




PROFILE OF EXHALED VOLATILE ORGANIC COMPOUNDS ASSOCIATED WITH BREAST CANCER

PERFIL DE COMPOSTOS ORGÂNICOS VOLÁTEIS EXALADOS ASSOCIADOS AO CÂNCER DE MAMA

PERFIL DE COMPUESTOS ORGÁNICOS VOLÁTILES EXHALADOS ASOCIADOS A CÁNCER DE MAMA

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ABSTRACT

Breast cancer is one of the leading causes of female mortality worldwide, due to late detection and limited access to diagnostic methods. This article reviews the feasibility of using volatile organic compounds (VOCs) present in exhaled breath as a complementary diagnostic tool through the use of electronic noses. These noninvasive technologies can detect specific chemical patterns related to metabolic alterations associated with cancer and could be integrated into current screening systems. The review covers recent studies that use techniques such as mass spectrometry and chemical sensors to identify VOC profiles characteristic of breast cancer. Compounds such as 2-propanol, heptanal, and cyclopentanone are highlighted, which demonstrate high sensitivity and specificity in differentiating between healthy and diseased patients. The metabolic pathways involved and the biological effects of different chemical groups are also explored. Although electronic nose technology still faces technical and standardization challenges, its advantages—such as speed, low cost, and ease of use—make it a promising alternative for improving early diagnosis and personalized medicine in oncology. It is concluded that further research is needed to validate its clinical applicability.

Keywords: Volatile Organic Compounds. Breast Cancer. Electronic Nose. Early Diagnosis.

RESUMO

O câncer de mama é uma das principais causas de mortalidade feminina em todo o mundo, devido à detecção tardia e ao acesso limitado a métodos diagnósticos. Este artigo analisa a viabilidade do uso de compostos orgânicos voláteis (COVs) presentes no ar exalado como ferramenta complementar de diagnóstico por meio do uso de narizes eletrônicos. Essas tecnologias não invasivas podem detectar padrões químicos específicos relacionados a alterações metabólicas associadas ao câncer e podem ser integradas aos sistemas de rastreamento atuais. A revisão abrange estudos recentes

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que utilizam técnicas como espectrometria de massas e sensores químicos para identificar perfis de COVs característicos do câncer de mama. Compostos como 2-propanol, heptanal e ciclopentanona são destacados, os quais demonstram alta sensibilidade e especificidade na diferenciação entre pacientes saudáveis e doentes. As vias metabólicas envolvidas e os efeitos biológicos de diferentes grupos químicos também são explorados. Embora a tecnologia do nariz eletrônico ainda enfrente desafios técnicos e de padronização, suas vantagens — como velocidade, baixo custo e facilidade de uso — a tornam uma alternativa promissora para aprimorar o diagnóstico precoce e a medicina personalizada em oncologia. Conclui-se que mais pesquisas são necessárias para validar sua aplicabilidade clínica.

Palavras-chave: Compostos Orgânicos Voláteis. Câncer de Mama. Nariz Eletrônico. Diagnóstico Precoce.

RESUMEN

El cáncer de mama representa una de las principales causas de mortalidad femenina a nivel mundial, debido a la detección tardía y al limitado acceso a métodos diagnósticos. Este artículo revisa la viabilidad del uso de compuestos orgánicos volátiles (COVs) presentes en el aliento exhalado como herramienta diagnóstica complementaria mediante el uso de narices electrónicas. Estas tecnologías no invasivas pueden detectar patrones químicos específicos relacionados con alteraciones metabólicas asociadas al cáncer, y podrían integrarse a los sistemas de tamizaje actuales. La revisión abarca estudios recientes que utilizan técnicas como la espectrometría de masas y sensores químicos para identificar perfiles de COVs característicos del cáncer de mama. Se destacan compuestos como el 2-propanol, heptanal y ciclo-pentanona, los cuales muestran alta sensibilidad y especificidad para diferenciar entre pacientes sanas y enfermas. Asimismo, se exploran las rutas metabólicas implicadas y los efectos biológicos de distintos grupos químicos. Aunque la tecnología de nariz electrónica aún enfrenta retos técnicos y de estandarización, sus ventajas —como la rapidez, bajo costo y facilidad de uso— la convierten en una alternativa prometedora para mejorar el diagnóstico temprano y la medicina personalizada en oncología. Se concluye que se requiere mayor investigación para validar su aplicabilidad clínica.

Palabras clave: Compuestos Orgánicos Volátiles. Cáncer de Mama. Nariz Electrónica. Diagnóstico Temprano.



1 INTRODUCTION

Breast cancer is among the leading causes of cancer death in women globally. According to the World Health Organization, 670,000 women died from this disease in 2022, with higher rates in women between 50 and 80 years of age. It is estimated that one in eight women could develop breast cancer in their lifetime, making it a significant global health problem^{1,2}. The main characteristics related to this are the lack of information, cultural differences, and economic differences among the population, which delimits a barrier that hinders the search for early care and follow-up treatment for those who suffer from it³.

The diagnosis is received from an abnormal screening study; however, sometimes alterations are detected by the finding of clinical data such as palpation of nodules or lumps in the breasts, sinking and changes in the texture of the skin or abnormal discharge from the nipple³. Medical attention is usually sought when cancer data are so advanced that they are detected as alarming by the patients themselves, and not when they are performed by control ⁴. There are factors that can increase the risk of developing breast cancer, such as advanced age, family history, excessive alcohol and tobacco consumption, reproductive factors and the use of postmenopausal hormone therapy⁵, however, approximately 50% of breast cancers are diagnosed in women who do not have any apparent risk factors. The WHO mentions that this may be related to mutations due to the aging process and not to hereditary mutations,¹ highlighting the complexity of the disease and the importance of early detection, regardless of the presence or absence of risk factors ^{2,6}.

There are several invasive and non-invasive diagnostic tests that have different levels of sensitivity and specificity ⁷. Screening and diagnosis for breast cancer in Mexico is based on clinical examination and breast self-examination, along with the use of mammographs, ultrasounds, and biopsies; however, there is a deficient number of available mammographers and specialist radiologists who interpret these studies, coupled with the population's lack of prevention culture, which contributes to late diagnosis even in those with suggestive clinical symptoms ^{3, 8, 9}. With the above, it has been seen the need to implement simpler, faster, cheaper and more convenient screening tools for users, taking into account that early detection is so far the most important point in the fight against breast cancer ¹⁰. In recent years, studies have been carried out



worldwide by groups of researchers who are exploring options to complement existing screening approaches ³.

Volatile organic compounds (VOCs) are compounds that contain carbon and other chemical elements such as hydrogen, oxygen, nitrogen, chlorine, sulfur, etc. and that at room temperature are gaseous. The diagnosis of breast cancer using ***volatile organic compounds from breath samples*** suggests a promising future, having the characteristic of being non-invasive, providing rapid results and having a greater reach in the general population ¹¹. Machine learning instruments using exhaled breath samples have been shown to have a high value in diagnosing diseases, and can be conclusive in profiling VOCs ¹².

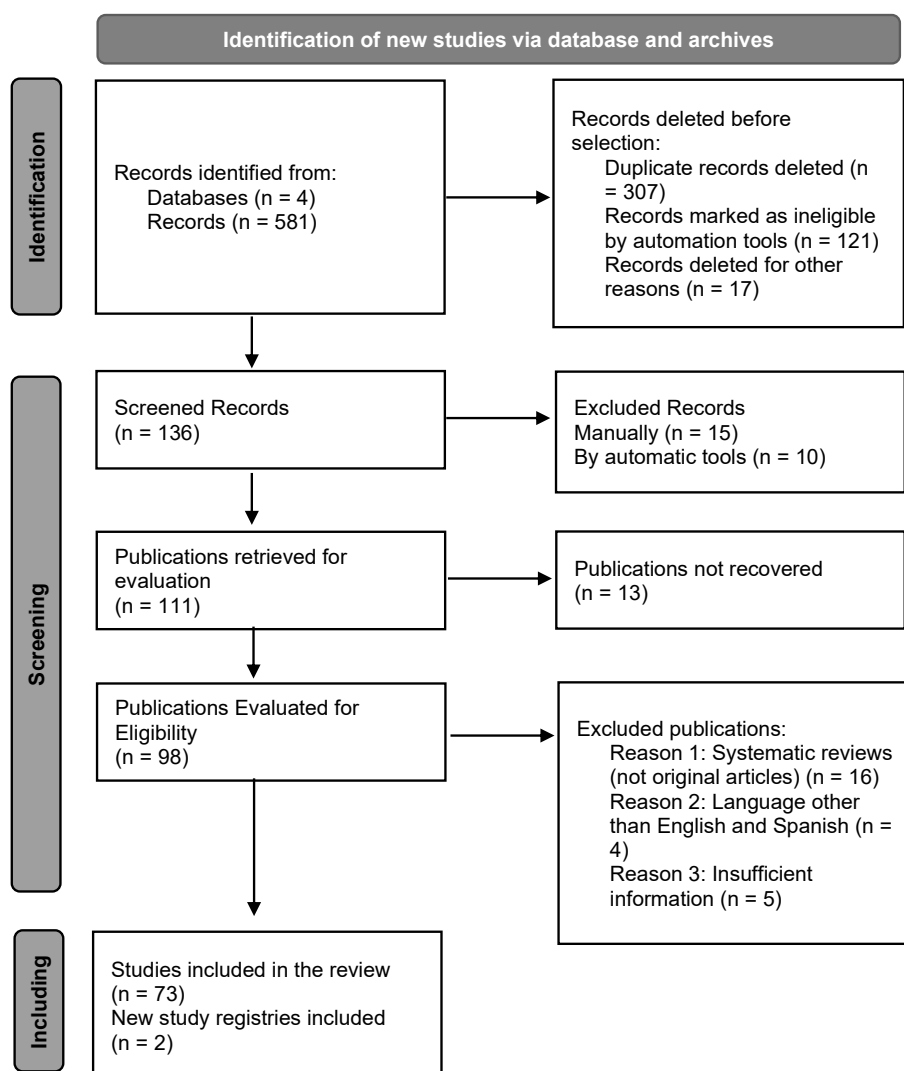
The aim of this review is to compile the information associated with assessing whether the use of electronic nose technology with a focus on the analysis of volatile organic compounds detected in biofluids, specifically in breath, could be a complementary tool for the diagnosis of pathologies of global importance such as breast cancer. Finally, we discuss the profile of exhaled volatile organic compounds associated with breast cancer.

2 MATERIALS AND METHODS

In the present review, a systematic search was performed in the databases PubMed, Web Of Science, Wiley Online Library and Science Direct. The keywords used were English terms: *volatile organic compounds, breath biomarkers, volatolomics, volatile, breast cancer, breast carcinoma, screening, detection and electronic nose*. We used search filters by year of publication from 01 January 2019 to 01 August 2024. The search was carried out in September 2024, where a total of 581 articles were found; of which 64 were obtained from PubMed, 44 from Web Of Science, 152 from Wiley Online Library and 321 from Science Direct. For the successful retrieval of useful items, duplicate items were removed.

Figure 1

PRISMA flowchart for the selection of reports analyzed for the detection of breast cancer using volatile organic compounds



3 RESULTS AND DISCUSSION

E-nose work as a multisensory system, composed of a panel or array containing gas-sensitive nanosensors. There are sensors based on metal-oxide and carbon nanoparticles that contain conductive polymers that achieve an analysis or creation of respiratory fingerprints by capturing a change in the electrical resistances detected by metals ¹³. The function of sensors is to detect components of a sample and transform them into a physical quantity, such as resistance, thus reflecting how much exposure or affinity the sensors have to the "odorous" sample to which they were subjected ¹⁴. As a



type of pattern recognition training is created, a mathematical model can be built capable of distinguishing between healthy and sick people, classifying them according to their respiratory footprint. Table I shows the classic techniques for quantifying VOCs.

Table 1

Methods for analysis of exhaled breath

Criterion	Classic techniques	Pattern Recognition Methods
Beginning	Accurate identification and quantification of specific compounds.	Pattern recognition in complex compound profiles.
Examples of techniques	PTR-MS, GC-MS	E-nose, IMS
Advantages	High precision and sensitivity; ability to quantify.	Fast, they do not require extensive pre-processing.
Limitations	High costs, require specialized personnel.	Lower specificity in compound identification.
Main applications	Detailed analysis of compounds in scientific research.	Rapid detection in medical diagnostics and air quality. Mostly used for the analysis of volatile and semi-volatile compounds

PTR-MS: Proton Transfer Reaction Mass Spectrometry, GC-MS: Gas Chromatography coupled to Mass Spectrometry, E-nose: Electronic nose, IMS: Ion Mobility Spectroscopy.

3.1 VOLATILE ORGANIC COMPOUNDS

The fluids we excrete from our bodies contain hundreds of volatile organic compounds (VOCs), which originate from various biochemical and metabolic pathways. If a metabolic pathway is altered, it can cause an altered VOC profile that can be perceived in some human biofluid ¹³. Volatile organic compounds are carbon-containing chemicals that evaporate easily at room temperature and can be considered as useful biomarkers in medicine ¹⁵. Biomarkers are biological molecules that can be detected in fluids, tissues, or blood. These include proteins, nucleic acids, and carbohydrates, which act as indicators of the onset or progression of diseases such as cancer ¹⁶. When we talk about a volatile biomarker, we refer to a compound or substance with high volatile characteristics or that is in gaseous form, being useful to interpret the current state of health of an individual. We continuously produce volatile organic compounds (VOCs) responsible for our chemical footprint ¹⁷. The production of VOCs originates in cell metabolism and can vary in their composition or quantity when cells experience

pathophysiological conditions that lead to neoplastic transformation. This can occur, for example: due to hypoxia, an increase in energy expenditure due to hyperproliferation or the production of reactive oxygen species ¹⁸. Several studies have shown that VOCs can differentiate pre- and post-disease states in patients with breast cancer, being useful in the detection of endogenous metabolites related to cancer.

3.2 PROFILE OF ORGANIC VOLUTILE COMPOUNDS RELATED TO BREAST CANCER

Volatile organic compounds (VOCs) have been investigated in relation to breast cancer due to their potential as diagnostic biomarkers. Several studies have shown that VOC profiles in breath and other body fluids may have the ability to differentiate between breast cancer patients and healthy patients ^{19, 20}.

Zhang et al. used mass spectrometry to detect VOCs in breath samples, showing high sensitivity and specificity in differentiating between patients with and without breast cancer, but with limited performance in differentiating pathological or molecular subtypes²⁰. *Gong et al.*, identified some key metabolites that correlate with breast cancer: N-acetyl-D-tryptophan, 2-arachidonoylglycerol, pipecolic acid, and oxoglutaric acid ²¹. On the other hand, in a study conducted by Park Jiwon, it was found that L-octanoylcarnitine, 5-oxoproline, hypoxanthine, and docosahexaenoic acid were potential biomarkers for breast cancer²². A wide variety of volatile organic compounds and metabolites with high predictive value for the detection of breast cancer have been found in the urine, some of them being 2-propanol and 2-butanone ²³.

In a paper published in 2014, *Wang et al.*, identified specific volatile metabolites in the breath that distinguish breast cancer patients from healthy individuals, suggesting their use as diagnostic biomarkers ²⁴. Another study by *Lavra et al.* analyzed VOCs in breast cancer cell lines, identifying volatile fingerprints that could offer important information about the molecular and tumor characteristics of cancer cells ²⁵.

Breast cancer-related VOCs are a variety of metabolites detected, as shown in Table 2 and Figure 2.



Table 2

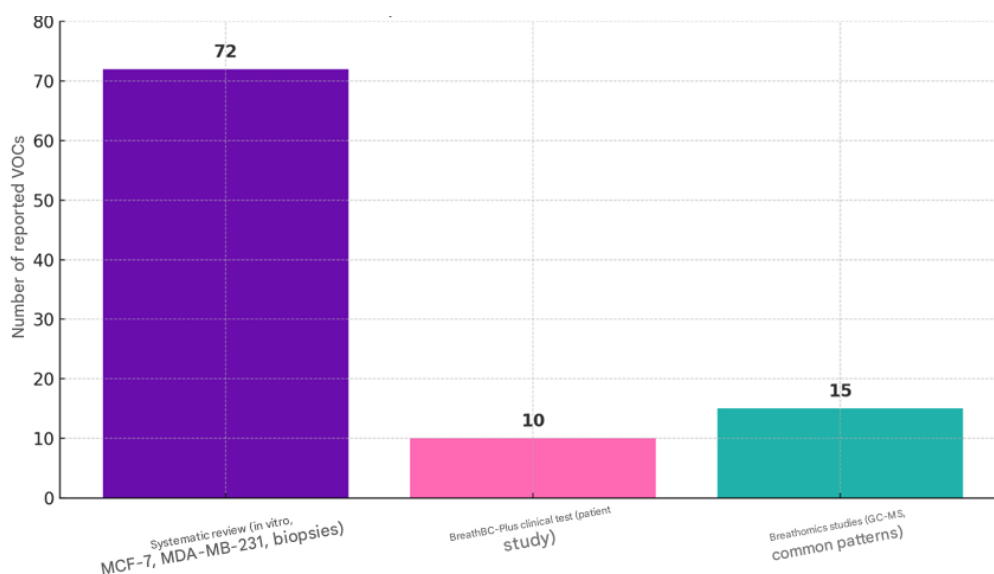
Volatile metabolites related to breast cancer

Metabolite Name	Guy	Metabolic Pathway Involved	Detection Method	Relevance in Breast Cancer
2-Propanol	Volatile	Lipid metabolism	GC-MS	Detected in urine, possible biomarker.
2-Butanone	Volatile	Ketone metabolism	GC-MS	Differentiation between patients and controls.
2-Ethyl-1-Hexanol	Volatile	Not determined	GC-MS	Present in invasive ductal carcinoma.
Isolongifolenone	Volatile	Not determined	GC-MS	Associated with aggressive tumor cells.
Furan	Volatile	Carbohydrate Breakdown	GC-MS	Related to oxidative stress.
Dodecanoic acid	Volatile	Lipid metabolism	GC-MS	Potential marker in invasive carcinoma.
2-Methoxy-Phenol	Volatile	Phenolic metabolism	GC-MS	Associated with tumor molecular characteristics.
Heptanal	Volatile	Fatty acid oxidation	GC-MS	Sensitive for invasive lesions.
Cyclopentanone	Volatile	Ketone metabolism	GC-MS	Detected in women with invasive lesions.
6-Methyl-5-hepten-2-one	Volatile	Isoprenoid metabolism	GC-MS	Present in women with benign lesions.
Ethanol	Volatile	Alcohol metabolism	GC-MS	Detected in breast cancer cell lines.
N-Propanol	Volatile	Alcohol metabolism	GC-MS	Identified in breast cancer cell lines.
Ethyl ethanoate	Volatile	Ester metabolism	GC-MS	Found in breast cancer cell lines.

C-MS: Gas Chromatography coupled to Mass Spectrometry.

Figure 2

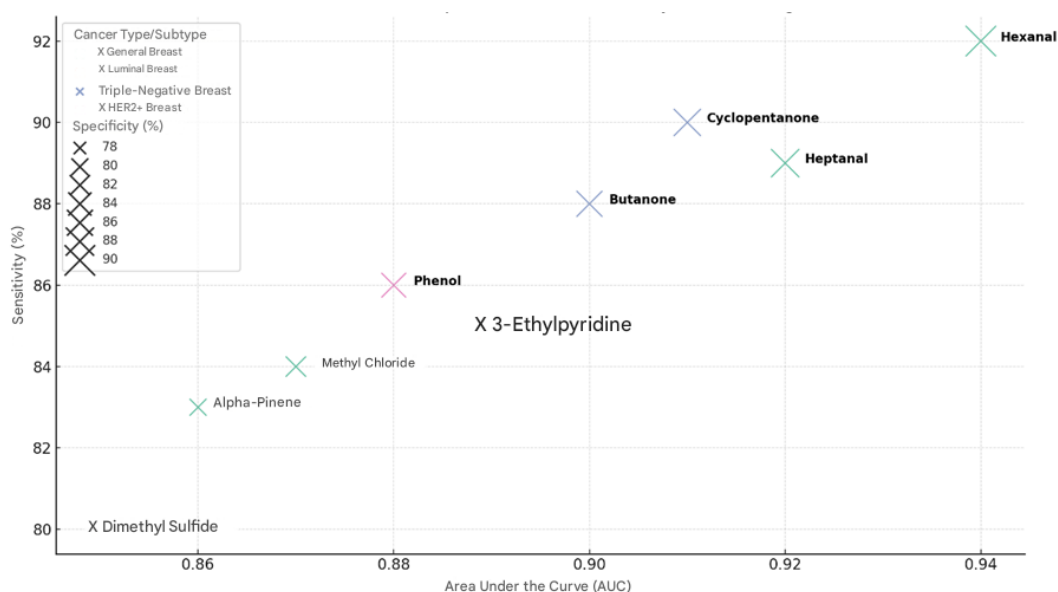
Number of VOCs reported in exhaled breath in breast cancer



The specific observations of what is reported in the literature are shown in Figure 3. Where you can see in the graph the different VOCs associated with different subtypes of cancer, where **Hexanal** and **Heptanal** have **high AUCs (>0.9)** and excellent sensitivity, being good general biomarkers.

Figure 3

Analysis of the relationship between VOCs, cancer subtypes and diagnostic metrics





Subsequently, Cyclopentanone stands out in triple-negative breast cancer, with a good balance between sensitivity and specificity. 3-methylpyridine and Phenol are more associated with the HER2+ subtype, and Alpha-pinene and Dimethyl sulfide have more modest but still useful values as part of multicomponent combinations. Finally, Table 3 shows a relationship between the chemical compound, the metabolic pathway involved and its biological effect, which can be associated with cell damage.

Table 3

Relationship between chemical compounds and their biological effect

Chemical Category	Main metabolic source	Key Biological Effect
Alkanes/Alkenes	Lipid peroxidation	Oxidative stress, membrane damage
Aldehydes	Lipid oxidation	Mutagenicity, chronic inflammation
Ketones	β -oxidation	Energy alteration (Warburg effect)
Alcohols	Aldehyde reduction	Redox imbalance, tumour signalling
Halogenated	Xenobiotic metabolism	Genotoxicity, induced detoxification
Aromatic	Aromatic AA catabolism	Hormonal alteration, epigenetics
Sulphurous / Ethers	Sulphur/microbial metabolism	Immunomodulation, redox stress

4 CONCLUSIONS

The advancement of technology in the medical field has allowed the development of innovative tools for the diagnosis and treatment of diseases such as breast cancer, offering new perspectives in early detection, molecular analysis and targeted therapies. The ability of electronic noses to identify unique "respiratory fingerprints" based on pattern recognition algorithms positions them as promising tools for non-invasive and inexpensive diagnostics, especially in diseases such as breast cancer. However, its accuracy for quantitative analysis still faces technical limitations. Despite the challenges that emerging technologies still face, such as the lack of standardization in volatologies or the complexity in the manufacture of nanomaterials, the advances made so far represent a significant step towards the future of personalized and precision medicine. Current studies suggest that volatile organic compounds have potential to complement current diagnostic tools, although more research is required to validate these findings and improve diagnostic accuracy.



5 ETHICAL CONSIDERATIONS

Protection of people and animals. The authors state that no experiments have been carried out on humans or animals for this research.

Confidentiality, informed consent and ethical approval. The study does not involve personal data of patients nor does it require ethical approval. SAGER guides do not apply.

Conflict of Interest Statement

The authors declare that they have no conflict of interest.

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