# GC/MS-TOF ANALYSIS OF ESSENTIAL OIL COMPOSITION OF THE *Allium schoenoprasum* L. BULBS CULTIVATED FROM QUANG TRI - VIETNAM

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## ABSTRACT

The research content of the study was an investigation of the chemical compositions from the essential oils of *Allium schoenprasum* L. bulbs collected from Quang Tri-Vietnam. The essential oils extracted by hydrodistillation method. The chemical components of essential oils were analyzed using of gas chromatography-time-of-flight mass spectrometry (GC/MS-TOF). The results show that the main ingredient of the oil is organic sulfur compounds, especially, allyl polysulfides, which account for more than 76% of substances identified. The results also show that solvents used to dissolve the essential oil affect the results of the analysis. Organic sulfur compounds are best soluble in n-hexane. Comparative analysis indicated that GC/MS-TOF could analyze more compound than GC/MS-Quadrupole.

*Keywords: Allium schoenoprasum* L., essential oil, GC/MS-TOF, chive, sulfide.

## 1. INTRODUCTION

*Allium schoenoprasum* L. known as chives is a perennial monocot in the onion genus. *Allium* is the largest and most important representative genus of the *Alliaceae* family and comprises 450 species, widely distributed in the northern hemisphere. In fact, *Allium* species are a rich source of phytonutrients, useful for the treatment or prevention of a number of diseases, including cancer, coronary heart disease, obesity, hypercholesterolemia, diabetes type 2, hypertension, cataract and disturbances of the gastrointestinal tract [1]. Comprises perennial herbs with globose to piriform bulbs. The leaves are flat to cylindrical while stems are cylindrical, trigonous, or flat. The flowers are white, yellowish, pink, or purple, holding six petals that might be free or slightly connate at the base [2].

*Allium* species have used for centuries for their exceptional flavor as vegetables and spices besides being valued as ornamentals, and ethnomedicine for prevention of various diseases. Members of this genus known for their sulfur compounds enriched volatile oil [3]. The essential oil and crude extract of several *Allium* species have demonstrated antibacterial, antifungal, antioxidant and cytotoxic activities [3-9]. On the other hand, previous investigations have reported a variety of compounds including thiosulfinates, organosulfur derivatives, steroidal saponins, and terpenes. *Allium* species recognized for the presence of sulfur compounds enriched volatile oil. The essential oil obtained from chives was found to be rich in sulphur compounds five (99.12% leaves) and four (98.32% roots) components were identified being bis-(2-sulfhydryl ethyl)disulfide (72.06% leaves, 56.47% roots) the major constituent on the two oil samples while 2,4,5-trithiahexane (5.45% leaves, 15.90% roots) and tris (methylthio)-methane (4.01% leaves, 12.81% roots) were detected in lower amounts [2,10-11].

In Vietnam, *Allium* has grown in Central Vietnam such as Quang Ngai, Quang Nam, Quang Tri, especially Nghe An and Ha Tinh. In recent studies, it has found that the essential oils and extracts of *Allium* collected from Vietnam have held significant amounts of antimicrobial, antifungal and antioxidant active ingredients [8, 12].

Currently, identification and analysis of chemical constituents of essential oils are carried out manually using GC/MS or GC/FID [10, 11], a very time-consuming process that can take a trained analytical chemist many hours, with a high risk of human error. GC/MS-TOF is the specific technical analysis that has high-resolution, accurately mass analysis, fastly full spectrum acquisition, and automate. The research content of the study was an investigation of the chemical compositions from the essential oils of *Allium schoenprasum* L. bulbs collected from Quang Tri-Vietnam using GC/MS-TOF and compare with GC/MS-Quadrupole.

## 2. EXPERIMENTAL

### 2.1. Apparatus

GC/MS 6890N Agilent Technologies system coupled to time-of-flight mass spectrometry detector (GC/MS -TOF). The column used was a non-polar column DB-5, 30 m, 0.25 mm i.d., 0.25 μm $d_f$, coated with 5% phenyl 95% methylpolysiloxane. The identification of the oil components was based on the MS database (NIST Version 2.0, 2011 and Wiley Registry 8th Edition) and Mass Hunter Software.

### 2.2. Materials and Reagents

*2.2.1. Plant material*

Research material is tubers of *Allium Schoenoprasum* L. fresh, uniform, average diameter 1-2 cm, collected in Quang Tri, cleaned, grinded by machine.

*Figure 1. Allium schoenoprasum* L. cultivated from Quang Tri-Vietnam

*2.2.2. Reagents*

All the chemicals used were of analytical grade: n-hexan (99.99% GC/MS, Merck), acetone (99.99% GC/MS, Merck), ethyl acetate (99.99% GC/MS, Merck).

## 2.3. Procedure

### *2.3.1. Isolation of essential oil*

The fresh bulbs were cut into small pieces and submitted to hydrodistillation for 4h using a Clevenger-type apparatus. The oils were dried over anhydrous sodium sulfate and stored at 4 ºC.

### *2.3.2. GC-MS analysis*

Dissolve the essential oil with acetone, ethyl acetate, n-hexane and use gas chromatography-mass spectrometry (GC/MS) to identify their chemical constituents. According to the references, these are the solvents commonly used to dissolve the oil for GC/MS analysis.

These analyses were performed by using a GC/MS 6890 N Agilent Technologies system: coupled to time-of-flight mass spectrometry detector (GC/MS-TOF). The column used was a non-polar column DB-5, 30 m, 0.25 mm i.d., 0.25 μm df, coated with 5% phenyl 95% methyl polysiloxane. This chromatographic column is a specialized column used for identification of analysis essential oil components by EI/MS. Injection of 1.0μL samples was carried out, the carrier gas was Helium and injection temperature was 260 ºC. The ionization mode used was the electronic impact at 70 eV and mass range between 35 and 400 was scanned. Identification was confirmed by comparison of their spectral mass with authentic samples, with those stored in the MS database (NIST 2008 (P/N: EQ-16050N08)) and with index retention literature data using the automatic mass spectral deconvolution and identification system software (Mass Hunter Software).

# 3. RESULTS AND DISCUSSION

## 3.1. Optimization of the GC/MS/TOF device parameters

Dissolved the essential oil with acetone, injection of 1.0 μL samples, GC/MS-TOF analysis was performed as Table 1.

*Table 1.* GC/MS/TOF parameters

| | Injection volume | Split ratio | Oven temperature program |
|---|---|---|---|
| TOF 1 | 0.5 μL | 300:1 | 50 °C, hold 1 min, increase 8 °C/min to 270 °C, hold 10 min |
| TOF 2 | 0.5 μL | 50:1 | 50 °C, hold 5 min, increase 8 °C/min to 270 °C, hold 5 min |
| TOF 3 | 0.5 μL | 20:1 | 50 °C, hold 1 min, increase 8 °C/min to 270 °C, hold 10 min |
| TOF 4 | 1.0 μL | 20:1 | 50 °C, hold 1 min, increase 8 °C/min to 270 °C, hold 10 min |
| TOF 5 | 1.0 μL | 20:1 | 60 °C, hold 3 °C/min to 240 °C |

After investigating GC/MS-TOF specimens, it was found that program number 5 was optimal for identifying with the *Allium* essential oil, the peaks the symmetric and separately relatively well, the peaks with small content appear more and more clearly (Figure 1), list of sulfur compounds identified in Table 2.

*Table 2.* List of sulfur compounds identified by GC/MS-TOF – 5 (acetone)

| S.No. | Compound name | R. Time (min) | % Area |
|---|---|---|---|
| 1 | Methyl propyl trisulfide | 10:45 | 13.37 |
| 2 | 1,5-Dithiocane | 08:40 | 6.54 |
| 3 | cis-Propenyl propyl trisulfide | 18:19 | 6.41 |
| 4 | 2-Methyl-2-methylthio-1-propanol | 21:10 | 5.78 |
| 5 | Trisulfide dimethyl | 05:17 | 5.69 |
| 6 | trans-Propenyl propyl trisulfide | 17:59 | 5.55 |
| 7 | Trisulfide dipropyl | 17:10 | 5.50 |
| 8 | 1,4-Dimethyl tetrasulfane | 14:33 | 4.97 |
| 9 | 2,4-Dimethyl-5,6-dithia-2,7-nonadienal | 30:57 | 4.41 |
| 10 | Disulfide methyl 1-(methylthio)propyl | 15:05 | 4.20 |
| 11 | 1-Propene, 1-(methylthio)-, (z)- | 11:39 | 3.12 |
| 12 | 1,3-Dithiane | 24:22 | 2.98 |
| 13 | 1,2,3-Trithiolane, 4-methyl- | 32:22 | 2.92 |
| 14 | 1-Propene 1-(methylthio)-, (e)- | 11:20 | 2.73 |
| 15 | Disulfide methyl propyl | 03:46 | 2.72 |
| 16 | Disulfide dipropyl | 08:04 | 2.61 |
| 17 | 3-Ethyl-5-methyl-1,2,4-trithiolane | 14:39 | 2.52 |
| 18 | 6-Ethyl-4,5,7,8-tetrathianonane | 29:53 | 2.41 |
| 19 | Methyl 1-propenyl disulfide, (z)- | 04:03 | 2.39 |
| 20 | 1-Propyl-2-(4-thiohept-2-en-5-yl) disulfide | 21:58 | 1.98 |
| 21 | Methyl 1-propenyl disulfide, (e)- | 03:50 | 1.64 |
| 22 | Disulfide dimethyl | 01:44 | 1.34 |
| 23 | 1,2-Dithiolane | 21:35 | 1.15 |
| 24 | 4,6-Diethyl-1,2,3,5-tetrathiolane | 28:53 | 1.07 |
| 25 | Thiophene, 2,4-dimethyl- | 03:19 | 0.87 |
| 26 | Trisulfide, methyl 2-propenyl | 33:32 | 0.75 |
| 27 | 2-Mercapto-3,4-dimethyl-2,3-dihydrothiophene | 23:12 | 0.70 |
| 28 | 8-Ethyl-4,5,6,7,9-pentathiadecane | 21:51 | 0.70 |
| 29 | Carboisopropoxy methoxy sulfide | 27:17 | 0.61 |
| 30 | Disulfide methyl 1-(methylthio)ethyl | 11:55 | 0.61 |
| 31 | Diallyl disulphide | 13:51 | 0.61 |
| 32 | Carboisopropoxy carbomethoxymethyl disulfide | 29:08 | 0.36 |
| 33 | 6-ethyl-4,5,7,8-tetrathia-2-nonene | 30:39 | 0.36 |
| 34 | Methyl methanesulfonylacetate | 25:53 | 0.34 |
| 35 | Disulfide methyl 2-propenyl | 03:39 | 0.10 |

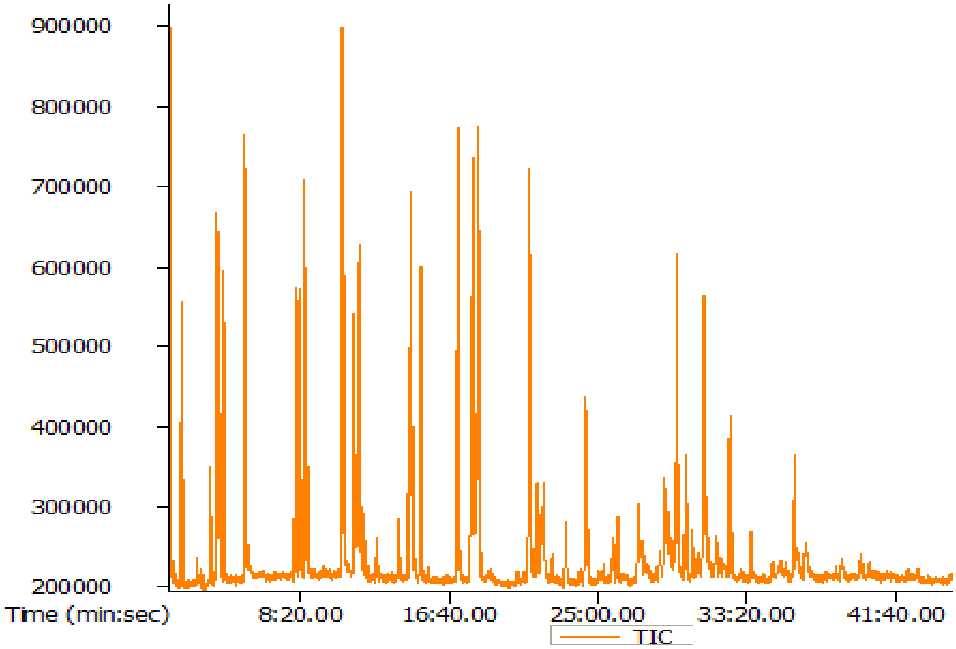


*Figure 2.* GC-MS chromatogram of program TOF – 5 (acetone)

Comparison of substances obtained with the universal library identified 46 volatile substances (excluding solvents). Of these, 35 sulfur compounds (Table 2) accounted for 76% of all identified compounds. Compared with the reference [5, 10] has the same components such as dipropyl trisulfide; dimethyl trisulfide; dipropyl disulfide; methyl propyl trisulfide; trans and cis propenyl propyl trisulfide. In addition, 1-propenyl methyl disulfide, 1, 3-dithiane; 3-ethyl-5-methyl-1, 2, 4-trithiolane; 1, 4-dimethyl tetrasulfide has been identified. These compounds are present in onions and garlic essential oil not yet mentioned in Allium essential oil in the reference. This is explained by the sealed distillation system and optimal analysis program should get more compound than the previous report.

## 3.2. Survey on influence of solvents dissolve essential oil

### *3.2.1. Allium essential oil was dissolved by ethyl acetate*

*Allium* essential oil dissolved by ethyl acetate, the investigator (Table 1, program TOF 5) performed GC/MS-TOF analysis, a list of sulfur compounds identified in Table 3.

*Table 3:* List of sulfur compounds identified by GC/MS- TOF – 5 (ethyl acetate)

| S.No. | Compound name | R. Time (min) | % Area |
|---|---|---|---|
| 1 | Methyl propyl trisulfide | 10:50 | 11.01 |
| 2 | Dimethyl trisulfide | 05:24 | 9.13 |
| 3 | cis-Propenyl propyl trisulfide | 18:01 | 8.37 |
| 4 | 1,4-Dimethyl tetrasulfane | 14:42 | 8.31 |
| 5 | trans-Propenyl propyl trisulfide | 18:22 | 8.29 |
| 6 | 2,4-Dimethyl-5,6-dithia-2,7-nonadienal | 28:29 | 6.74 |
| 7 | 1-Propene, 1-(methylthio)-, (z)- | 11:48 | 6.35 |
| 8 | 1-Propene, 1-(methylthio)-, (e)- | 11:27 | 6.17 |

| S.No. | Compound name | R. Time (min) | % Area |
|---|---|---|---|
| 9 | Dimethyl tetrasulfide | 21:15 | 5.82 |
| 10 | Methyl 1-propenyl disulfide, (z)- | 04:09 | 4.10 |
| 11 | Trisulfide dipropyl | 17:12 | 3.72 |
| 12 | 1-Propyl-2-(4-thiohept-2-en-5-yl) disulfide | 21:59 | 2.34 |
| 13 | Methyl 1-propenyl disulfide, (e)- | 03:54 | 2.13 |
| 14 | 2-Mercapto-3,4-dimethyl-2,3-dihydrothiophene | 12:13 | 1.67 |
| 15 | [2-13c]-1,3-Dithiane | 24:23 | 1.61 |
| 16 | 1,2,3-Trithiolane, 4-methyl- | 12:39 | 0.96 |
| 17 | 1-Propene, 3,3'-thiobis- | 18:28 | 0.77 |
| 18 | Disulfide dipropyl | 08:06 | 0.77 |
| 19 | Disulfide methyl 1-(methylthio)propyl | 15:07 | 0.69 |
| 20 | Diallyl disulphide | 13:53 | 0.67 |
| 21 | 1-Methyl-2-(3,5-dimethylthien-4-yl) disulfide | 25:45 | 0.61 |
| 22 | 2-Propenyl sulphide | 18:59 | 0.58 |
| 23 | 6-Ethyl-4,5,7,8-tetrathia-2-nonene | 30:39 | 0.55 |
| 24 | Disulfide dimethyl | 01:45 | 0.55 |
| 25 | Pentasulfide dimethyl | 25:04 | 0.51 |
| 26 | Disulfide methyl propyl | 03:48 | 0.48 |
| 27 | Disulfide 1-methylethyl propyl | 27:17 | 0.39 |
| 28 | 6-Ethyl-4,5,7,8-tetrathianonane | 29:53 | 0.32 |
| 29 | Trisulfide methyl 2-propenyl | 33:32 | 0.27 |
| 30 | Thiophene 2,4-dimethyl- | 03:21 | 0.19 |

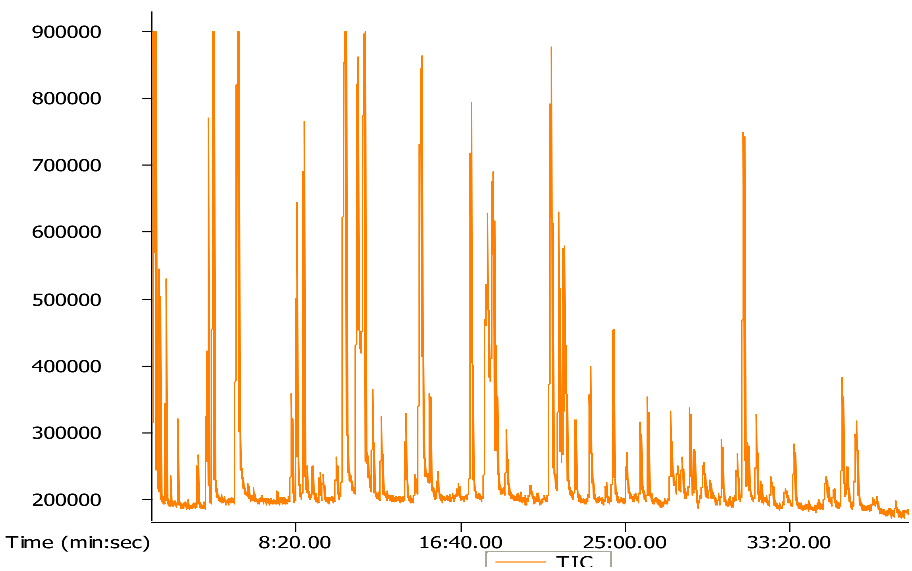


*Figure 3.* GC-MS chromatogram of program TOF – 5 (ethyl acetate)

Comparison of substances received with the universal library identified 38 substances (excluding solvent). Of these, 30 sulfide compounds (Table 3) accounted for 80% of all identified compounds, more than reference materials. Compared to the reference [5, 10] has the same components as dimethyl disulfide; disulfide methyl propyl; methyl 1-propenyl disulfide, (e) -; methyl 1-propenyl disulfide, (z) -; dimethyl trisulfide; dipropyl disulfide; cis and trans propenyl propyl disulfide; methyl propyl trisulfide; dipropyl trisulfide. In addition, compounds such as trans and cis propenyl propyl trisulfide, methyl propyl disulfide; 1,3-dithiane; 2,4-dimethyl-5,6-dithio-2,7-nonadiene; 1,4-dimethyl tetra sulfide are identified. These are substances found in onions and garlic but not identified in *Allium* essential oil in previous studies.

### *3.2.2. Allium essential oil was dissolved by n-hexane*

*Allium* essential oil dissolved in n-hexane, the investigator (Table 1, program TOF 5) performed GC/MS-TOF analysis, a list of sulfur compounds identified in Table 4.

*Table 4.* List of sulfur compounds identified by GC/MS-TOF-5 (n-hexane)

| S.No. | Compound name | R. Time (min) | %Area |
|---|---|---|---|
| 1 | 1-Propene 1-(methylthio)-, (z)- | 11:27 | 15.8 |
| 2 | Methyl propyl trisulfide | 10:51 | 10.0 |
| 3 | 3-Ethyl-5-methyl-1,2,4-trithiolane | 14:41 | 7.79 |
| 4 | Disulfide methyl propyl | 21:16 | 6.55 |
| 5 | Dimethyl trisulfide | 05:21 | 5.31 |
| 6 | 2,4-Dimethyl-5,6-dithia-2,7-nonadienal | 30:59 | 4.91 |
| 7 | trans-Propenyl propyl disulfide | 08:44 | 4.82 |
| 8 | 1-Propyl-2-(4-thiohept-2-en-5-yl) disulfide | 22:00 | 3.47 |
| 9 | Trisulfide dipropyl | 17:11 | 3.26 |
| 10 | Methyl 1-propenyl disulfide, (z)- | 04:07 | 3.17 |
| 11 | 1,5-Dithiocane | 08:21 | 3.11 |
| 12 | Disulfide methyl 2-propenyl | 21:39 | 3.08 |
| 13 | Trisulfide di-2-propenyl | 18:18 | 3.06 |
| 14 | Cis propenyl propyl trisulfide | 18:01 | 2.71 |
| 15 | 1,3-Dithiane | 24:24 | 2.51 |
| 16 | Allyl n-propyl sulphide | 17:55 | 2.41 |
| 17 | Ethene, 1,2-bis(methylthio)- | 21:54 | 2.32 |
| 18 | 2-Mercapto-3,4-dimethyl-2,3-dihydrothiophene | 12:12 | 1.89 |
| 19 | Methyl 1-propenyl disulfide, (e)- | 03:52 | 1.87 |
| 20 | Disulfide methyl 1-(methylthio)propyl | 15:07 | 1.74 |
| 21 | Disulf dipropyl | 08:05 | 1.64 |
| 22 | Diallyl disulphide | 18:29 | 1.46 |
| 23 | Diallyl sulfide | 18:58 | 1.14 |
| 24 | Carboisopropoxy methoxy sulfide | 27:18 | 0.74 |
| 25 | 10,11-dioxatricyclo[6.2.2.0(1,6)]dodecane-7,7,8-tricarbonitrile, 9-imino-12-thiophen-2-yl- | 23:13 | 0.73 |
| 26 | 2-Vinyl-1,3-dithiane | 09:09 | 0.65 |
| 27 | Diallyl tetrasulfide | 27:53 | 0.58 |
| 28 | Pentasulfide dimethyl | 25:04 | 0.55 |

| S.No. | Compound name | R. Time (min) | %Area |
|---|---|---|---|
| 29 | 4,6-Diethyl-1,2,3,5-tetrathiolane | 28:59 | 0.51 |
| 30 | 1,2,3-Trithiolane, 4-methyl- | 12:38 | 0.41 |
| 31 | Disulfide methyl 1-(methylthio)ethyl | 11:58 | 0.40 |
| 32 | Methyl allylthioacetate | 09:30 | 0.39 |
| 33 | Diallyl disulphide | 13:52 | 0.33 |
| 34 | 6-Ethyl-4,5,7,8-tetrathia-2-nonene | 30:38 | 0.24 |
| 35 | Disulfide dimethyl | 01:44 | 0.17 |
| 36 | Thiophene 2,4-dimethyl- | 03:20 | 0.14 |
| 37 | Diallyl trisulfide | 33:32 | 0.07 |

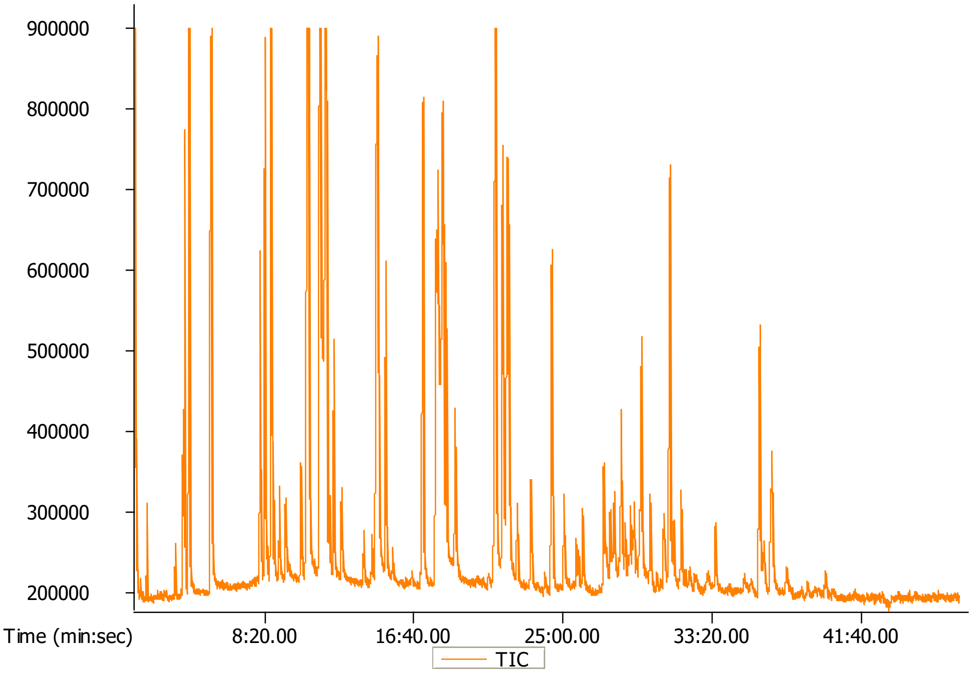


*Figure 4.* GC-MS chromatogram of program TOF – 5 (n-hexane)

Comparison of substances obtained with the universal library identified 40 substances (excluding solvent). Of these, 37 sulfide compounds (Table 4) accounted for 93% of all identified compounds, 17% more than acetone, and 13% as compared to ethyl acetate and reference materials. The results of the identified components are similar to references [5, 10] disulfide dimethyl; methyl 1-propenyl disulfide, (e) -; methyl 1-propenyl disulfide, (z) -; dimethyl trisulfide; disulfide, dipropyl; trans-propenyl propyl disulfide; trisulfide, dipropyl; diallyl disulphide; diallyl sulfide disulfide, methyl propyl; diallyl trisulfide.

In addition, common compounds found in garlic bulbs but not yet identified in previous reports have also been identified in *Allium* essential oil as methyl propyl trisulfide; 1,3-dithiane; 2,4-dimethyl-5,6-dithia-2,7-nonadiene; 3-Ethyl-5-methyl-1,2,4-trithiolane.

Many allyl sulfide compounds not yet mentioned in *Allium* essential oil in the reference have been identified such as: thiophene, 2,4-dimethyl; 1,5-dithiocane; 2-vinyl-1,3-dithiane; methyl allylthioacetate; methyl propyl trisulfide; 1-propene, 1- (methylthio) -, (z) -; disulfide, methyl 1-methylthio) ethyl; 2-mercapto-3,4-dimethyl-2,3-dihydrothiophene; 1,2,3-trithiolane, 4-methyl-; 3-ethyl-5-methyl-1,2,4-trithiolane; disulfide, methyl 1- (methylthio) propyl; allyl n-propyl sulphide; cis propenyl propyl trisulfide; trisulfide, di-2-propenyl; disulfide, methyl

2-propenyl; ethene, 1,2-bis (methylthio)-; 1-propyl-2- (4-thiohept-2-en-5-yl) disulfide; 3 (2h) -furanone; 1,3-dithiane; pentasulphide,...

*3.2.3. Comparison and evaluation*

The results of the investigations on the effect of solvents using soluble essential oils showed that acetone was the best soluble oil as 46 compounds were identified in *Allium* essential oils. Although when dissolving the essential oils with ethyl acetate and n-hexane, the number of compounds was less identified than the acetone solvent with 38 and 40 compounds, respectively. However, when compared to the total number of compounds detected, the number of organic sulfur compounds in n-hexane and ethyl acetate was higher when dissolved with acetone (Table 5). This problem is explained by the effect of solvent polarization on the soluble compounds in essential oils. The results show that disulfide compounds are highly soluble in acetone (polar aprotic solvents), while ethyl acetate (polar aprotic solvents but significantly less polar than acetone) dissolves trisulfide and tetrasulfide; compounds mainly soluble in n-hexane (non-polar solvents) are monosulfides, disulfide, and trisulfide (Figure 5).

*Table 5.* Comparison and evaluation of the effect of solvents using soluble essential oils

| | Acetone | Ethyl acetate | N-hexane |
|---|---|---|---|
| Total | 46 | 38 | 40 |
| Organic sulfur compound | 35 | 30 | 37 |
| Percentage of sulfur compounds | 76% | 80% | 93% |

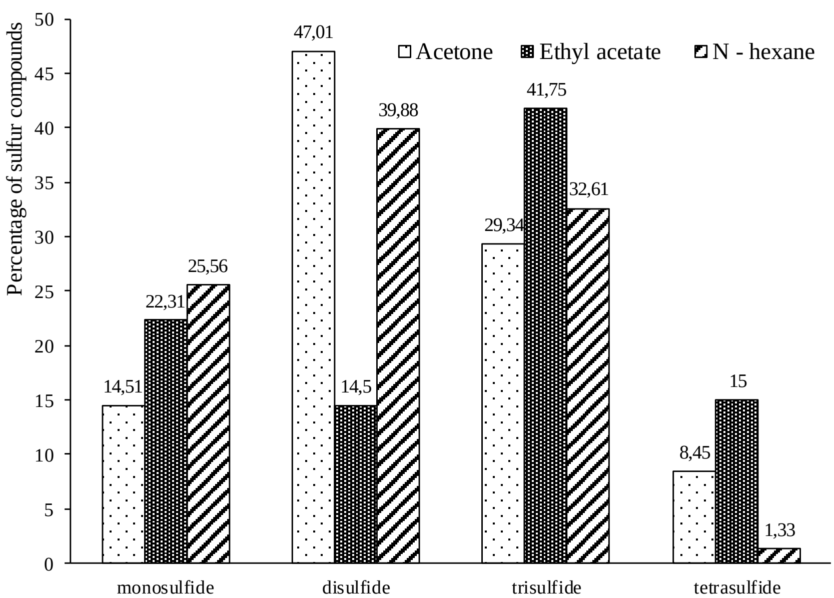


*Figure 5.* Effect of solvents using soluble essential oils

## 3.3. Comparison of GC/MS-TOF and GC/MS-quadrupole

A sample of the solvated oil extracted by solvent analyzed on GC/MS-TOF and GC/MS-quadrupole with the following investigations to determine the chemical composition of the essential oil in Table 6. As a result, all three compound solvents determined by TOF are always more than quadrupole.

*Table 6.* Comparison of the number of compounds identified from the two methods

| Solvent | TOF | | Quadrupole | |
|---|---|---|---|---|
| | Total compounds | Organic sulfur compounds | Total compounds | Organic sulfur compounds |
| Acetone | 46 | 35 | 40 | 35 |
| Ethyl acetat | 38 | 30 | 35 | 32 |
| N-hexan | 40 | 37 | 38 | 34 |

## 4. CONCLUSION

Research results and chemical composition analysis of essential oils from *Allium schoenprasum L.* showed that the main constituents of the essential oil were sulfur compounds, especially allyl polysulfides, which accounted for more than 76% of all identified substances. Compared with the reference, the survey program identified more compounds, many allyl sulfide compounds not yet mentioned in *Allium* essential oil in previous studies. The results also show that solvents used to dissolve the essential oil affect the results of the analysis. Comparing Q-TOF GC/MS and GC/MS-quadrupole, Q-TOF GC/MS can analyze more compounds than quadrupole.

However, research is still limited, it is necessary to investigate the following issues: the impact of geographic conditions, seasons, and conditions of separation of essential oils to ingredients in essential oils.

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## TÓM TẮT

PHÂN TÍCH THÀNH PHẦN TINH DẦU CỦ NÉN (*Allium schoenoprasum* L.)
ĐƯỢC TRỒNG Ở QUẢNG TRỊ BẰNG PHƯƠNG PHÁP GC/MS-TOF

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Nội dung nghiên cứu của báo cáo là phân tích thành phần hóa học của tinh dầu củ nén (*Allium schoenprasum* L.) được trồng ở Quảng Trị-Việt Nam, tinh dầu được chiết xuất bằng phương pháp chưng cất lôi cuốn hơi nước. Kết quả phân tích tinh dầu bằng phương pháp GC/MS-TOF cho thấy thành phần chính trong tinh dầu là hợp chất lưu huỳnh hữu cơ, đặc biệt là allyl polysulfides, chiếm hơn 76% trong tổng số các chất được xác định. Kết quả nghiên cứu cũng cho thấy dung môi sử dụng để hòa tan tinh dầu có ảnh hưởng đến kết quả phân tích. Khi so sánh trên tổng chất nhận danh được thì kết quả khảo sát cho thấy các hợp chất lưu huỳnh hữu cơ tan tốt trong n-hexan. So sánh kết quả phân tích trên GC/MS-TOF và GC/MS-Quadrupole cho thấy GC/MS-TOF có độ phân giải tốt nên nhận danh được nhiều chất hơn, thích hợp hơn trong phân tích thành phần tinh dầu.

*Từ khóa: Allium schoenprasum* L., tinh dầu, GC/MS-TOF, củ nén, sulfide.