# Substance Characterisation Report

Test Item: Anti-mold Chip (WS)

**Sponsor**:
Wan Shuen Company
Abt.: Hsin-Yi Wang
No. 158 Yichang E. Rd., Taiping Dist
411 Taichung City

**Test Facility:**
LAUS GmbH
Auf der Schafweide 20
D-67489 Kirrweiler, Germany

**Monitor:**
Wan Shuen Company
Abt.: Hsin-Yi Wang
No. 158 Yichang E. Rd., Taiping Dist
411 Taichung City

**Managing Director:**

21 SEP 2017

Date Dr. Dietmar Kuhn

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# 1 PURPOSE OF THE STUDY

This study was performed in order to characterise Anti-mold Chip (WS). Different spectra and chromatograms were measured.

# 2 MATERIALS AND METHODS

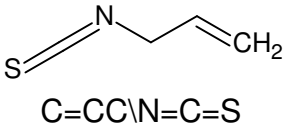
## 2.1 Test Item

### 2.1.1 Specification

The following information concerning identity and composition of the test item was provided by the sponsor.

| | |
|---|---|
| Name | Anti-mold Chip (WS) |
| Batch no. | 3102 |
| Appearance | not stated |
| Composition | not stated |
| CAS No. | 57-06-7 |
| EINECS-No. | not stated |
| Molecular formula | C4H5NS |
| Molecular weight | 99.15 g/mol |
| Purity | <= 100 % |
| Homogeneity | not stated |
| Vapour pressure | not stated |
| Stability | not stated |
| Solubility | not stated |
| Production date | 04. 2017 |
| Expiry date | 01.04.2018 |
| Storage | not stated |
| Hazard information | not stated |
| P-phrases | not stated |
| H-phrases | not stated |
| Number of reports | 2 |

2.1.2 Structure, SMILES Code, etc. generated for Anti-mold Chip (WS) (CAS 57-06-7) by ACD/ChemSketch




C=CC\N=C=S

| | |
|---|---|
| Molecular Formula: | $C_4H_5NS$ |
| Formula Weight: | 99.1542 |
| Composition: | C(48.45%) H(5.08%) N(14.13%) S(32.34%) |
| Molar Refractivity: | 31.17 ± 0.5 $cm^3$ |
| Molar Volume: | 108.8 ± 7.0 $cm^3$ |
| Parachor: | 249.8 ± 8.0 $cm^3$ |
| Index of Refraction: | 1.484 ± 0.05 |
| Surface Tension: | 27.7 ± 7.0 dyne/cm |
| Density: | 0.91 ± 0.1 $g/cm^3$ |
| Dielectric Constant: | Not available |
| Polarizability: | 12.35 ± 0.5 $10^{-24}cm^3$ |
| RDBE: | 3 |
| Monoisotopic Mass: | 99.014269 Da |
| Nominal Mass: | 99 Da |
| Average Mass: | 99.1542 Da |
| M+: | 99.013721 Da |
| M-: | 99.014818 Da |
| [M+H]+: | 100.021546 Da |
| [M+H]-: | 100.022643 Da |
| [M-H]+: | 98.005896 Da |
| [M-H]-: | 98.006993 Da |

2.1.3 Storage

The test item was stored in a closed vessel at room temperature.

## 2.2 Instruments

2.2.1 GC/MS

| | |
|---|---|
| Injector/sampler | Gerstel KAS4/MPS2-L |
| GC | Agilent 7890 |
| Capillary Column | Restek Rxi 624, 30 m x 0.18 mm x 1 µm film |
| MS | Agilent 59777 A Quadrupol MS |

## 2.3 Reagents

None reagents of analytical grade were used.

# 3 PERFORMANCE OF THE STUDY

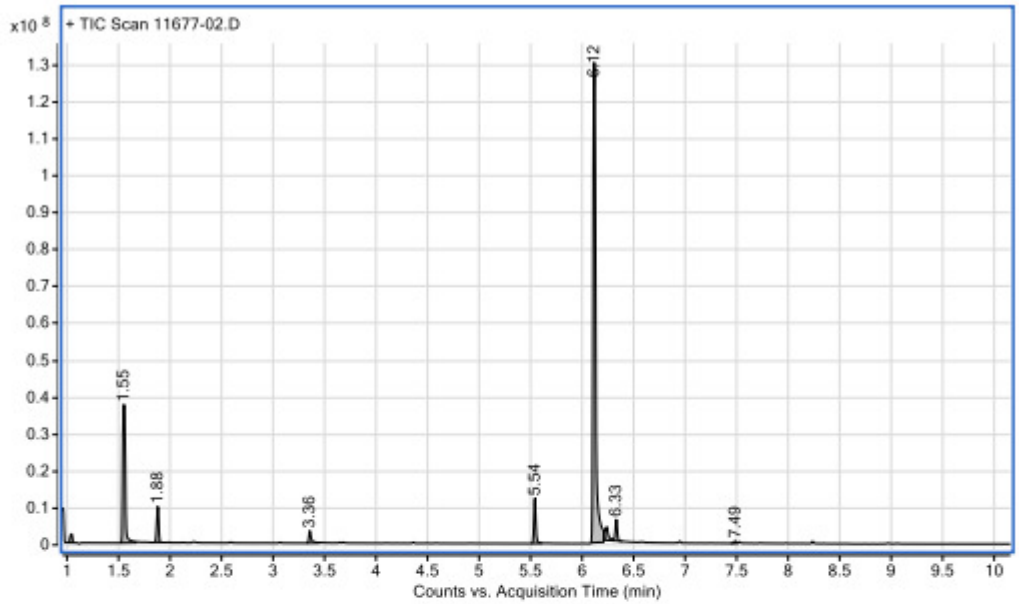
## 3.1 GC-MS

| | |
|---|---|
| Sample Preparation | Remove 1 adhesive sticker from its carrier and transfer it into a 20 mL headspace vial. |
| GC Oven program | 50 °C for 0.5 min<br>then 15 °C/min to 150 °C for 0 min.<br>30 °C/min to 180 °C for 2 min. |
| GC-Injector | |
| Carrier gas | Hydrogen |
| Mode | split |
| Injector temp. | 180 °C |
| Flow | 0.9 mL/min |
| Split ratio | 80:1 |
| Inj. volume | 500 µL Headspace |
| GC Headspace Incubation | 6 min @ 60 °C |
| MS Parameters | |
| Ionization | EI 70 eV |
| Mode | Scan m/z 35 – 240 |
| Signal used for peak integration | Total Ion Current m/z 35 – 240 |
| Peaks considered | > 0.1 area % of largest peak |
| Mass spectra database | NIST14: National Institute of Standards and Technology 2014 |

# 4 FINDINGS

## 4.1 GC-MS

### 4.1.1 Chromatogram 17082503S: Anti-mold Chip (WS)




| Peak | RT [min] | Area Sum % |
|---|---|---|
| 1 | 1.05 | 0.94 |
| 2 | 1.55 | 18.62 |
| 3 | 1.88 | 3.56 |
| 4 | 3.36 | 1.51 |
| 5 | 5.54 | 4.31 |
| 6 | 6.12 | 66.62 |
| 7 | 6.24 | 2.06 |
| 8 | 6.33 | 2.16 |
| 9 | 7.49 | 0.21 |

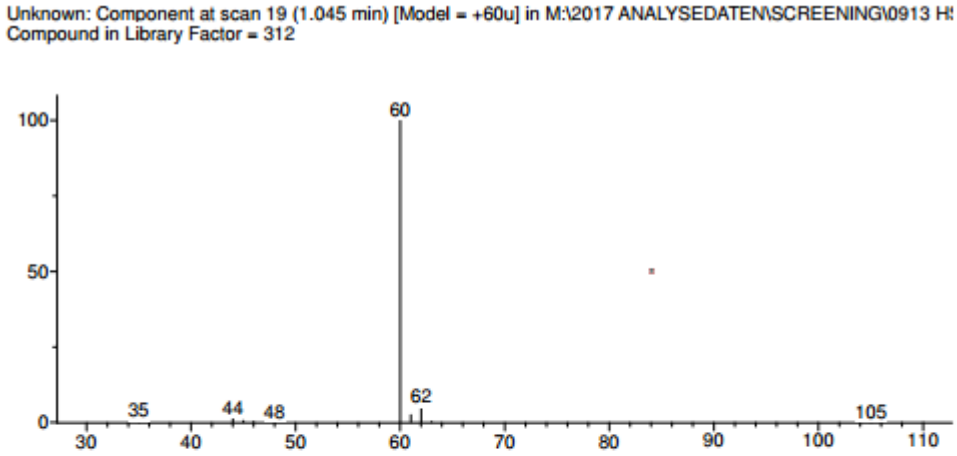
Sample peaks below 0.1 area sum % and system background peaks are not included.

**Mass Spectra Library Search Results**

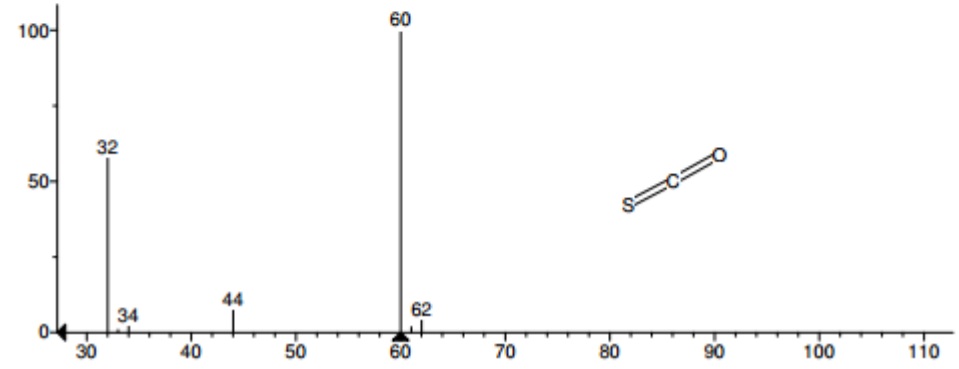
**Contained in attached reports.**
Library search results items for each reported peak:
Deconvoluted mass spectrum at peak apex, mass spectrum and structural formula of 2 best library hits.
Similarity (forward: MF and reverse: RMF) with score range 0 to 1000.

### 4.1.2 MS-Spectra

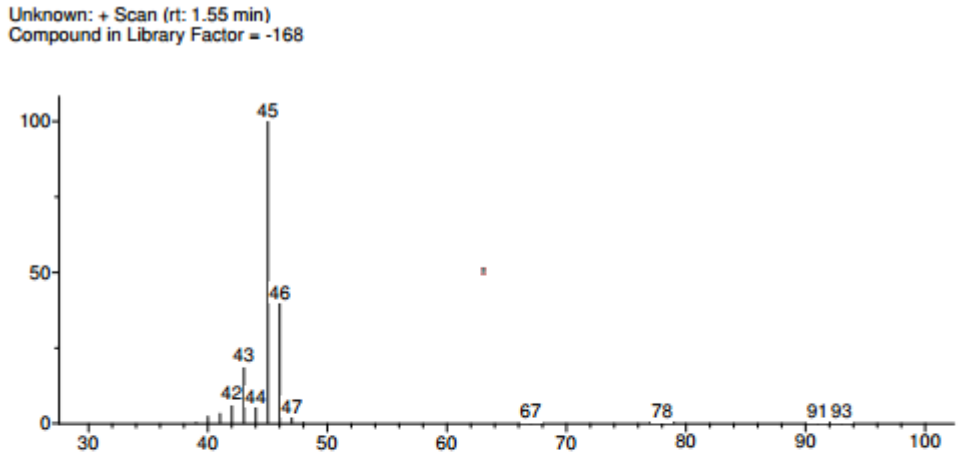
Peak 1 at 1.045 min.: identified as Carbonyl sulfide (CAS 463-58-1)

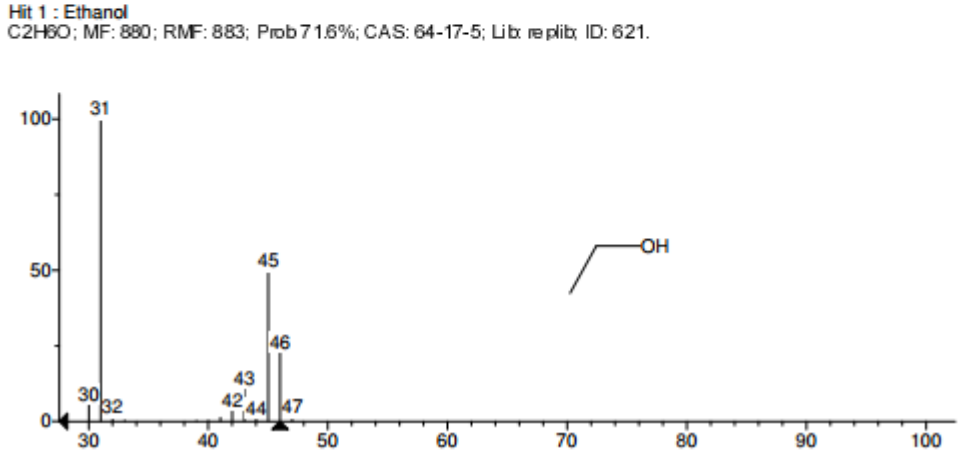



Hit 1 : Carbonyl sulfide
COS; MF: 940; RMF: 943; Prob 90.0%; CAS: 463-58-1; Lib: mainlib; ID: 30818.



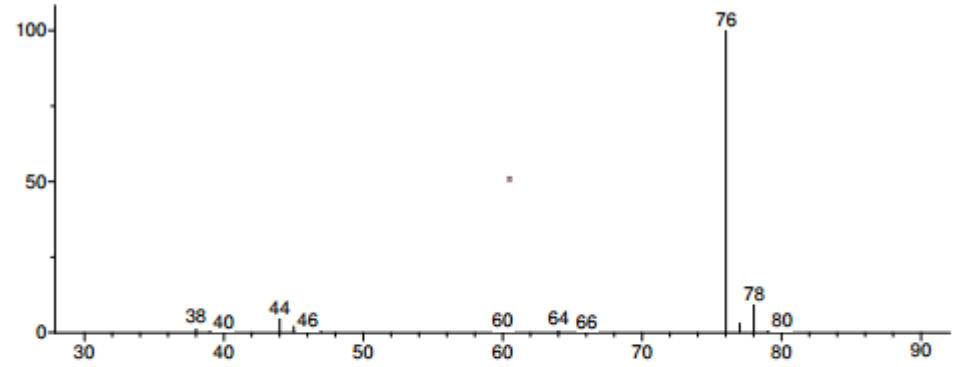
Peak 2 at 1.55 min.: identified as Ethanol (CAS 64-17-5)



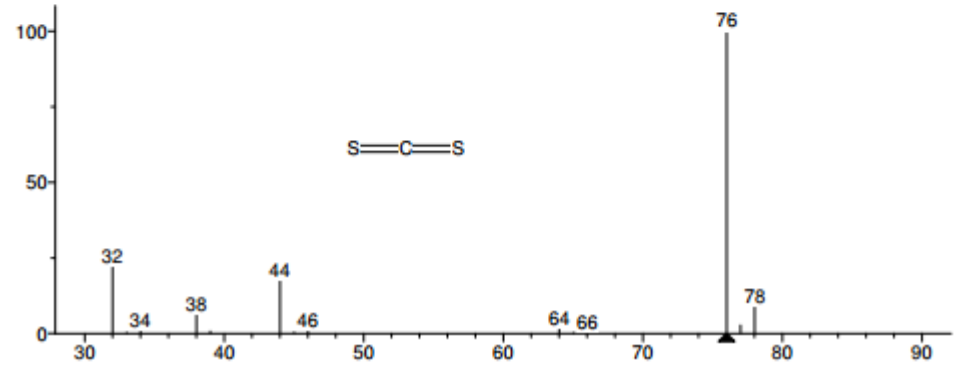



Peak 3 at 1.884 min.: identified as Carbon disulfide (CAS 75-15-0)

Unknown: Component at scan 192 (1.884 min) [Model = +76u] in M:\2017 ANALYSEDATEN\SCREENING\0913 I
Compound in Library Factor = 293

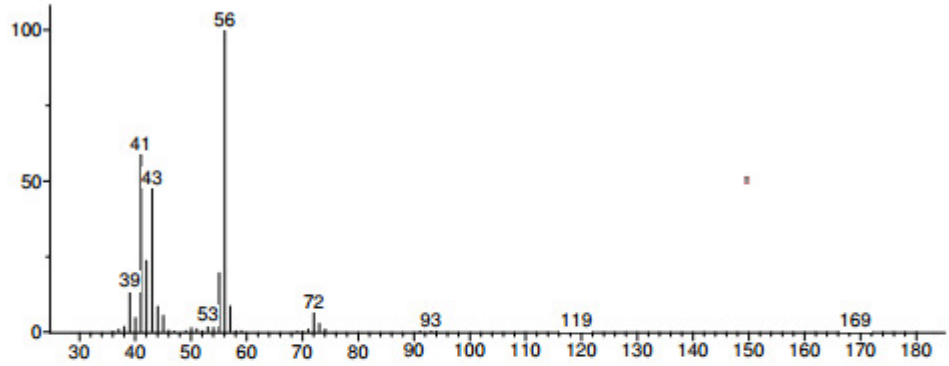



Hit 1 : Carbon disulfide
CS2; MF: 872; RMF: 875; Prob 95.2%; CAS: 75-15-0; Lib: replib; ID: 10767.

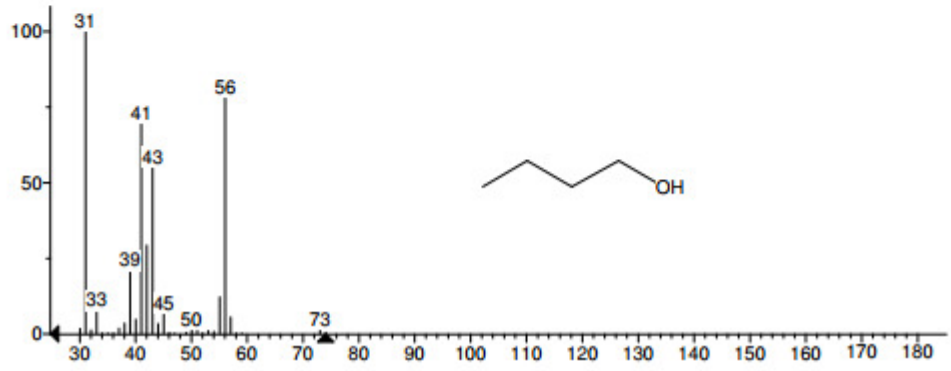


Peak 4 at 3.360 min.: identified as 1-Butanol (CAS 71-36-3)

Unknown: Component at scan 497 (3.360 min) [Model = +56u] in M:\2017 ANALYSEDATEN\SCREENING\0913 I
Compound in Library Factor = 135

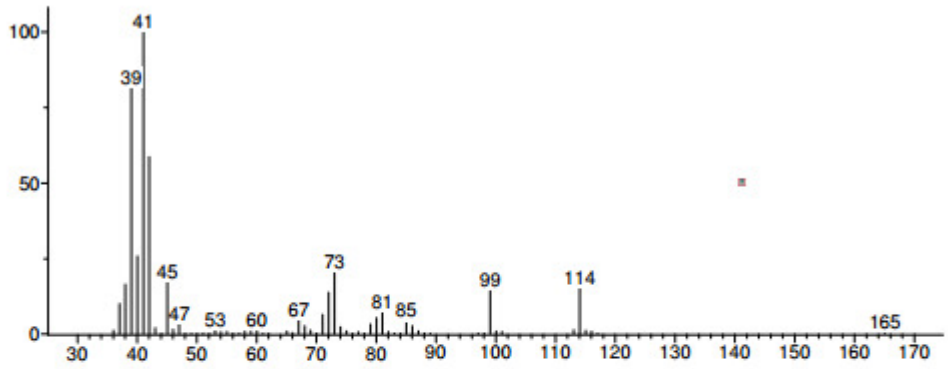



Hit 1 : 1-Butanol
C4H10O; MF: 903; RMF: 923; Prob 67.8%; CAS: 71-36-3; Lib: replib; ID: 630.

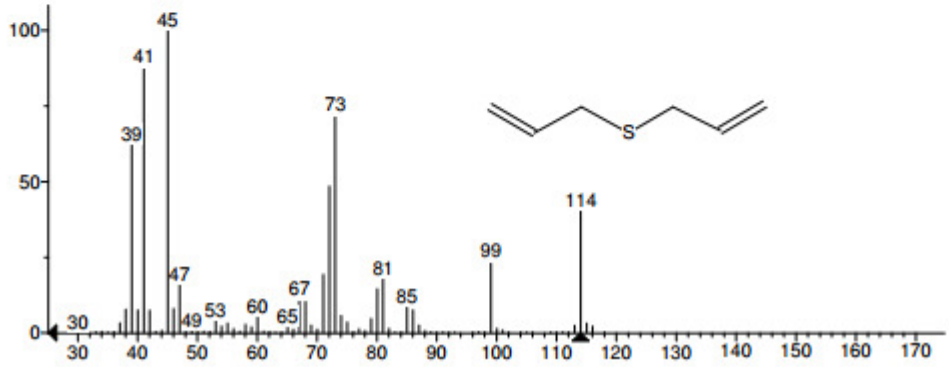


Peak 5 at 5.544 min.: identified as Diallyl sulfide (CAS 592-88-1)

Unknown: Component at scan 949 (5.544 min) [Model = +41u] in M:\2017 ANALYSEDATEN\SCREENING\0913 I
Compound in Library Factor = -136

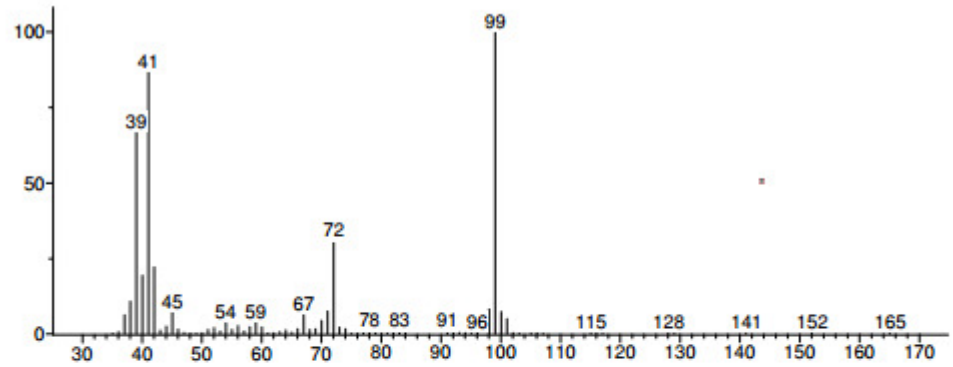



Hit 1 : Diallyl sulfide
C6H10S; MF: 827; RMF: 827; Prob 86.5%; CAS: 592-88-1; Lib: replib; ID: 3966.

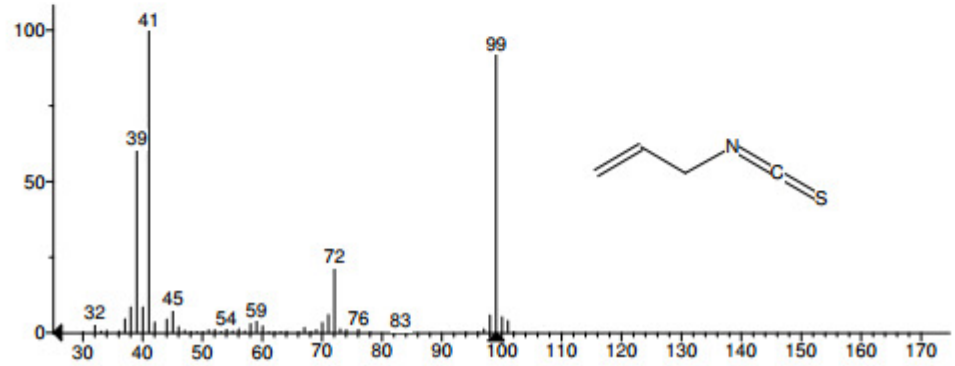


Peak 6 at 6.12 min.: identified as Allyl Isothiocyanate (CAS 57-06-7)

Unknown: + Scan (rt: 6.12 min) 11677-02.D
Compound in Library Factor = 362

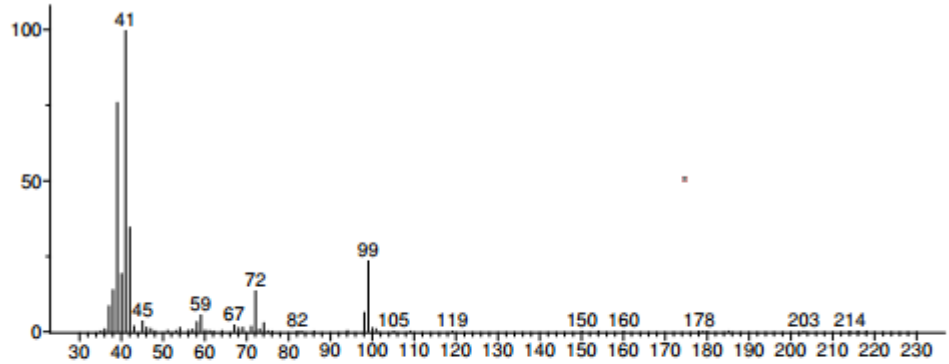



Hit 1 : Allyl Isothiocyanate
C4H5NS; MF: 891; RMF: 897; Prob 78.6%; CAS: 57-06-7; Lib: replib; ID: 1355.

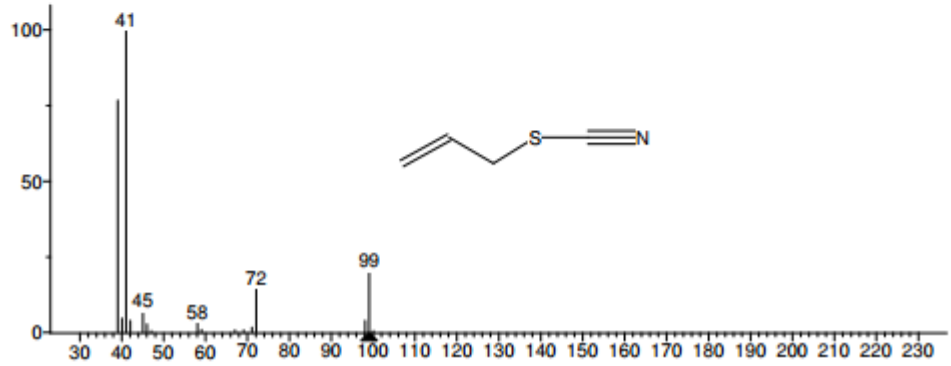


Peak 7 at 6.243 min.: identified as 2-Propenylester Thiocyanic acid (CAS 764-49-8)

Unknown: Component at scan 1093 (6.243 min) [Model = +41u] in M:\2017 ANALYSEDATEN\SCREENING\0913
Compound in Library Factor = -324

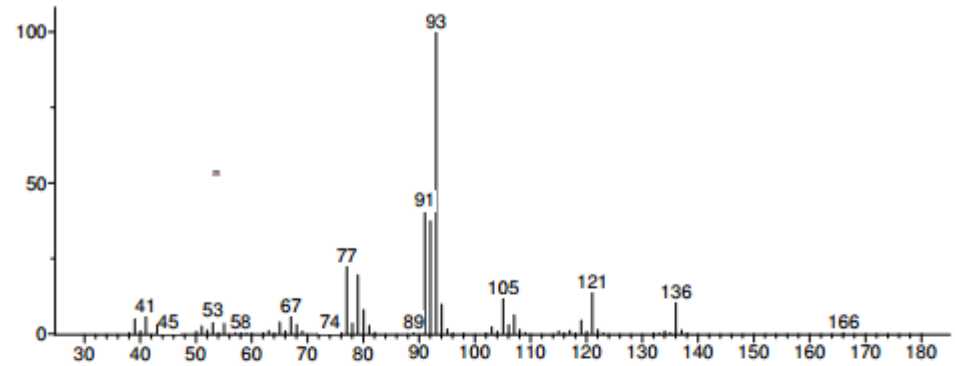



Hit 1 : Thiocyanic acid, 2-propenyl ester
C4H5NS; MF: 797; RMF: 833; Prob 75.2%; CAS: 764-49-8; Lib: mainlib; ID: 2231.

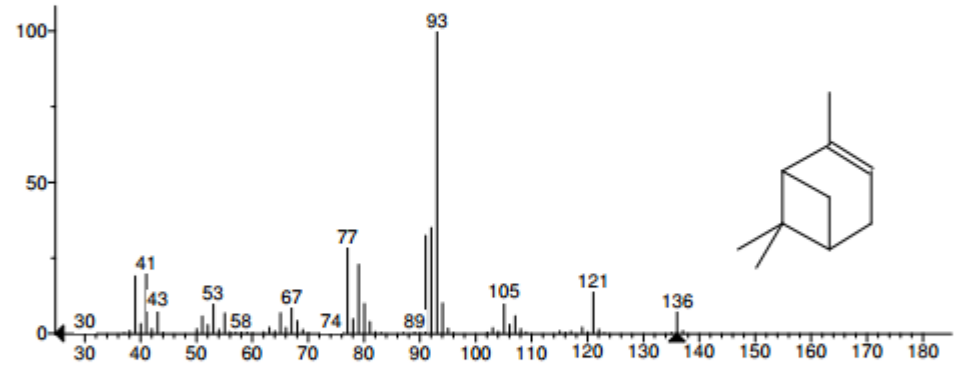


Peak 8 at 6.243 min.: identified as α-Pinene (CAS 80-56-8) or 3-Carene (CAS 13466-78-9)

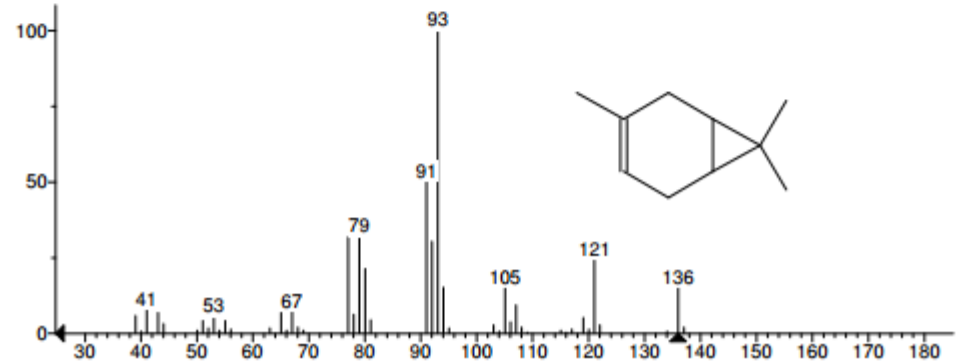
Unknown: Component at scan 1112 (6.335 min) [Model = +93u] in M:\2017 ANALYSEDATEN\SCREENING\0913
Compound in Library Factor = -117



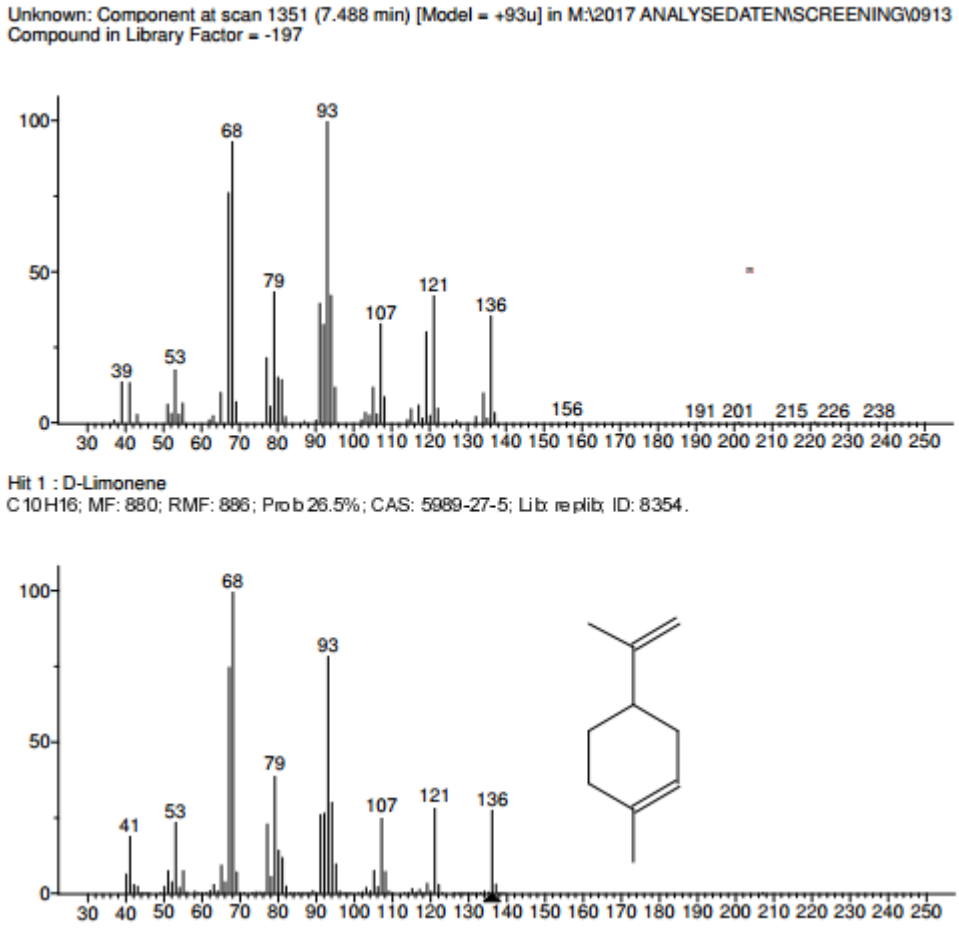

Hit 1 : α-Pinene
C10H16; MF: 929; RMF: 931; Prob 13.1%; CAS: 80-56-8; Lib: replib; ID: 14130.




Hit 2 : 3-Carene
C10H16; MF: 922; RMF: 927; Prob 10.0%; CAS: 13466-78-9; Lib: mainlib; ID: 66203.



Peak 9 at 7.488 min.: identified as D-Limonene (CAS 5989-27-5)




Hit 1 : D-Limonene
C10H16; MF: 880; RMF: 886; Prob 26.5%; CAS: 5989-27-5; Lib: replib; ID: 8354.

## 5 SUMMARY

The test item Anti-mold Chip (WS) showed up to 9 peaks by using GC-MS Headspace which could all assigned.

| Peak | Peak area % | Assignment |
|---|---|---|
| 1 | 0.94 | Carbonyl sulfide |
| 2 | 18.62 | Ethanol |
| 3 | 3.56 | Carbon disulfide |
| 4 | 1.51 | 1-Butanol |
| 5 | 4.31 | Diallyl sulfide |
| 6 | 66.62 | Allyl Isothiocyanate |
| 7 | 2.06 | 2-Propenylester Thiocyanic acid |
| 8 | 2.16 | α-Pinene or 3-Carene |
| 9 | 0.21 | D-Limonene |