

Effectiveness of the MonoTrap Collection Method for VOC Analysis in Exhaled Breath Using GC-MS

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User Benefits

- ◆ Comprehensive analysis of VOCs from non-invasive breath samples is feasible with this system.
- ◆ No equipment such as sampling pumps is required, enabling breath collection in remote locations.
- ◆ Internal standards support consistent comparison of analytical results across sample groups.

Introduction

Exhaled breath is a non-invasive sample that is easy to collect and imposes minimal burden on subjects. It is known to contain volatile organic compounds (VOCs) that reflect metabolic states and disease conditions within the body. More than 1,000 types of VOCs exist in breath, and numerous studies have reported the search for breath markers across various disease areas, including inflammatory diseases¹, cancer², and metabolic disorders³. Consequently, extensive research is being conducted in the field of breathomics.

While GC-MS is widely used for comprehensive and highly sensitive analysis of trace components in breath, differences in pretreatment steps, such as sample collection, affect measurement results. Therefore, optimizing analytical protocols to enhance reproducibility and consistency is essential.

This Application Note compares breath collection methods using Tenax tubes and MonoTrap using a thermal desorption-GC-MS system (Fig. 1) to determine the optimal collection method. Additionally, breath samples from healthy subjects and subjects with inflammatory conditions were analyzed using this analytical system to evaluate the usefulness of measuring and comparing VOC profiles with this approach.



Fig. 1 GCMS-QP2020 NX and TD-30

MonoTrap

MonoTrap provided from GL Sciences (Fig. 2) is an adsorption device based on a silica monolith structure, characterized by efficient VOC capture. It features a large specific surface area, enabling adsorption of a wide range of compounds from low-molecular-weight to medium-to-high boiling point components, and supports diverse analytical techniques such as solvent extraction and thermal desorption. Compact and lightweight for easy handling, it is well-suited for gas sampling



Fig. 2 Ampoule with MonoTrap (left) and MonoTraps (right)

of biological gases and environmental gases, enabling simple and reproducible sample pretreatment.

Exhaled Breath Sampling and Pretreatment

A comparison of collection methods was conducted using breath samples from healthy subjects. Breath samples were collected using two different methods.

In the Tenax tube method, after collecting exhaled breath in a 2 L sampling bag (A031-G2H24, GL Sciences), the breath components were captured in a Tenax collection tube (1/4" x 3.5" Glass ATD Tube, Tenax TA 35/60, CAMSCO) at a flow rate of 100 mL/min.

For the MonoTrap method, subjects blew exhaled breath into a 2 L sampling bag containing a MonoTrap (RGC 18TD, GL Sciences). The MonoTrap was then left at room temperature for 3 h or 24 h to adsorb VOCs from the exhaled breath. After collection, the MonoTrap was retrieved and transported in a GC vial. For the comparative study between healthy subjects and subjects with inflammatory conditions, breath samples were collected from both groups at Jikei University School of Medicine. The collection was performed using one MonoTrap under a 24 h static condition.

Table 1 Instrument Configuration and Analytical Conditions

Autosampler:	TD-30R
GC-MS Model:	GCMS-QP2020 NX
[TD-30R]	
Tube Desorb Temp.:	250 °C / 350 °C
Tube Desorb Flow:	60 mL/min
Sampling Time:	7 min
Trap Cooling Temp.:	-20 °C
Trap Desorb. Temp.:	250 °C
Trap Desorb. Time:	5 min
Trap Tube:	TENAX-TA
Joint Temp.:	250 °C
Valve Temp.:	250 °C
Transfer Line Temp.:	250 °C
Internal Standard:	Add Toluene-d8 at a flow rate of 20 mL/min over 0.30 min.
[GC]	
Column:	SH-Rxi-5Sil MS (Length 30.0 m, 0.25 mm I.D., df = 0.1 µm)
Column temperature:	60 °C(1min)→(5 °C/min)→200 °C →(30 °C/min)→320 °C(2 min)
Injection Mode:	Split
Split Ratio:	10
Carrier Gas:	Helium
Carrier Gas Control:	Linear velocity 36.5 cm/s
Purge flow rate:	5 mL/min
[MS]	
Ion source Temp.:	230 °C
Interface Temp.:	280 °C
Measurement Mode:	Scan
Event Time:	0.30 sec
Detector voltage:	Autotuning + 0.2kV
Scan range:	m/z 35-600

Note that our company was not involved in sample collection for this study and did not receive any personal information.

■ Analytical Conditions

After collection, MonoTrap and Tenax collection tubes were thermally desorbed using the TD-30R thermal desorption device and analyzed by GC-MS (GCMS-QP2020 NX). Toluene-d8 was added as an internal standard to confirm analytical stability. Detailed analytical conditions are shown in Table 1.

■ Results

1. Comparison of Detected Peak Numbers Based on Different Collection Methods

Analysis of breath from the same healthy subject using Tenax and MonoTrap revealed clear differences in the chromatograms obtained by both methods (Fig. 3). When using Tenax, 58 peaks were detected. In contrast, when using the MonoTrap, the number of detected peaks was comparable to the Tenax after a 3 h holding time. However, under a 24 h holding condition, the number of detected peaks increased to 152.

With the Tenax, exhaled breath collected in a sampling bag must be passed through the trap. Therefore, increasing the collection volume is necessary to improve sensitivity.

On the other hand, the sampling method using MonoTrap allows for extended collection periods simply by leaving the sampling bag stationary, and is expected to improve sensitivity. Furthermore, MonoTrap can be sealed in a GC vial for transport, making it useful when collection and analysis occur at different locations.

2. Optimization of MonoTrap Collection Conditions

To optimize breath collection conditions using MonoTrap, we evaluated the effects of varying the number of MonoTraps and the incubation time, simulating actual analytical operations. At a 3 h incubation time, using two MonoTraps showed no significant difference in peak species count, but a trend toward increased peak intensity was observed (data not shown). In contrast, at a 24 h incubation period, no significant differences in peak intensity or the number of detected peak species were observed even when varying the number of MonoTraps used (Fig. 4). These results indicate that under 24 h incubation conditions, adsorption of breath components reaches a consistent level with a single MonoTrap.

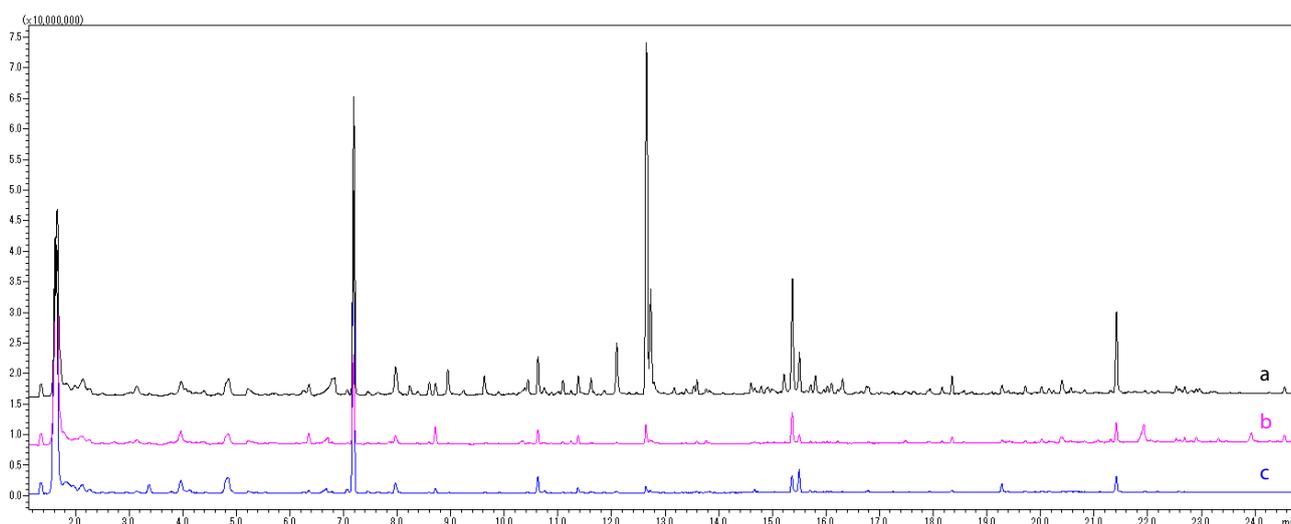


Fig. 3 Chromatograms Comparison of Healthy Subjects' Breath Using the Tenax and the MonoTrap Method.
a: MonoTrap (24 h incubation), b: MonoTrap (3 h incubation), c: Tenax

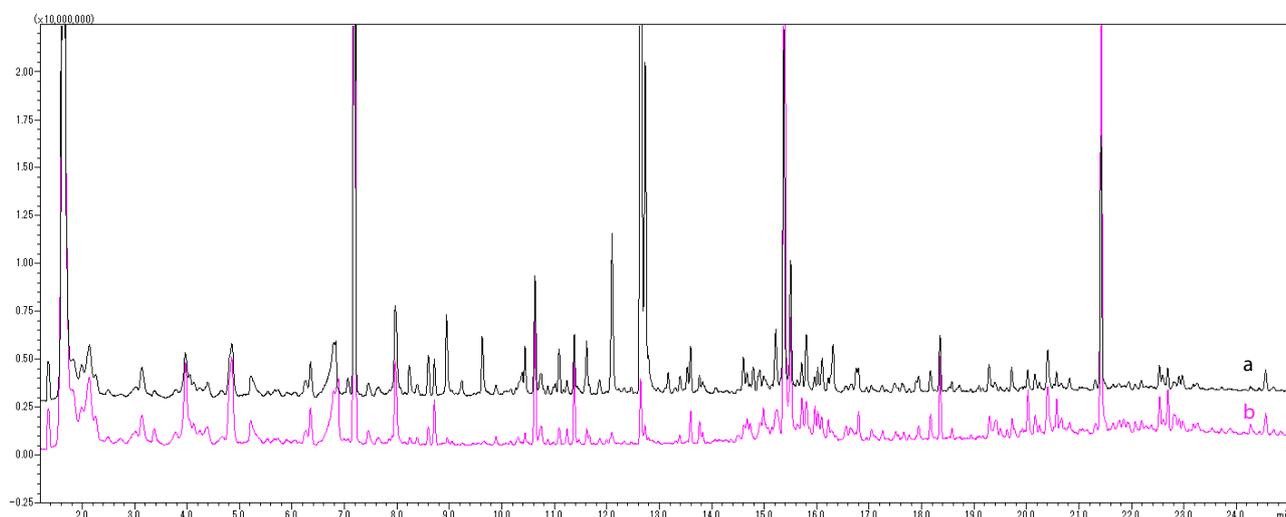


Fig. 4 Chromatograms Comparison Based on MonoTrap Quantity (24 h Static Incubation).
a: one MonoTrap, b: two MonoTraps

3. Comparison of Breath from Healthy Subjects and Subjects with Inflammatory Conditions.

Breath samples from healthy subjects and subjects with inflammatory conditions were analyzed using a single MonoTrap under 24 h collection protocol. The results revealed differences in peak intensity and detection for multiple volatile components. These differences were not limited to specific individual components; variations were observed in the overall profile of VOCs in the breath. As representative examples, chromatograms of dimethyl dodecane and methyl propyl nonane in the breath of healthy subjects and subjects with disease are shown (Fig. 5). This analysis system confirmed the ability to visualize differences in breath component profiles as measurable results. Note that these results are not intended for the diagnosis, differentiation, or severity assessment of specific diseases.

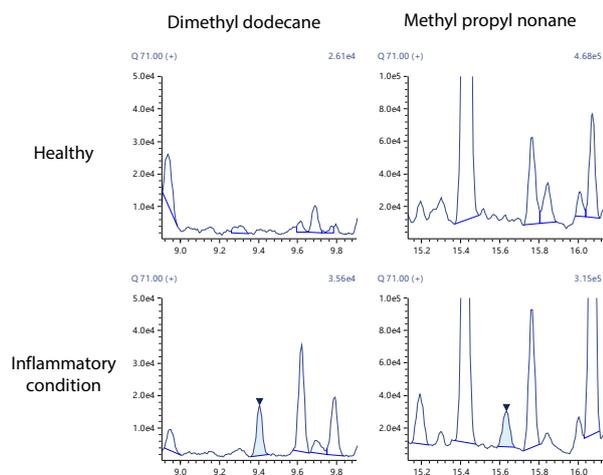


Fig. 5 Comparison of corresponding components between a healthy subject and a subject with an inflammatory condition.

■ Summary

This application news evaluated a breath VOC analysis system using thermal desorption–GC–MS with MonoTrap. MonoTrap detected a larger number of VOCs in exhaled breath from healthy subjects compared with the conventional Tenax tube method. Optimization of collection conditions indicated that static collection using one MonoTrap for 24 h is a practical and efficient protocol. Under these conditions, differences in VOC profiles were observed between healthy subjects and subjects with inflammatory conditions. MonoTrap enables breath collection without sampling pumps, and collected samples can be easily stored and transported, making the method suitable for remote sampling. Overall, this system demonstrated the capability for comprehensive VOC profiling of exhaled breath.

<References>

- 1) Kensuke Tsutsui, Masami Nemoto, Midori Kono, Takako Sato, Yukio Yoshizawa, Yoko Yumoto, Ryo Nakagawa, Takeo Iwamoto, Hiroshi Wada, Takashi Sasaki, "GC-MS analysis of exhaled gas for fine detection of inflammatory diseases", *Analytical Biochemistry*, June 2023.
- 2) Elina Gashimova, Anna Osipova, Azamat Temerdashev, Vladimir Porkhanov, Igor Polyakov, Dmitry Perunov, Ekaterina Dmitrieva, "Exhaled breath analysis using GC-MS and an electronic nose for lung cancer diagnostics", *Anal Methods*, Oct. 2021.
- 3) Alessia Di Gilio, Jolanda Palmisani, Marirosa Nisi, Valentina Pizzillo, Marco Fiorentino, Stefania Rotella, Nicola Mastrofilippo, Loreto Gesualdo, Gianluigi de Gennaro, "Breath Analysis: Identification of Potential Volatile Biomarkers for Non-Invasive Diagnosis of Chronic Kidney Disease (CKD)", *Molecules*, Oct. 2024.

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