue, indicating foundational but aging areas of research (Figure 2c).

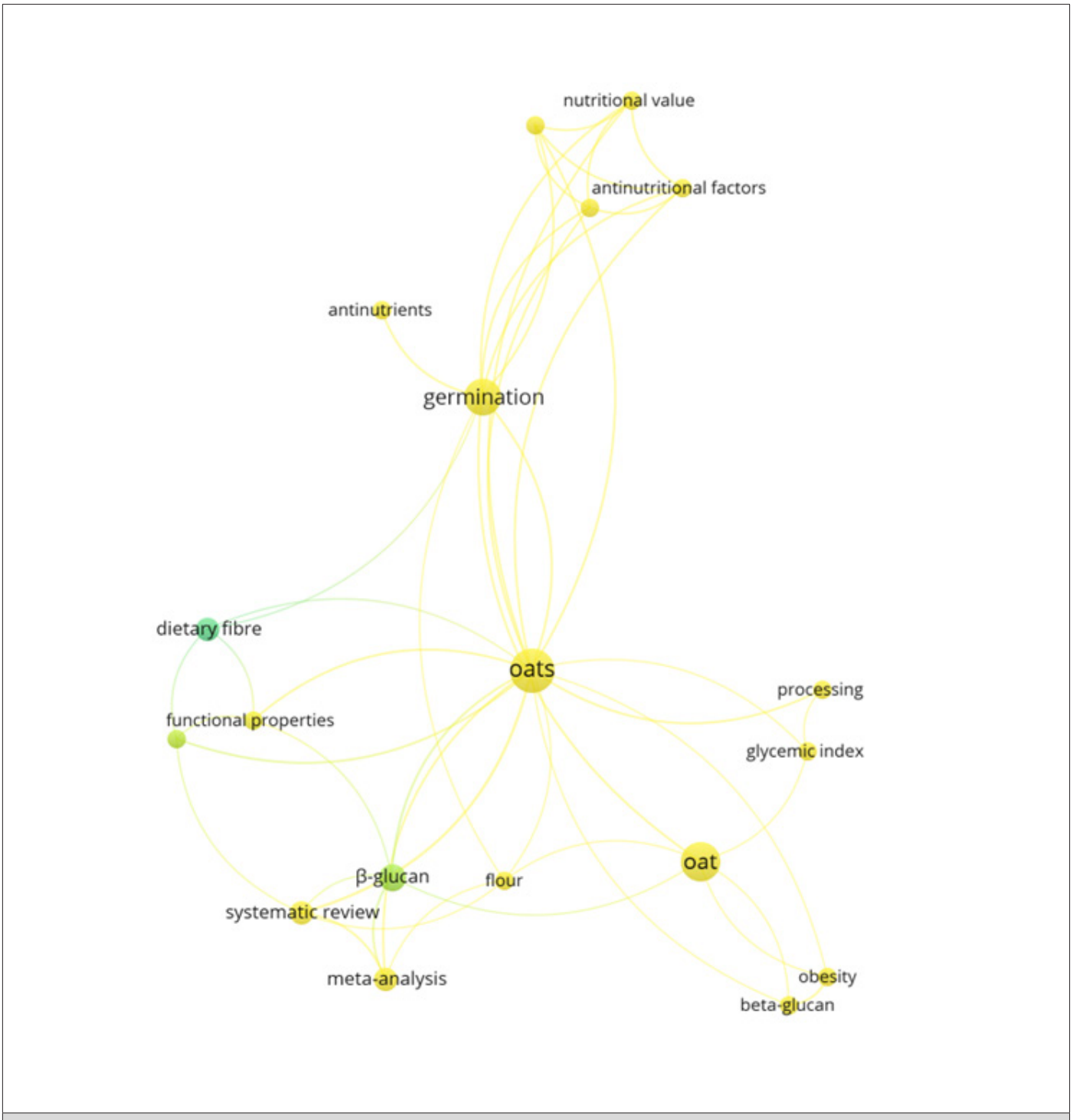

Figure 2(c)

Density visualization was used to assess the intensity and frequency of research activity. Keywords located in yellow regions of the map indicated high-frequency and high-density research zones. These included "oats," "β-glucan," "meta-analysis," "functional properties," and "glycaemic index," confirming that these areas are well-established and have been extensively studied. Green zones represented moderate research interest and contained keywords like "germination," "antinutritional factors," and "nutritional value," which are increasingly being investigated, particularly for their relevance to functional food development. Blue areas signified low-density regions, including peripheral or under-represented terms such as "antihyperglycaemia activity," underscoring gaps in literature connecting germinated oats directly with glycaemic control (Figure 2d).

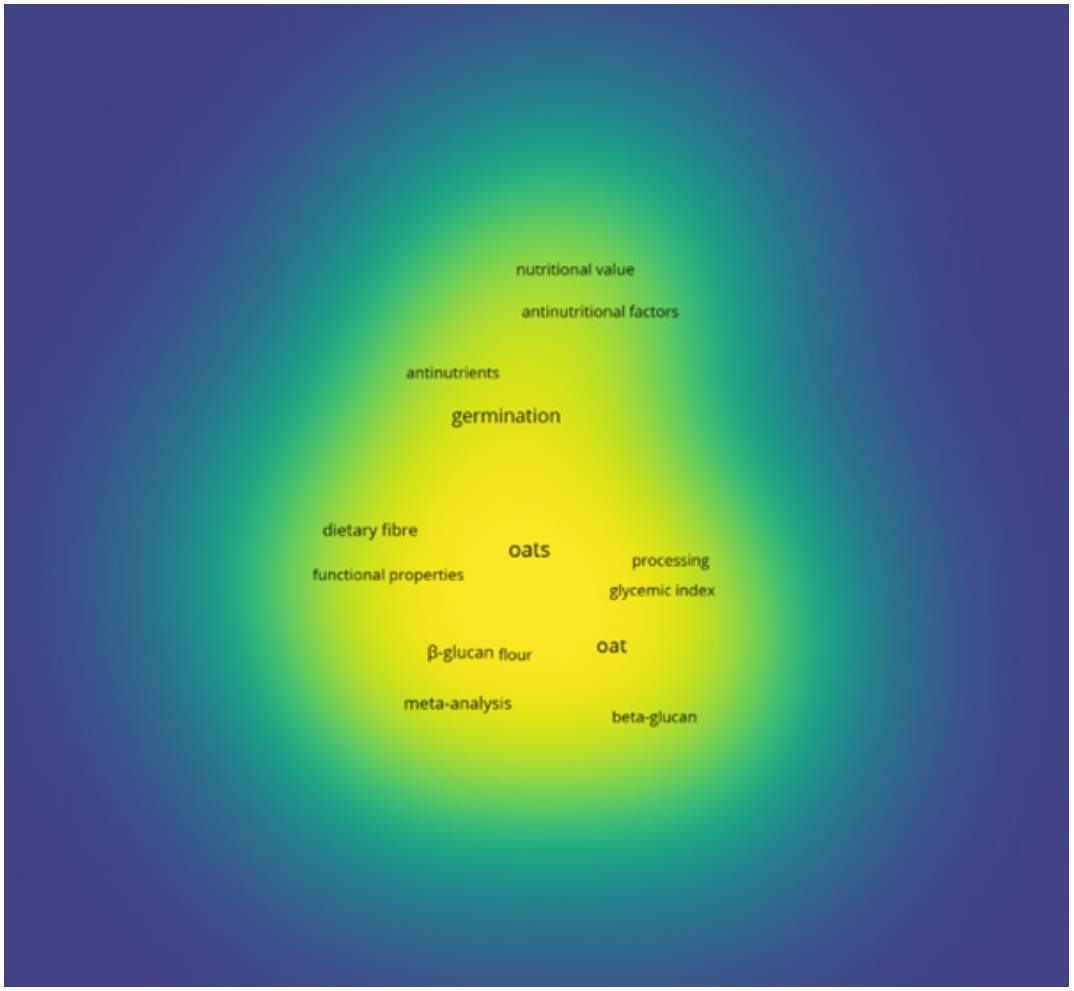

Figure 2(d)

Figure 2: Bibliometric Visualizations from VoSViewer Software.

ADME Analysis

The ADME (Absorption, Distribution, Metabolism, and Excretion) analysis of four bioactive compounds- β-glucan, avenanthramides, ferulic acid, and GABA, was conducted using the SwissADME tool. These compounds, known to increase during oat germination, were evaluated for their physicochemical properties, pharmacokinetics, drug-likeness, bioavailability, and synthetic accessibility to determine their potential as antidiabetic agents.

Table 2 summarizes the pharmacokinetic and drug likeness properties of the four key bioactive compounds of germinated oats (Table 2)

Table 2: Summary of properties of four key bioactive compounds of germinated oats.

Parameter	β-Glucan	Avenanthramides	Ferulic Acid	GABA
GI Absorption	Low	High	High	High
BBB Permeant	No	No	Yes	No
P-gp Substrate	No	No	No	No
CYP Inhibition	None	None	None	None
Log Kp (Skin Permeation)	–8.34 cm/s	–6.51 cm/s	–6.41 cm/s	–9.18 cm/s
Water Solubility	Soluble	Soluble	Soluble	Highly soluble
Lipinski Rule	No; 3 violations	Yes; 0 violations	Yes; 0 violations	Yes; 0 violations
Bioavailability Score	0.17	0.55	0.85	0.55
Synthetic Accessibility	6.78	3.11	1.93	1
TPSA (Å²)	180.57	116.14	66.76	63.32

Discussion

Bibliometric Analysis

"Oats" appears centrally in co-occurrence networks, strongly linked with terms like "β-glucan," "functional properties," "dietary fibre," and "systematic review," indicating a mature research area focused on metabolic health benefits such as cholesterol-lowering and satiety.

"Germination" also emerges as a relevant theme, mostly associated with improved nutritional value, reduced antinutritional factors, and altered physico-chemical properties. However, it remains largely disconnected from clinical or health-related terms such as "diabetes" or "glycaemic index," suggesting that its potential health benefits, particularly for glycaemic control, are underexplored. Terms like "glycaemic index" and "ant hyperglycaemia activity" appear only peripherally or in isolation, reinforcing the gap between compositional studies on germinated oats and their health outcomes. Despite β-glucan's known role in modulating postprandial glucose levels, its enhancement through germination and associated clinical impacts remain insufficiently studied.

Density mapping reveals that while oats and β-glucan are well-studied, germination lies in a moderate-density zone, highlighting a clear opportunity for integrative research that connects germination processing with functional health outcomes.

ADME Analysis

β-Glucan, while effective in modulating glucose levels through its fiber-related viscosity, demonstrated poor oral bioavailability due to its high molecular weight and polarity.

Avenanthramides showed excellent pharmacokinetic properties, including high GI absorption and minimal toxicity, passing all major drug-likeness rules. With a bioavailability score of 0.56, they are strong candidates for oral antidiabetic therapies or enriched foods. Ferulic acid emerged as the most drug-like, with high absorption, good BBB permeability, and a bioavailability score of 0.85. GABA had moderate bioavailability (0.55) and excellent water solubility but limited permeability and drug-likeness due to its small size and polarity.

Overall, ferulic acid and avenanthramides are suited for drug development, while β-glucan and GABA are better positioned for nutraceutical and functional food applications. A combined formulation approach may offer the most effective strategy for diabetes management using germinated oat components.

Conclusion

This study integrated bibliometric analysis and ADME profiling to evaluate the antidiabetic potential of germination-enhanced oat compounds. While literature strongly supports the nutritional benefits of oats and germination, there remains a clear research gap linking germinated oats to glycaemic control. ADME analysis revealed ferulic acid and avenanthramides as promising oral drug candidates, while β-glucan and GABA showed potential for functional food applications due to their safety and biochemical relevance despite pharmacokinetic limitations.

Future research should focus on conducting in vitro and in vivo validation of antidiabetic effects of these compounds. Synergistic formulations may be investigated combining multiple bioactives. Clinical trials may be explored to assess efficacy of germinated oat-based functional foods or nutraceuticals in diabetic populations. Such multidimensional approaches will help bridge the gap between nutritional science and metabolic disease management.

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Conflict of Interest

Authors declare no conflict of interest.

Author Contributions

a) Conceptualization: RP, AKS

b) Intellectual content definition: RP, AKS

c) Data acquisition: AKS

d) Data analysis and visualization: AKS

e) Manuscript – original draft: AKS

f) Manuscript – review and editing: RP, AKS

g) Final approval of manuscript: RP, AKS

h) Supervision: RP

All authors have read and approved the final manuscript.

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