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Framing thematic trends around computational methods research in health sciences

Delineando las tendencias temáticas en torno a la investigación de métodos computacionales en ciencias de la salud

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ABSTRACT

In this study, we adopted the term co-occurrence analysis method to explore the thematic trends in the literature regarding computational methods applied to health science. We will outline the key topics and subtopics that characterize this area of research. The Visualization of Similarities (VOS) algorithm was utilized to represent the relationships between keywords, identifying thematic clusters. Five clusters were identified: computational methods and modeling, computational chemistry and molecular dynamics, computational biology and data analysis, computational methods and biological models, and computational modeling and drug design. The study indicates that integrating computational methods in health sciences is a continuously expanding field. Key applications include modeling biological processes, simulating molecular interactions, and optimizing medical treatments. The various clusters analyzed demonstrate that computational tools enhance the exploration of biomedical phenomena and improve the accuracy of diagnoses, the personalization of therapies, and the efficiency of pharmaceutical research.

Keywords: computational methods; health sciences; health informatics; term co-occurrence analysis; bibliometrics

RESUMEN

En este estudio, adoptamos el término método de análisis de coocurrencia para explorar las tendencias temáticas en la literatura sobre métodos computacionales aplicados a las ciencias de la salud. Esbozamos los temas y subtemas clave que caracterizan esta área de investigación. Se utilizó el algoritmo Visualization of Similarities (VOS) para representar las relaciones entre palabras clave en sus grupos temáticos. Se detectaron cinco grupos: métodos computacionales y modelización, química computacional y dinámica molecular, biología computacional y análisis de datos, métodos computacionales y modelos biológicos, y modelización computacional y diseño de fármacos. El estudio indica que la integración de métodos computacionales en las ciencias de la salud es un campo en continua expansión. Las aplicaciones clave incluyen la modelización de procesos biológicos, la simulación de interacciones moleculares y la optimización de tratamientos médicos. Los diversos grupos analizados demuestran que las herramientas computacionales mejoran la exploración de los fenómenos biomédicos y aumentan la precisión de los diagnósticos, la personalización de las terapias y la eficiencia de la investigación farmacéutica.

Palabras clave: métodos computacionales; ciencias de la salud; informática médica; análisis de coocurrencia de términos; bibliometría

1. INTRODUCTION

Advanced computational methods include various categories, such as machine learning and numerical simulation, which employ complementary methodological approaches. While machine learning focuses on pattern recognition and data prediction, numerical simulation is part of mathematical modeling, providing approximate solutions to complex problems. Together, these techniques enable the analysis and prediction of systems through mathematical models, algorithms, and advanced computational tools (Krzywanski et al., 2024; Oscuvilca Tapia et al., 2024). According to Giorgetti et al. (2012), computational methods range from systems biology to bioinformatics and molecular simulation, assisting in analyzing characteristics that are difficult or impossible to measure directly.

The substantial generation of scientific literature highlights these topics' importance from theoretical and practical perspectives. Bibliometrics, as a method for analyzing scientific literature (Vaishya et al., 2024), helps to reveal intrinsic patterns across various research areas. This led Shukla et al. (2020) to perform a bibliometric analysis of the journal *Computer Methods and Programs in Biomedicine* (CMPB) from its inception in 1970 to 2017, to identify trends in computational biomedical research. By examining keyword co-occurrence, co-citation, and bibliographic coupling, the authors demonstrated that CMPB is among the most influential publications in the field, with strong connections to *IEEE Transactions on Biomedical Engineering* and *IEEE Transactions on Medical Imaging*. The findings suggest that, in the past decade, machine learning has dominated health research, particularly in medical image processing and analysis. Furthermore, the journal's international character is emphasized by a growing volume of articles from Europe, the USA, and Asia.

In another measure, Solorzano and Plevris (2022) present a bibliometric analysis based on data concerning the use of computational intelligence (CI) techniques in modeling and simulating structures. By utilizing a database of approximately 8,000 publications from 1990 to 2022, the authors identified research trends and gaps in the literature, emphasizing the increasing adoption of alternative methods to the Finite Element Method (FEM) to address the complexity of modern constructions. The results indicate that strategies based on CI are gaining traction in structural engineering due to their ability to tackle complex numerical problems, thereby enhancing the precision and efficiency of structural design.

Meanwhile, Faust (2018) analyzes the thematic evolution in the journal *Computers in Biology and Medicine (CBM)* from 1990 to the present by examining keywords provided by the authors. Through automated term clustering, the author identified Support Vector Machine (SVM), Electroencephalography (EEG), and image processing as the primary research areas. The findings reveal a shift in artificial intelligence methods, highlighted by the replacement of Artificial Neural Networks (ANN) with SVM in 2006, which has become the most relevant algorithm in CBM.

In this study, we will adopt the term co-occurrence analysis method to explore the thematic trends in the literature regarding computational methods applied to health science. We will outline the key topics and subtopics that characterize this area of research.

2. MATERIALS AND METHODS

In this study, we used a bibliometric approach that employs the co-occurrence of terms to identify the thematic structure of research on computational methods applied to health. The data were extracted from the Scopus database using the following search strategy: TITLE (“computational method”) AND PUBYEAR > 1946 AND PUBYEAR < 2025 AND (LIMIT-TO (DOCTYPE, “ar”) OR LIMIT-TO (DOCTYPE, “cp”) OR LIMIT-TO (DOCTYPE, “re”) OR LIMIT-TO (DOCTYPE, “ch”) OR LIMIT-TO (DOCTYPE, “cr”)).

The records obtained were exported in CSV format and processed using VOSviewer software. We normalized each term, unifying plurals and singulars, and removed generic words with little semantic weight. A minimum threshold of ten occurrences was established for a term to be included in the map. The

Visualization of Similarities (VOS) algorithm was utilized for the graphical representation of the relationships between keywords, identifying thematic clusters. In this exercise, we applied metrics of link strength and occurrence frequency to identify the most relevant terms and their connections.

Based on the co-occurrence analysis, we identified both generic and specific thematic clusters—specifically, topics and subtopics. These clusters were interpreted manually, with representative names assigned according to the predominant terms within each group. The results were illustrated on a map featuring 1,074 nodes. Larger nodes indicated terms with higher frequencies of appearance, and stronger links showcased significant relationships between the keywords.

3. RESULTS AND DISCUSSION

We present a detailed analysis of the clusters identified in the term co-occurrence map (Figure 1), highlighting the themes and subthemes they represent (Table 1).

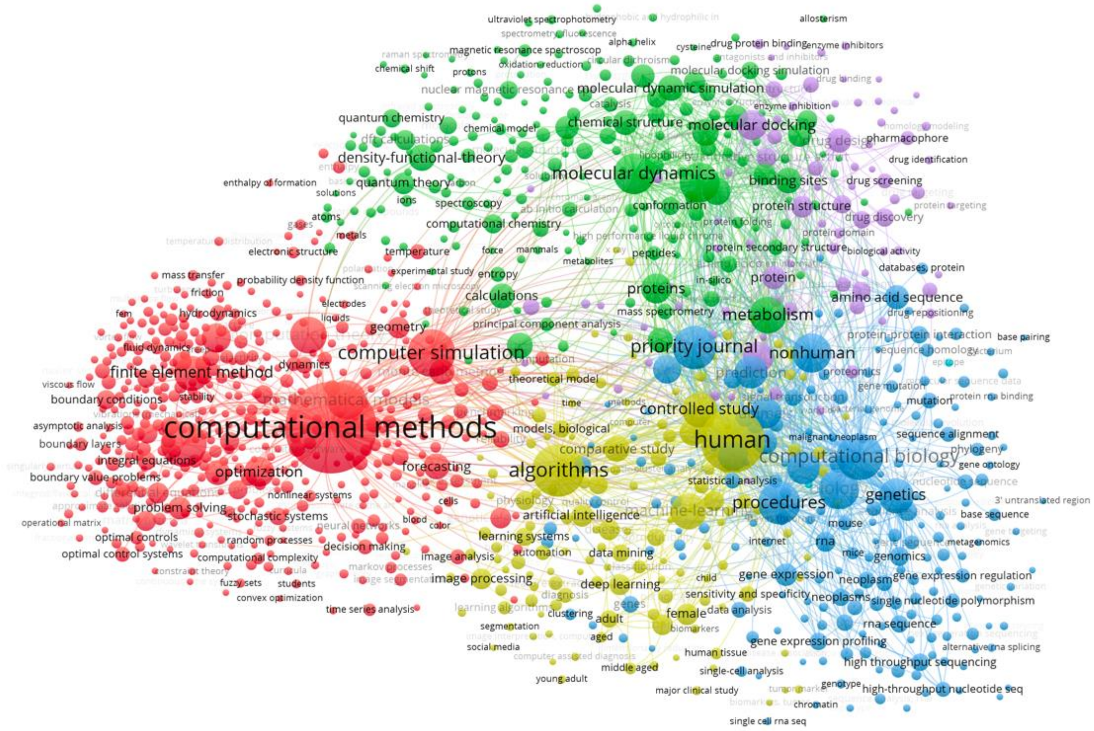

Figure 1. Clustering map derived from the co-occurrence analysis of computational methods research in health sciences

Cluster 1: "Computational methods and modeling"

This cluster is the largest on the entire map and illustrates a highly interconnected network of keywords related to the application of computational methods in biomedical research, biological systems modeling, and medical processes optimization. Here lie the terms that most broadly represent the literature on the subject. The terms with the highest connectivity and occurrence are "computational methods" (10,081), "computer simulation" (4,613), "mathematical models" (2,605), "numerical methods" (2,287), and "computation theory" (1,745). Their presence indicates that computational techniques play a crucial role in tackling biomedical problems through digital simulations, numerical modeling, and advanced algorithms (Piana, 2009; Lin, 2022).

The term "computational methods" (10,081) establishes the strongest connections with several subdisciplines in bioengineering and medical informatics. It has a significant link to "computer simulation"

(4,613). This thematic association reflects the critical role of computer simulations in studying physiological processes, evaluating treatments, and optimizing medical devices (Cheng et al., 2019; Wu, Krishnan & Ghoraani, 2022). Additionally, the relationship with “numerical methods” (2,287) and “finite element method (FEM)” (1,365) indicates a substantial presence of numerical techniques for solving differential equations in modeling biological structures and tissues (Usyk & McCulloch, 2003; Bardini & Di Carlo, 2024). Conversely, the high connectivity of “mathematical models” (2,605) with “biomechanics” (1,231), “tissue engineering” (1,119), and “blood flow” (1,034) underscores the application of mathematical models in simulating biological systems. Meanwhile, the connection with computational fluid dynamics (CFD) (1,112) highlights the importance of simulating flows in organs and circulatory systems.

The term computation theory (1,745) is closely linked to machine learning (1,563) and artificial intelligence (1,489). This connection may arise from the increasing application of machine learning techniques in the analysis of medical data (Ghassemi et al., 2020). These methodologies aid in developing assisted diagnosis systems, treatment personalization, and predictive models for diseases. Furthermore, it is essential to note that the connection to “data visualization” (1.003) and “image analysis” (1.012) underscores research into processing medical images, such as magnetic resonance imaging and computed tomography (Angenent, Pichon, & Tannenbaum, 2006; Tang, 2019).

We identified a group of keywords that indicate, due to their relationship, that this cluster has subthemes (ST). We named ST 1 of this cluster “mathematical modeling and simulation of biological processes," based on the presence of terms such as “mathematical models” (2,605), “numerical simulation” (1,312), and “partial differential equations” (980). These terms reflect techniques that are essential for simulating living tissue, predicting cell behavior, and modeling cardiovascular systems, for example. ST 2 is “fluid dynamics and blood flow analysis," signified by the presence of terms like “computational fluid dynamics (CFD)” (1,112), closely related to “blood flow” (1,034), and “vascular modeling” (968), indicating that these methods are widely used to analyze flow dynamics in arteries and predict thrombus or aneurysm formation. The third ST pertains to “biomechanics and tissue modeling," indicated by the keywords “biomechanics” (1,231) and “tissue engineering” (1,119), which are closely associated with simulating the mechanical response of biological tissues and developing computational models for designing implants and biomaterials. For instance, methods like the finite element method (FEM) (1,365) are used to analyze tissue deformation under mechanical loads and enhance the efficiency of prostheses and medical devices (Boccaccio et al., 2011).

ST 4 addresses “artificial intelligence and medical data analysis," underscored by the significant connection among terms such as “machine learning” (1,563), “artificial intelligence” (1,489), and “big data” (1,232). Here, we encounter techniques that aid in the development of diagnostic algorithms, the identification of patterns in clinical data, and the personalization of medical treatments based on a patient's genetic profile. Additionally, TS 4 is closely related to the “visualization of data and processing of medical images," as shown by the frequency of terms like “image analysis” (1,012), “data visualization” (1,003), and "computed tomography” (986). These techniques enhance the accuracy of disease diagnoses through the segmentation and reconstruction of 3D medical images, thereby improving the interpretation of clinical results (Udupa, 2005; Poiate et al., 2011).

Cluster 2: “Computational chemistry and molecular dynamics”

This cluster represents a subject area where computational chemistry, molecular dynamics, and metabolism seem to play a fundamental role. The most frequently co-occurring term in the network is “chemistry” (5,049). Its relationship with “molecular dynamics” (4,258) indicates that dynamic simulation methods are essential for predicting the behavior of molecules in biological environments. Similarly, the strong presence of “metabolism” (4,604) suggests a connection with metabolic studies that seek to understand how chemical reactions in the body can be influenced by pharmacological therapies and biomolecules (Bonafe et al., 2018).

Within the cluster, the connection between "molecular models" (2,564) and “proteins” (2,588) underscores the approach taken in the literature on computational modeling for analyzing proteins and their behavior in cellular environments. The link between “ab initio calculations" (412) and “quantum mechanics” (1,015) further illustrates the significance of theoretical methods in predicting molecular structures and optimizing drugs through quantum mechanics calculations (Mazurek, Szeleszczuk, & Pisklak, 2020).

In this cluster, TS 1: “molecular modeling and computational simulation” is evident from the presence of terms such as "molecular models" (2,564), “molecular docking” (1,976), and “computational chemistry” (1,863), which highlight the importance of computational tools in predicting biomolecular interactions. These techniques are crucial for identifying new drugs and assessing the structural stability of chemical compounds in biological environments (Jiao et al., 2021). In TS 2: “molecular dynamics and quantum mechanics applied to biochemistry," there is a strong correlation between “molecular dynamics” (4,258) and “quantum mechanics” (1,015). It is important to note that employing these methods to model proteins and enzymes supports the prediction of molecular interactions and enhances our understanding of the mechanisms underlying chemical reactions in living organisms (Quesne, Borowski, & de Visser, 2016; Souza et al., 2017).

A third subtopic, “metabolism and computational biochemistry," is highlighted by the significance of the term “metabolism” (4,604) and its co-occurrence with “biochemical networks” (1,748) and “systems biology” (1,536). This emphasizes the growing importance of computational methods in integrating experimental data to model complex metabolic processes. Meanwhile, TS 4, “protein-ligand interactions and drug design," arises from the connections between keywords such as “proteins” (2,588), “ligand binding” (1,879), and “drug discovery” (1,690). Lastly, TS 5, “computational chemistry in biomedical materials," illustrates the potential application of the technique “ab initio calculation” (412) alongside “density functional theory (DFT)” (876). This highlights research focused on predicting the electronic and structural properties of biomaterials, which is crucial for developing medical devices, therapeutic nanoparticles, and biocompatible coatings.

Cluster 3: “Computational biology and data analysis”

This cluster reflects the increasing significance of computational biology, genetic analysis, and the utilization of computational models to interpret biological data in the context of health. The most frequently co-occurring term in the network is “computational biology” (7,038), which connects the most terms within the cluster. Its strong relationship with “genetics” (4,117) and “bioinformatics” (2,882) suggests that the analysis of genomic information and the application of computational algorithms are fundamental pillars in this discipline.

A key concept in this cluster is “animals” (3,025), which implies that many computational biology studies incorporate model organisms like mice to grasp genetic and evolutionary processes. Its association with “gene expression” (3,978) signifies that animal models are essential in biomedical research, confirming genetic findings and assessing therapeutic interventions.

Among the subthemes of this cluster, we see TS 1, “gene expression analysis," due to the connection between the terms “genetics” (4,117), “gene expression” (3,978), and “sequence analysis” (3,245). This reflects an area related to the application of computational models in exploring the genetic code and gene regulation (Wang, 2008). ST 2 pertains to “bioinformatics and big data," which we infer from the presence of the term “bioinformatics” (2,882), strongly linked to “data analysis” (3,487) and “machine learning” (3,212). Meanwhile, ST 3 refers to the “prediction of biological phenomena." The key term “prediction” (3,459) indicates that computational models are utilized to predict biological structures and functions, as well as cellular and physiological responses to external stimuli. Its association with “computational models” (2,891) and “systems biology” (3,126) suggests a focus on the mathematical representation of biological networks and metabolic processes. Lastly, “computational evolutionary and phylogenetic biology” represents TS 4, due to the presence and connection between the terms “phylogenetics” (2,951), “evolutionary biology” (2,805), and “molecular evolution” (2,479).

Cluster 4: “Computational methods and biological models”

In cluster 4, the most influential term is “support vector machines” (1,273), a classification technique used in medical data analysis. Its strong connection to “biological model” (1,184) and “models, biological” (969) indicates that these methods are employed to represent physiological processes and simulate diseases. Furthermore, the mention of “diseases” (1,020) highlights the importance of these approaches in studying pathologies and their progression. Another key concept is “reproducibility” (1,016), which is closely linked to “data analysis” and “statistical models.” This emphasizes an area where computational techniques are being explored to ensure the reliability of results obtained in clinical research.

The first topic segment (TS) is closely linked to “computer modeling in biology and medicine." Here, we notice a connection between the terms “biological model” (1,184), “models, biological” (969), and "simulation," emphasizing the use of mathematical representations to understand biological processes. These models are used in studying diseases, predicting treatment responses, and optimizing medical interventions (Day, 2006; Mathews et al., 2007). TS 2 is titled “disease and pathology modeling,” where a strong link is evident between the term “diseases” (1,020) and the concepts of “classification” and “predictive modeling." It is acknowledged that computational models assist in early disease detection and personalized treatment approaches. TS 3 pertains to the “reproducibility and validation of studies," a practice integral to the scientific production and publication process and crucial in health sciences. Here, we observe the relationship among “reproducibility” (1,016), “statistical methods," and “data analysis." Finally, TS 4 focuses on “classification and prediction methods in health," as highlighted by the term “support vector machines” (1,273) and its connection with “classification” and “predictive modeling." This reflects a research area dedicated to the application of these methods in automated diagnosis, patient segmentation, and pattern detection within extensive clinical data.

Cluster 5: Computational modeling and drug design

This cluster strongly emphasizes computational modeling, drug design, and protein structure. The term "computer model" occurs most frequently (3,359 times). Its close association with “molecular docking” (2,941) and “drug design” (2,044) suggests that these models are used to analyze the affinity of compounds with target proteins, facilitating the identification of promising candidates for new drug development (Sheng & Zhang, 2013; Wang et al., 2024). Another important concept in this cluster is “protein” (1,924), which closely relates to “protein structure” (1,707). This link highlights the significance of structural protein analysis in drug discovery, as many therapeutic strategies depend on the inhibition or modulation of specific proteins. Modeling the structure and function of proteins enhances our understanding of drug mechanisms of action and allows for the optimization of their design to increase effectiveness and reduce side effects (Tiwari et al., 2004).

Here we note four subtopics, the first of which (ST 1) pertains to “computational modeling in drug discovery.” There is a strong link between “computer model” (3,359), “molecular docking” (2,941), and “simulation.” TS 2 is defined as “drug design and evaluation of molecular interactions," reflecting the close relationship among the terms “drug design” (2,044), “binding affinity," and “computational chemistry." This area demonstrates that drug design is also based on computational analyses to assess the stability and efficiency of interactions between molecules. ST 3, “structural analysis of proteins," encompasses the term “protein structure” (1,707), which is closely linked to “protein” (1,924) and “molecular modeling." Here, we see the delineation of a topic that addresses the analysis of the three-dimensional structure of proteins to understand the function of biomolecules and design more selective inhibitors. The final topic (ST 4) is titled “molecular simulation and modeling of biomolecular interactions” because of the presence of relevant terms such as “molecular simulation” and “binding studies." This suggests that simulating interactions between proteins and drugs is a vital technique and is, therefore, well-explored in scientific literature.

Table 1. Summary of the topical clustering composition

Cluster label	Subtopics (ST)	Top 20 keywords
Cluster 1: Computational methods and modeling	ST 1: Mmathematical modeling and simulation of biological processes	computational methods, computer simulation, numerical methods, mathematical models, computation theory, finite element method, optimization, computational fluid dynamics, forecasting, iterative methods, Monte Carlo method, problem solving, geometry, genetic algorithms, differential equations, nonlinear equations, finite difference method, matrix algebra, heat transfer, inverse problems
	ST 2: Fluid dynamics and blood flow analysis	
	ST 3: Biomechanics and tissue modeling	
	ST 4: Artificial intelligence and medical data analysis	
	ST 5: Visualization of data and processing of medical images	
Cluster 2: Computational chemistry and molecular dynamics	TS 1: Molecular modeling and computational simulation	molecular dynamics, chemistry, metabolism, proteins, unclassified drug, models molecular, density-functional theory, binding sites, molecular dynamic simulation, simulation, chemical structure, calculations, mathematical analysis, thermodynamics, hydrogen bonding, protein conformation, protein binding, ligands, molecular model, quantum theory
	TS 2: Molecular dynamics and quantum mechanics applied to biochemistry	
	TS 3: Metabolism and computational biochemistry	
	TS 4: protein-ligand interactions and drug design	
	TS 5: Computational chemistry in biomedical materials	
Cluster 3: Computational biology and data analysis	TS 1: Gene expression analysis	computational biology, priority journal, procedures, biology, nonhuman, genetics, prediction, bioinformatics, animals, software, mathematical computing, computer program, amino acid sequence, gene expression, RNA, genomics, accuracy, sequence analysis, DNA, computer analysis
	TS 2: Bioinformatics and big data	
	TS 3: Prediction of biological phenomena	
	TS 4: Computational evolutionary and phylogenetic biology	
Cluster 4: Computational methods and biological models	TS 1: Computer modeling in biology and medicine	human, algorithms, machine learning, controlled study, methodology, comparative study, artificial intelligence, female, deep learning, image processing, male, diseases, support vector machines, biological model, physiology, learning systems, models biological, data mining, adult, reproducibility
	TS 2: Disease and pathology modeling	
	TS 3: Reproducibility and validation of studies	
	TS 4: Classification and prediction methods in health	
Cluster 5: Computational modeling and drug design	TS 1: Computational modeling in drug discovery	computer model, molecular docking, drug design, protein, protein structure, quantitative structure-activity relation, protein analysis, drug discovery, structure-activity relationship, drug development, drug structure, computer-aided design, ligand binding, virtual screening, drug screening, antineoplastic agents, docking, high throughput screening, protein function, pharmacophore
	TS 2: Drug design and evaluation of molecular interactions	
	TS 3: Structural analysis of proteins	
	TS 4: Molecular simulation and modeling of biomolecular interactions	

CONCLUSIONS

The study indicates that integrating computational methods in health sciences is a continuously expanding field. Key applications include modeling biological processes, simulating molecular interactions, and optimizing medical treatments. The various clusters analyzed demonstrate that computational tools enhance the exploration of biomedical phenomena and improve the accuracy of diagnoses, the personalization of therapies, and the efficiency of pharmaceutical research.

One of the most significant findings is that computational simulation and mathematical modeling have become crucial approaches in analyzing biological systems. Similarly, the analysis emphasizes the increasing intersection of artificial intelligence and health sciences. The strong link between machine learning, artificial intelligence, and big data indicates that machine learning algorithms are playing a key role in analyzing clinical data, diagnosing based on medical images, and identifying biological patterns.

Another key point is the significance of computational chemistry and molecular dynamics in drug discovery and optimization. Tools such as molecular docking and quantum mechanics highlight the importance of theoretical calculations and molecular simulations in predicting biomolecular interactions. The study also underscores the relevance of computational models in personalized biology and medicine. Computational biology and bioinformatics have made advances in genomic analysis, biomarker identification, and treatment response prediction possible.

Ultimately, the research highlighted the critical importance of reproducibility and validation of computational models in healthcare. The connection between terms like reproducibility, statistical methods, and data analysis underscores the necessity of ensuring the reliability of results obtained from simulations and biomedical data analysis. Transparency in computational methodologies and the experimental validation of models continue to pose fundamental challenges for integrating these approaches into clinical and pharmaceutical practices.

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest related to the development of the study.

AUTHORSHIP CONTRIBUTION

Conceptualization; Data curation; Formal analysis; Research; Methodology; Visualization; Writing - original draft; Writing - review and editing: Oscuvilca-Tapia, E. C, Bermejo-Sánchez, F. R., Noreña-Lucho, M. M., and Estrada-Choque, E. A.

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