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

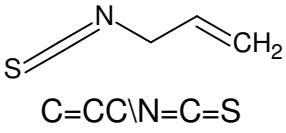
2.1 Test Item

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

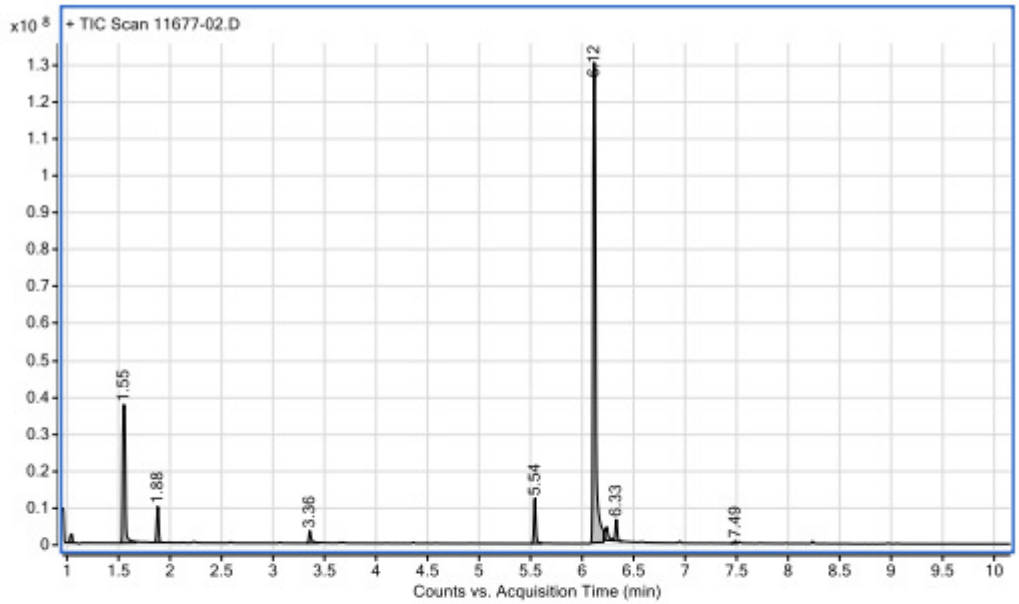
3.1 GC-MS

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 then 15 °C/min to 150 °C for 0 min. 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

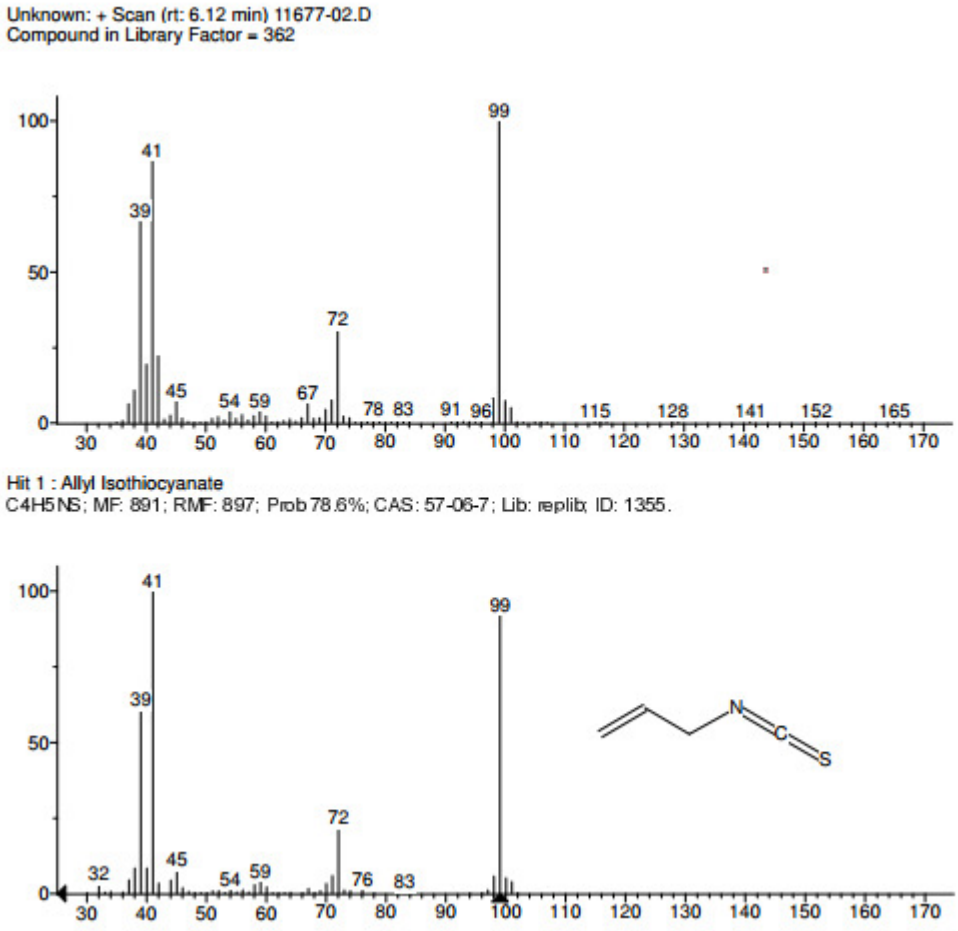
Sample peaks below 0.1 area sum % and system background peaks are not included.

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

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



5 SUMMARY

The test item Anti-mold Chip (WS) assigned an amount of Allyl Isothiocyanate as > 66.62 %.

Peak	Peak area %	Assignment
Major peak	66.62	Allyl Isothiocyanate