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# Characterization of Gandapura Oil by GC and Analysis of Nitration Product Structure Using FTIR Spectroscopy

Theresia Novianti Marpaung*, Marham Sitorus

Chemistry Department, Faculty of Mathematic State University of Medan, Medan 20221

*Corresponding author: therempg@gmail.com

**ABSTRACT**

*A study has been conducted on the orientation of the nitration reaction of methyl salicylate from wintergreen oil (Gaultheria Procumbens L.) with sulfuric acid catalyst. The research method was carried out through a reflux process between gandapura oil, $HNO_3$, and $H_2SO_4$ at a temperature of 56-60°C for 60 minutes, followed by a washing and recrystallization stage using ethyl acetate. The product obtained was then analyzed using FT-IR. The nitration product is a white crystal, indicating that the compound is relatively pure with a melting point of 100-109°C. Based on the FTIR spectrum, it was confirmed that a nitration reaction had occurred with the appearance of characteristic nitrate ($NO_2^+$) absorption at 1537 $cm^{-1}$ (asymmetric).*

*Keywords: Methyl salicylate, nitration, and acid catalysis.*

## 1. INTRODUCTION

Wintergreen oil is a natural essential oil obtained from the distillation or extraction of *Gaultheria* leaves and is known for its remarkably high methyl salicylate content. Wintergreen oil has significant industrial value, particularly in the fragrance, pharmaceutical, and traditional therapeutic sectors. The presence of methyl salicylate contributes to its characteristic aroma as well as its analgesic and anti-inflammatory properties. In addition to its medicinal and cosmetic applications, wintergreen oil is also utilized in topical formulations, aromatherapy products, insect control preparations, and as an active ingredient in mosquito repellent formulations.[3]

Wintergreen oil derived from *Gaultheria procumbens* L. is predominantly composed of methyl salicylate, with reported concentrations reaching approximately 99%.[8] Methyl salicylate is an ester compound that appears as a colorless liquid under ambient conditions and is characterized by its distinctive aromatic odor. Physically, wintergreen oil exhibits a pale yellow appearance and possesses well defined physicochemical properties. It has a boiling point of approximately 223°C, a melting point of -8.6°C, a density of 1.18 g/mL, and a molecular weight of 152.15 g/mol.[4,5,7]

Gas chromatography (GC) is an analytical technique used to separate and analyze volatile and thermally stable compounds in a sample. In this method, an inert carrier gas serves as the mobile phase, transporting the vaporized sample through a heated column coated with a liquid stationary phase. The components are separated based on differences in their interaction with the stationary phase and their respective retention times. Each compound is then detected as it elutes from the column, producing a chromatogram that reflects the composition of the sample.[1,2]



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Fourier Transform Infrared (FT-IR) spectroscopy is a widely applied analytical method for structural characterization and functional group identification of chemical compounds. The technique produces an infrared spectrum representing molecular vibrational transitions, which can be utilized for qualitative identification and, in certain applications, quantitative analysis. FT-IR measurements are generally conducted in transmission or reflectance modes. In transmission mode, the absorption of infrared radiation by the sample is recorded, and the sample may be analyzed in solid, liquid, or gaseous form depending on the preparation technique. Solid samples are typically prepared as KBr or NaCl pellets, while liquid samples or suspensions may be analyzed using appropriate media.[9]

**Table 1.** Infrared Absorption Region of Several Functional Groups.[6]

| Group | Compound | Wave Number ($cm^{-1}$) |
|---|---|---|
| O-H | Fenol (broad) | 3250-3650 $cm^{-1}$ |
| O-H | Fenol (bend) | 1300-1600 $cm^{-1}$<br>600-800 $cm^{-1}$ |
| C-O | Ester $COOCH_3$ (stretch)<br>Fenol (stretch) | 1000-1200 $cm^{-1}$<br>>1200 $cm^{-1}$ |
| =C-H | $sp_2$ (stretch)<br>$sp_2$ (bend) | 3000-3250 $cm^{-1}$<br>650-1000 $cm^{-1}$ |
| -C-H | $sp_3$ (stretch) | 2850-2960 $cm^{-1}$ |
| C=C | Aromatic (stretch) | 1600-1650 $cm^{-1}$ |
| C=O | Ester (stretch) | 1725-1750 $cm^{-1}$ |
| $-NO_2$ | Asymmetric (stretch)<br>Symmetric (stretch) | 1485-1555 $cm^{-1}$<br>1320-1355 $cm^{-1}$ |

## 2. EXPERIMENTAL

### *2.1. Chemicals, Equipment and Instrumentation*

The materials used included commercial wintergreen oil (Gaultheria Procumbens L.), 98% sulfuric acid ($H_2SO_4$), 68% nitric acid ($HNO_3$), ethyl acetate ($C_4H_8O_2$), distilled water, and ice cubes. The equipment used in this study included an analytical balance, laboratory glassware, a Buchner funnel, a magnetic stirrer hotplate (Thermo Fisher Scientific), an ice container, a set of reflux apparatus, a stirrer bar, petroleum jelly, filter paper, an oven, Fourier Transform Infrared Spectroscopy (FT-IR) Bruker Invenio and Gas Chromatography (GC).

### *2.2. Research Procedure*

Commercial gandapura oil was analyzed using Gas Chromatography (GC) and Fourier Transform Infrared spectroscopy (FT-IR). A total of 5 mL of gandapura oil and 11 mL of nitric acid ($HNO_3$) were prepared in separate containers placed in ice. A total of 3 mL of sulfuric acid ($H_2SO_4$) was placed in a three-neck flask, which was then placed in a container filled with ice and salt to lower the freezing point. The flask was cooled to a temperature of 5°C for 30 minutes.

Once the temperature was reached, a magnetic stir bar was placed in the flask, and stirring was carried out at a speed of 200 rpm. Cold nitric acid was added slowly drop by drop while maintaining the temperature at 2°C for 30 minutes. Next, cold camphor oil was also added slowly drop by drop and cooled again to a temperature of 2°C for 30 minutes. After that, the stirrer bar is replaced with a boiling stone, a reflux apparatus is assembled, and the mixture is heated at 50°C for 1 hour to continue the nitration reaction.

The reaction solid is washed with cold distilled water to remove residual acid, then filtered using filter paper. The solid obtained is dissolved in ethyl acetate with the addition of boiling stones and heated until completely dissolved. The solution is then cooled in a container filled with ice until crystals form. The resulting crystals are dried in an oven at 40°C


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for 1 hour. The reaction product is then weighed, tested for its melting point, and characterized using gas chromatography (GC) and FT-IR spectroscopy.

## 3. RESULTS AND DISCUSSION

### *3.1. Gas Chromatography (GC)*

The characterization of commercial gandapura oil was performed using gas chromatography (GC) to identify the composition of its constituent compounds and determine the relative content of methyl salicylate as the main component.

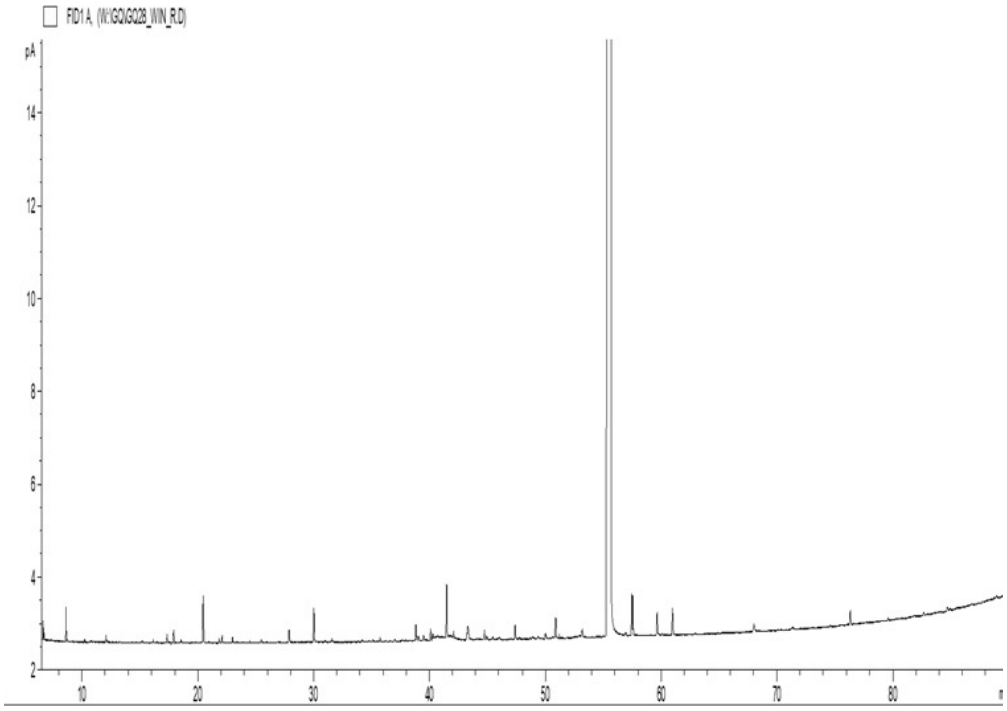


**Figure 1.** GC Spectra of Gandapura Oil.

**Table 2.** Composition of Gandapura Oil Compounds Based on GC Analysis.

| Peak | RT (Min) | Compound Name | % |
|---|---|---|---|
| 1 | 8,63 | Alpha-Pinene | 0,03 |
| 2 | 12,09 | Beta-Pinene | 0,01 |
| 3 | 17,35 | Limonene | 0,01 |
| 4 | 17,91 | 1,8-Cineole | 0,02 |
| 5 | 20,47 | Gamma-Terpinene | 0,06 |
| 6 | 27,88 | 1-Hexanol | 0,02 |
| 7 | 30,02 | 3-Hexen-1-ol | 0,05 |
| 8 | 38,82 | Ethyl Methylpentanol | 0,02 |
| 9 | 40,10 | Ketone Compound Mw=192 | 0,02 |
| 10 | 41,49 | Linalool | 0,07 |
| 11 | 43,34 | 2,4-Nonanedione | 0,04 |
| 12 | 44,77 | Beta-Caryophyllene | 0,01 |



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| | | | |
|---|---|---|---|
| 13 | 50,89 | Alpha-Terpineol | 0,03 |
| 14 | 55,67 | Methyl Salicylate | 99,45 |
| 15 | 57,51 | Ethyl Salicylate | 0,06 |
| 16 | 59,64 | Geraniol | 0,03 |
| 17 | 60,98 | Benzyl Alcohol | 0,04 |
| 18 | 76,35 | Eugenol | 0,02 |
| | | Total | 99,98 |

GC analysis of *Gaultheria procumbens* L. essential oil revealed methyl salicylate as the major constituent (99.45%), while minor components such as linalool (0.07%), geraniol (0.03%), and eugenol (0.02%) were detected in trace amounts. This result is consistent with previous reports indicating methyl salicylate as the predominant compound in wintergreen oil.[8]

*3.2. Fourier Transform Infrared Analysis (FT-IR)*

Based on the FT-IR analysis results obtained, the spectrum shows the presence of functional groups in commercial gandapura oil samples, nitration reaction products, and crystallized nitration products. Functional group identification was performed based on infrared absorption patterns at specific wave numbers, as shown in the following figure.

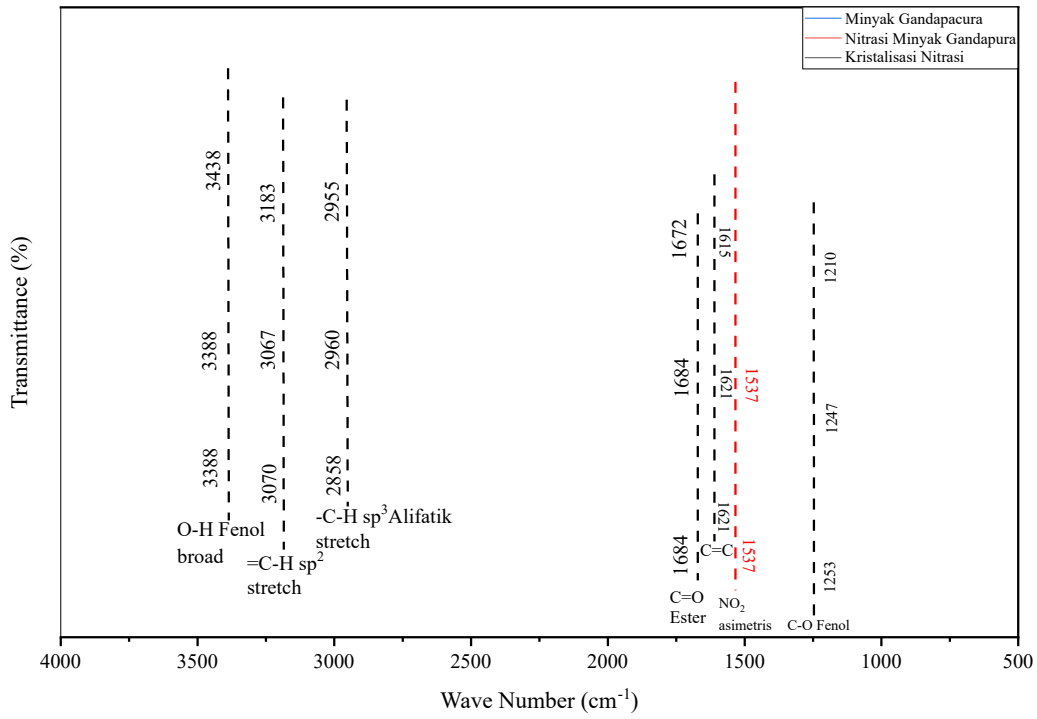


**Figure 2.** Analysis of FT-IR Spectra of Gandapura Oil, Nitration, and Recrystallized Products.

**Figure 2** shows differences in absorption peaks between commercial gandapura oil, nitration products, and recrystallization products, indicating changes in functional groups after the reaction. In commercial gandapura oil, a characteristic peak appears at a wavelength of 3383 $cm^{-1}$, which is identified as the strain of the phenolic -OH group (broad). In the nitration and recrystallization products, the absorption band still appears around 3383 $cm^{-1}$, indicating the presence of phenolic -OH stretching vibrations.


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The stretching vibration =C-H $sp^2$ in the range of 3000-3250 $cm^{-1}$ shifted from 3183 $cm^{-1}$ in gandapura oil to 3067 $cm^{-1}$ and 3070 $cm^{-1}$ in the nitration and recrystallization products. This shift indicates a change in the aromatic C-H bond environment due to the introduction of the -$NO_2$ group into the aromatic ring. The aliphatic C-H ($sp^3$) stretching band also underwent a small shift from 2955 $cm^{-1}$ to 2960 $cm^{-1}$ in the nitration product and 2858 $cm^{-1}$ in the recrystallization product, indicating that the methoxy group (-$OCH_3$) of the ester remained unchanged.

Strong absorption at 1672 $cm^{-1}$ in gandapura oil indicates the presence of C=O ester groups, which shifted to 1684 $cm^{-1}$ after nitration due to the electron withdrawal effect of the nitro group bound to the aromatic ring. The aromatic C=C band also shifts slightly from 1615 $cm^{-1}$ to 1621 $cm^{-1}$, indicating that the benzene ring structure is maintained after the nitration reaction.

A significant change is observed with the appearance of new bands at 1537 $cm^{-1}$, which are absent in the gandapura oil spectrum, indicating the successful nitration reaction. In addition, the absorption band of the phenol C-O group shifted from 1210 $cm^{-1}$ in gandapura oil to 1247 $cm^{-1}$ in the nitration product and 1253 $cm^{-1}$ in the recrystallization product.

The following table presents reference data showing the differences in absorption peaks among commercial wintergreen oil, the nitration product, and the recrystallized product, indicating changes in functional groups after the reaction.

**Table 3.** Comparative FT-IR Spectra of Wintergreen Oil, Nitration Product, and Recrystallized Product.

| Spectral Region ($cm^{-1}$).[6] | Functional Group | Peak Absorption ($cm^{-1}$) | | |
|---|---|---|---|---|
| | | Wintergreen Oil | Nitration | Recrystallization |
| 3250-3650 $cm^{-1}$ | O-H Fenol (*broad*) | 3438 $cm^{-1}$ | 3383 $cm^{-1}$ | 3383 $cm^{-1}$ |
| 3000-3250 $cm^{-1}$ | =C-H $sp^2$ (*stretch*) | 3183 $cm^{-1}$ | 3067 $cm^{-1}$ | 3070 $cm^{-1}$ |
| 2850-2960 $cm^{-1}$ | C-H $sp^3$ Alifatik (*stretch*) | 2955 $cm^{-1}$ | 2960 $cm^{-1}$ | 2858 $cm^{-1}$ |
| 1725-1750 $cm^{-1}$ | C=O Ester (*stretch*) | 1672 $cm^{-1}$ | 1684 $cm^{-1}$ | 1684 $cm^{-1}$ |
| 1600-1650 $cm^{-1}$ | C=C (*stretch*) | 1615 $cm^{-1}$ | 1621 $cm^{-1}$ | 1621 $cm^{-1}$ |
| 1485-1555 $cm^{-1}$ | -$NO_2$ Asimetris (*stretch*) | - | 1537 $cm^{-1}$<br>1440 $cm^{-1}$ | 1537 $cm^{-1}$ 1440 $cm^{-1}$ |
| >1200 $cm^{-1}$ | C-O Fenol (*stretch*) | 1210 $cm^{-1}$ | 1247 $cm^{-1}$ | 1253 $cm^{-1}$ |

The FT-IR spectral results indicate that nitro groups (-$NO_2$) have formed in the nitration and recrystallization products, as evidenced by the appearance of new absorption bands at 1537 $cm^{-1}$. The presence of these characteristic absorption bands suggests the formation of -$NO_2$ bonds on the aromatic ring, confirming that the nitration reaction of gandapura oil successfully produced methyl nitrosalicylate compounds.

## 4. CONCLUSION

Based on GC analysis, gandapura oil was confirmed to contain methyl salicylate as the dominant component with a composition of 99.45%, indicating high purity of the starting material. The FT-IR analysis of the nitration product showed the appearance of characteristic absorption bands corresponding to nitro (-$NO_2$) functional groups, along with the preservation of ester and aromatic functional groups. These results indicate that the nitration reaction successfully produced a nitro-substituted derivative of methyl salicylate.



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