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GROWER SUMMARY

Headlines

- Relationships were identified between chemical volatile constituents of watercress and the profile of sensory attributes. These are significant as they provide a means to predict the sensory properties of watercress from the results of analysis.
- Some attributes were found to be strongly correlated to the concentration of individual chemical components. Thus the intensity of these flavour attributes may be predicated from the intensity of these indicator compounds.
- The work has provided valuable information regarding the likely drivers of consumer liking for watercress as well as the basis for an analytical approach to monitor these sensory attributes.
- The results provide a platform for progression to phase 2 of the study in which the effect of agronomic effects on flavour will be determined.

Background

A study was carried out to determine the links between sensory attributes, consumer preference and chemical compositional analysis in watercress. Previous work had established that consumer preference was influenced by both flavour and texture of the samples, including crisp and chewy textures and hot, sweet, and grassy/green flavours. Phenylethylisothiocyanate (PEITC) levels were also investigated, due to its proven health benefits.

This study set out to determine the possible effects of agronomic treatments on the resulting flavour profiles of the samples and the possible result on consumer preference. Its objective was to optimise certain volatile compounds in the crop, particularly PEITC, with them aim of increasing consumer preference, and hence increasing the level of consumption, which would result in health benefits for the population.

Approach

There were 3 main stages to the work: The first stage involved a scoping trial in which commercial sulphur treatments were used alongside a waterstress treatment. This was to ascertain the concentrations of products that could be utilised in subsequent trials. Two commercial sulphur treatments were used: Hortisul and Sulphomex. The second stage of work used a replicated trial design to understand how repeated applications of sulphur product, used throughout the growing period, could influence the level of flavour volatiles in the crop. The final phase of work utilised a validation trial, in which two treatments identified in stage 2, were used to determine consumer preference against the control.

Data from all tests were statistically analysed and related in order to understand perceptual differences and consumer acceptance in terms of chemical composition (flavour volatiles).

The study design for trials is summarised below:

Samples generated	Objective	Chemistry	Sensory
Trial 1 – 1. Control 2. Sulphomex 5l/ha 3. Sulphomex 15l/ha 4. Hortisul 20kg/ha 5. Hortisul 40kg/ha 6. Waterstress	To identify agronomic treatments e.g sulphur products, concentrations and waterstress, to be used in subsequent trials.	Chemical analysis of flavour volatiles and total sulphur content.	Discrimination testing (triangle test)
Trial 2 – 1. 4 x 30kg/ha Hortisul 2. 4 x 50kg/ha Hortisul 3. 2 x 30kg/ha Hortisul 4. 2 x 50kg/ha Hortisul 5. Control	To determine the effect of repeated sulphur applications to the growing crop on the flavour volatiles	Chemical analysis of flavour volatiles	None
Trial 3 – 1. 4 x 30kg/ha Hortisul 2. Control 3. 4 x 50kg/ha Hortisul	To validate trial 2 objectives and generate samples for consumer trial	Chemical analysis of flavour volatiles	Consumer preference test

Table 1. Treatments and samples generated in each of the trials.

Discussion

Initial scoping studies (stage 1) indicated that applications of sulphur compounds to growing watercress produced a trend of increased levels of total sulphur in the plant tissue. These increases ranged from 4 to 14%. Sulphomex appeared to give a higher level of total sulphur in the resulting plant tissue compared to Hortisul. However, Hortisul tended to yield larger amounts of PEITC in the watercress than Sulphomex from these initial scoping trials. As PEITC was of particular interest in this piece of work, Hortisul was utilised in subsequent trials.

In terms of sensory discrimination test carried out during the initial scoping trial, there were no significant differences between the treatment samples and the control sample. Although the triangle test revealed no significant differences, waterstress treatment did appear to have a larger impact on sensory perception than the sulphur treatments, with more assessors correctly identifying a difference between the waterstress and control samples.

Results of stage 2 showed trends which suggested that four repeated applications of Hortisul yielded higher levels of PEITC than 2 repeated applications in the replicated trials. However, this difference was not significant.

The application of stress to the crop by withholding water seemed to have a greater effect on flavour profiles than sulphur applications, as indicated by the large number of volatiles showing significant differences between the waterstressed sample and the remaining samples.

In terms of stage 3, there were no significant differences in consumer preference between the three samples generated (i.e. 4 low applications, 4 high applications and the control). All 3 samples recorded acceptable levels of liking across all the attributes, but no sample was significantly liked more than another. Sample 2 (the control sample), was the least liked sample across all attributes, but again these values were not significant. From the consumer data, sample 3 (where there had been 4 repeated applications of Hortisul at a high level) generally, appeared to be the most favoured sample.

In terms of chemical analysis, the results from the initial scoping trial appeared to indicate a clear trend for an increase in sulphur-containing compounds, including 2-phenylethyl isothiocyanate (PEITC), in watercress subjected to waterstress or treated with high levels of Hortisul. This trend was still apparent, though less pronounced, in the waterstressed samples analysed for trial 2, but was not observed in the samples analysed for trial 3. The reason for this is unknown. This particular sulphur-containing compound, 2-phenylethyl isothiocyanate, considered to possess anti-carcinogenic properties, was found to be by far the largest volatile peak detected in all of the watercress samples analysed. This could be considered the most important volatile within the full range that have been analysed. Results of trial 2 seemed to suggest that 2-phenylethyl isothiocyanate could be increased using the 4 low application and 4 high application treatments. However, this was not confirmed during the validation study in phase 3, in which control samples had higher levels. This may be a reflection of the metabolic state of the crop utilised, under the prevailing environmental conditions within each trial. Despite the lack of significance in trial 2, it was decided to continue with the validation trial in order to investigate this trend further and determine its impact on consumer preference.

Studies on the effect of ageing and cooking of watercress indicated that both processes, particularly cooking, significantly reduced the levels of many volatile compounds in watercress, and that the sulphur-containing compounds were among those most affected. For 2-phenylethyl isothiocyanate ageing watercress for 4 days resulted in a 10% drop in the peak area of this compound, while cooking watercress resulted in a drop in 2-phenylethyl isothiocyanate to less than 1% of its level before cooking. It was therefore clear that this and other volatiles were very susceptible to effects of storage and heating. This should be a consideration in the processing of watercress samples in relation to the health benefits of the crop.

From a commercial viewpoint, the variability in trial results and lack of significant preference between samples, make it difficult to issue specific recommendations relating to the specific agronomic treatment of watercress, for both enhancing sensory and consumer perception and increasing the levels of PEITC. However, trends generally suggested that higher repeated levels of sulphur applications could increase levels of PEITC and that waterstress could also have an effect on the flavour profile. From an agronomic viewpoint, results from trial 2, in which a replicated block design was used, may have given more reliable results than those from the other trials. This therefore suggested that repeated applications of higher concentrations of sulphur products, could have an effect on PEITC content, as these treatments resulted in the higher peak areas, following chemical analysis. This could therefore suggest that there is a possible cumulative effect of sulphur applications in terms of PEITC formation in the growing crop.

Regarding the impact of the agronomic treatments investigated on sensory quality, results from stage 1 suggest that differences in agronomic treatments (within the scope of those studied) may not lead to significant perceivable differences between watercress samples. Furthermore, based on the selected group of consumers, results of stage 3 appear to indicate that the selected agronomic treatments may not have a large impact on consumer preference of the watercress. Therefore, we could perhaps suggest that decisions on the type of agronomic treatments to utilise, can focus instead on economic or health factors, as these may not necessarily be having a negative influence on the consumer.

It is possible that increasing the concentration or application timings of the sulphur products could have resulted in a corresponding increase in levels of PEITC. Similarly an increase in the level of waterstressing could have had the same effect.

These approaches were outside of the scope of this present study, but could form the basis of further field trials.

Summary

The sulphur compounds utilised in this study did have an effect upon the total sulphur content of the watercress samples when applied to the growing crop. This however, did not result in significant increases in levels of the sulphur-containing compound PEITC. Results from the stage 1 trial did suggest that PEITC was increased in watercress by sulphur applications. However, this was not supported in the volatile analysis results of the final validation trial. There was no indication that agronomic treatments had any effect in increasing consumer acceptability of watercress.

PEITC was found to be the largest volatile peak detected in all of the watercress samples analysed. The levels of PEITC within watercress were shown to be significantly reduced during storage of watercress and by cooking. These are therefore important considerations for processing in terms of the proven health benefits of this volatile compound.

Sulphur applications to the growing crop did not appear to alter its sensory perception to any significant level. In difference tests assessors were unable to identify significant differences between the treated samples and the untreated samples. Although the triangle test revealed no significant differences, waterstress treatment did appear to have a larger impact on sensory perception within the initial trial than the sulphur treatments, with more assessors correctly identifying a difference between the waterstress and control samples.

Summary of results

The data from this study indicated that sulphur applications to the growing crop resulted in an increase in the level of total sulphur in the growing crop. This indicated that it could result in an increase in sulphur-containing phenylethylthiocyanate (PEITC), which has proven health benefits. PEITC was found to be the largest volatile peak detected in all of the watercress samples analysed. The levels of PEITC within watercress were shown to be significantly reduced during storage of watercress and by cooking. These are therefore important considerations for processing in terms of the proven health benefits of this volatile compound.

Sulphur applications to the growing crop did not appear to alter its sensory perception to any significant level. In difference tests assessors were unable to identify significant differences between sulphur or waterstress treated samples and untreated samples. Although the difference was not significant, application of stress to the crop by withholding water before harvest, did appear to have a larger impact on sensory perception within the initial trial than the sulphur treatments, with more assessors correctly identifying a difference between the waterstress and control samples.

Further work

Further work could involve the utilisation of differing agronomic factors that might influence flavour volatiles in the growing crop. This could include the more extensive use of concentrations of sulphur products and more regular applications to the growing crop. This might lead to a greater increase in PEITC than was measured in this current study.

Action Points for Growers

Although there are not direct results for this project that can be utilised, growers should be alert to PEITC being a unique selling point for watercress (increased flavour and health benefit) which is found at highest levels in uncooked watercress.

SCIENCE SECTION

1. Background

This report represents the second phase of project work for the HDC on “Predicting the effect of agronomic production factors on the flavour acceptability of watercress to consumers” (project FV 255). The first phase of project work, carried out in 2004, had investigated the links between sensory attributes, consumer preference and chemical compositional analysis. The work had established that consumer preference was influenced by both the flavour and texture of the watercress samples, which included crisp and chewy textures and hot, sweet and grassy/green flavours. This second phase of work reported here utilised agronomic treatments in a series of field trials in order to generate samples for chemical and sensory analysis, concentrating upon the use of agronomic factors that might influence the volatile components of the watercress crop and the resulting flavour profiles. In turn, the work set out to determine whether the agronomic factors utilised in the field trials could influence consumer acceptability of the resulting product. If the levels of certain volatile components can be optimised in the crop it will be seen as a means of improving flavour preferences or marketability, and hence increasing the consumption of the crop. This would be of great commercial significance to growers and would have obvious health benefits for consumers.

2. Materials and Methods

2.1 Agronomy

There were 3 main stages involved in the agronomic treatments of the watercress. The first stage represented a scoping trial, which aimed to determine the range of sulphur applications and type of commercial product to be used in subsequent investigations. The second stage represented a replicated trial whereby the optimum applications of product types utilised in the scoping trial were identified and the level of volatiles in the treated samples was determined. Selected treatment levels were used in the final stage of trial work. The third and final stage utilised the optimised concentrations of specified sulphur products, in order to attempt to increase the Phenylethylisothiocyanate (PEITC) levels in the growing crop and determine consumer preference. All stages of the agronomic treatments sought to compare the levels of volatiles, such as PEITC, in the growing crop, with the final stage also looking to correlate these levels with consumer preference. In addition, the

possibility that consumer preference may be correlated with some other sensory aspect and chemical volatile in the watercress, was explored. All trial work was carried out in collaboration with Vitacress Salads, St Mary Bourne, Hampshire, during May-September, 2005.

2.1.1 Agronomy Stage 1.

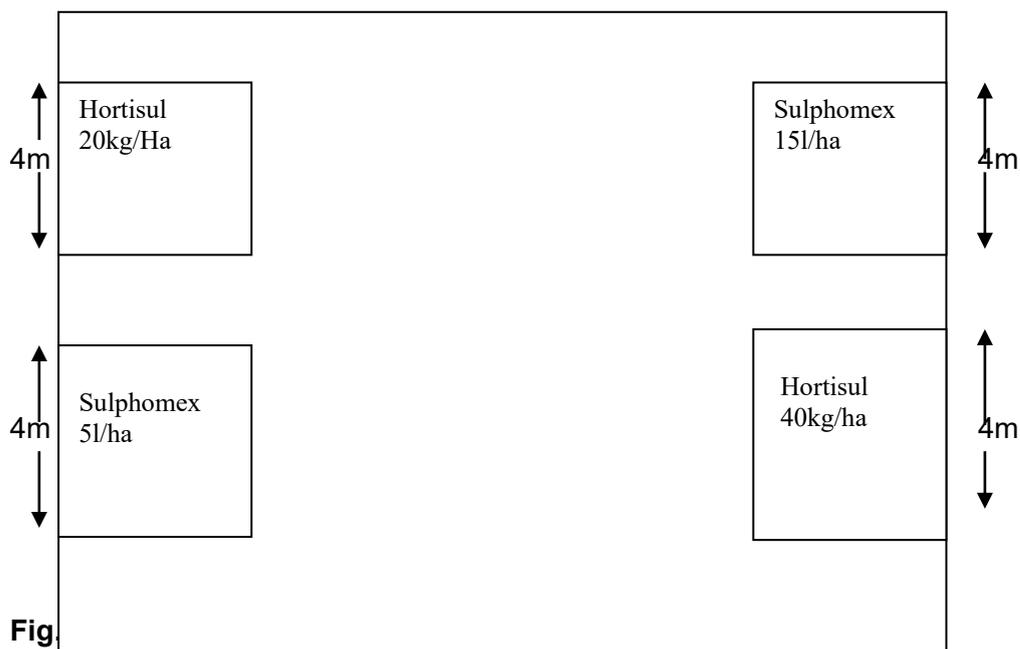
This trial was carried out in order to determine the range of sulphur concentrations that could be used on the watercress crop in subsequent studies and identify any possible phytotoxic effects following application. In addition, two commercially available sulphur products were used in this study and this initial stage served to identify which product should be used in subsequent studies. The scoping trial included both chemical and sensory discrimination testing.

Two different sulphur products were utilised in this initial scoping trial. These were both commercially sourced and were as follows:

- Sulphomex – Nitrogen 12.0 % w/w, 15.8 %w/v, Sulphur 65.0% w/w, 85.0% w/v. A liquid formulation
- Hortisul – K₂O (52%), S (18%), a granulated powder.

The scoping trial involved the application of sulphur products at the following rates: Sulphomex at 5l/ha, Sulphomex at 15l/ha, Hortisul at 20kg/ha, Hortisul at 40kg/ha. 4 x 2m plots were treated in each case. Applications were made using a knapsack boom sprayer May 27th 2005.

The trial plan is shown below:



Fig

Plots were harvested 3 days following the sulphur applications. A crop was also subject to waterstress, whereby the base of the crop stayed damp but the flow of water was restricted for 48 hours. No visible wilting or symptoms were apparent as a result of this treatment. Waterstressed samples were harvested the following day. An untreated control sample was also included for analysis. All crops were harvested by hand and were cut just above the level of the gravel bed following commercial practice.

Samples from this trial were evaluated by a sensory panel of 18 persons using a triangle test on May 31st 2005. Samples were also analysed using chemical volatile analysis.

2.1.2 Agronomy - Stage 2.

In the 2nd stage of applications Hortisul was used as the only sulphur application to the watercress crop. The results in stage 1 suggested that greater levels of Phenylethylisothiocyanate (PEITC) were detected in Hortisul treated compared to Sulphomex. The approach to the second phase of applications was to apply a high rate vs. a low rate of Hortisul, with 4 repeated applications compared to 2 repeated applications. This was detailed following guidance from the National Farmers Union (NFU) watercress group and allowed determination of the effect of the concentration of the product or the application period, on the level of volatile compounds in the crop. Application rates utilised were 30kg/ha (low) and 50kg/ha (high). The 4 repeated applications were made at weekly intervals for a period of 4 weeks. The 2 repeated applications were made in the last 2 weeks of the growing period. This trial utilised applications and products identified in phase 1 of the study. This was a fully replicated trial that used four sulphur applications: 4 high applications (50kg/ha), 4 low applications (30kg/ha), 2 high applications (50kg/ha) and 2 low applications (30kg/ha). This was to determine the relative effects of concentration and applications timings on the level of volatiles of the resulting crop. As with Stage 1, a waterstressed and untreated control sample were also included in the study design, both fully replicated within the trial. Chemical analysis alone was used in stage 2 of this investigation.

The trial plan is shown in fig.2.

Plot 1 (4 x high)	Plot 2 (control)	Plot 3 (2 x low)
Plot 4 (4 x low)	Plot 5 (2 x high)	Plot 6 (4 x high)
Plot 7 (2 x high)	Plot 8 (4 x high)	Plot 9 (control)
Plot 10 (2 x low)	Plot 11 (4 x low)	Plot 12 (2 x high)
Plot 13 (control)	Plot 14 (2 x low)	Plot 15 (4 x low)

All crops were harvested by hand on July 29th 2005 and were cut just above the level of the gravel bed as in commercial practice.

2.1.3 Agronomy - Stage 3.

In the final phase of experimental work, only two sulphur treatments were used. Four applications of Hortisul at high rate (50kg/ha) and four applications at low rate (30kg/ha). These were applied at weekly intervals over a period of 4 weeks. In addition, an untreated control sample was included in the trial.

Selection of sulphur treatments was based upon results obtained from the cumulative effect of repeated applications of the sulphur compounds in stage 2. Sulphur applications were made on a weekly basis for a period of 4 weeks with samples sourced five days after the last application of Hortisul to the growing crop. 8kg of watercress was harvested from each of the plots on September 28th 2005. The trial plan is shown below:

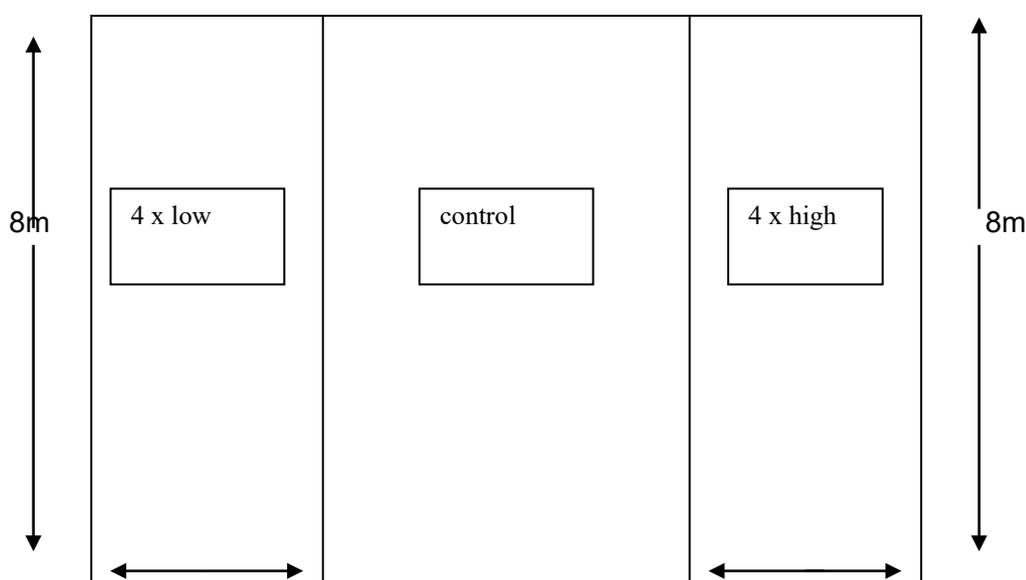


Fig. 3 Trial design for stage 3

Sulphur applications were made from the sides of the plots at the width of the boom (2 metres).

Analysis involved chemical determination of volatiles and level of consumer preference of the watercress samples.

The study design for trials is summarised below:

Samples generated	Objective	Chemistry	Sensory
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<p>Trial 1 –</p> <ol style="list-style-type: none"> 1. Control 2. Sulphomex 5l/ha 3. Sulphomex 15l/ha 4. Hortisul 20kg/ha 5. Hortisul 40kg/ha 6. Waterstress 	<p>To identify agronomic treatments e.g. sulphur products, concentrations and waterstress, to be used in subsequent trials.</p>	<p>Chemical analysis of flavour volatiles and total sulphur content.</p>	<p>Discrimination testing (triangle test)</p>
<p>Trial 2 –</p> <ol style="list-style-type: none"> 6. 4 x 30kg/ha Hortisul 7. 4 x 50kg/ha Hortisul 8. 2 x 30kg/ha Hortisul 9. 2 x 50kg/ha Hortisul 10. Control 	<p>To determine the effect of repeated sulphur applications to the growing crop on the flavour volatiles</p>	<p>Chemical analysis of flavour volatiles</p>	<p>None</p>
<p>Trial 3 –</p> <ol style="list-style-type: none"> 4. 4 x 30kg/ha Hortisul 5. Control 6. 4 x 50kg/ha Hortisul 	<p>To validate trial 2 objectives and generate samples for consumer trial</p>	<p>Chemical analysis of flavour volatiles</p>	<p>Consumer preference test</p>

Table 1. Treatments and samples generated in each of the trials.

2.2 Chemical analysis: Extraction of Volatiles by Headspace Solid Phase Micro Extraction (SPME)

Samples from all three stages of the study were analysed for volatile content.

2.2.1 Sample Preparation

For each sample, 50g of watercress was weighed into a metal beaker. The watercress was pushed down into the beaker until all the watercress was in the bottom half. Sufficient liquid nitrogen was then added to the beaker to completely cover the watercress, and the resulting mixture was thoroughly blended using an overhead macerator. After blending, the beaker was left to allow any liquid nitrogen remaining in the sample to evaporate. This was encouraged by occasional gentle stirring with a spatula. Once the liquid nitrogen had evaporated, 20g of salt and 50ml of distilled water was added to the watercress and mixed to a homogeneous state by stirring with a spatula. 10g portions of the watercress mixture were then transferred into 20ml headspace vials, where 100µl of 100ppm 1-bromohexane solution in ethanol was added. The vials were then sealed, and either put on the GC/MS autosampler immediately for analysis or placed in chilled storage to await analysis.

In addition as part of trial 2, some watercress samples were cooked. These samples were boiled for two minutes, drained and then prepared in the same manner as the other samples.

2.2.2 Sample Analysis

Each vial was equilibrated at 75°C for 15 minutes with agitation. The headspace of the vial was then sampled for 15 minutes at 75°C (with agitation) using a carboxen / polydimethylsiloxane coated SPME fibre. The volatiles adsorbed onto the fibre were analysed by thermal desorption at 250°C in the injector port of a GC/MS.

2.2.3 GC/MS Analysis of Volatiles

Analyses were carried out on a Varian 3800 gas chromatograph (GC) and Varian Saturn 2000 ion trap mass spectrometer (MS) via a CTC Combi-Pal autosampler.

GC/MS conditions were as follows:

Column:	60m x 0.25mm fused silica with VF-5MS stationary phase
Helium carrier gas flow rate:	1ml. Min ⁻¹
Desorption temperature:	250°C
Column temperature:	2 mins at 50°C; then 5°C. min ⁻¹ to 250°C
MS analysis mode:	SCAN 29-350 <i>m/z</i>

All peaks considered to be of sufficient size to allow accurate measurement of peak area were tentatively identified by spectral matching with the Wiley library of mass spectral data. The peak areas obtained were then subjected to statistical analysis to determine what differences, if any, existed between the volatile profiles of the samples.

This chemical analysis was carried out for all 3 stages of the trial work.

2.2.4 Statistical analysis: Chemistry data

The chemistry data were analysed using analysis of variance (ANOVA) to determine if there were significant differences between the samples with respect to volatile

content. Following ANOVA, a Newman-Keuls multiple comparison test was undertaken to establish which samples were different at the 10% level of significance. Samples with the same letters are not significantly different from each other.

2.3 Sensory assessment

2.3.1 Stage 1 - Sensory discrimination testing

For stage 1 of the practical phase of work a simple triangle test was carried out to determine whether there were perceivable differences between the samples. Three samples were taken from the trial: Sulphomex at 15l/ha, Hortisul at 40kg/ha and the waterstressed sample. These represented extremes from the range of samples that were supplied (i.e. high applications). Each of these samples was assessed against the control (untreated). For a triangle test using 18 judgements, a minimum of 10 correct judgements are required to establish a significant difference between samples at the 5% level of significance (British Standard 5929: Part 3: 1984/ISO 4120 – 1983).

2.3.2 Stage 2

There was no sensory assessment of the stage 2 trial samples.

2.3.3 Stage 3 – Consumer preference testing

For assessment of the stage 3 samples a consumer panel was used. Three samples of watercress from the field trial were assessed. All attributes were assessed as individual samples. All samples were refrigerated at a temperature between 1 and 4°C. Products were sampled in rotation according to a defined experimental design. Samples were pre-coded and the same codes were used for all respondents. Samples were presented on white coded plates.

A total of 111 consumer respondents were recruited, being split over 2 locations, with 49% from Chester and 50% from Surrey. All respondents had eaten watercress within the last 12 months and all indicated that they would eat watercress in the future.

Sample Codes were as follows:

		Consumer
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SF Code	Name	Treatment	ID Code
AG/85493/T3/1	4 x Low	4 x Low	240
AG/85493/T3/2	Control	Control	637
AG/85493/T3/3	4 x High	4 x High	921

2.3.3.1 Sample Preparation

Prior to the assessment the samples were washed thoroughly and the young centre stalks removed for assessment. Each respondent was presented with 3-4 sprigs of watercress on a coded plate. Water and cream crackers were given as palate cleansers. Respondents were requested to use the palate cleansers between samples.

2.3.3.2 Test Method Consumer

A total of 111 consumer respondents were recruited. The test was a street recruited central location test. Each respondent was asked to assess the three samples of watercress.

Respondents were asked to evaluate each of the samples and complete a questionnaire.

Degree of liking was measured for overall liking, flavour and aftertaste. Consumer satisfaction (just about right) was also measured for bitterness, hotness of flavour and strength of aftertaste. The consumer data were analysed to identify the most and least acceptable samples.

A 9-point hedonic scale was used to capture respondents degree of liking of the products characteristics. A 5-point "Just about Right" scale was used for specific attributes.

Hedonic Scale

Like extremely 9
much

Like very much 8
much

Like moderately 7

Just about Right

5 Much too strong / too

4 A little too strong / too

3 Just about right

Like slightly	6	2	A little too mild / not enough
Neither like or dislike	5	1	Much too mild / not enough
Dislike slightly	4		
Dislike moderately	3		
Dislike very much	2		
Dislike extremely	1		

2.3.3.3 Data Analysis : Consumer data

The data was analysed by a number of methods, which are described below. The statistical package used was S-Plus and SPSS.

The data were tabulated to indicate the count and percentage of responses for each of the scores per sample, for both the hedonic and just about right questions. Summary statistics were provided on each sample.

ANOVA

The hedonic data were then analysed using analysis of variance (ANOVA) to determine if there were significant differences between the samples with respect to acceptability. Following ANOVA, a Newman-Keuls multiple comparison test was undertaken to establish which samples were different at the 5% level of significance. Samples with the same letters are not significantly different from each other.

T-Test

A t-test was performed on the just about right attributes; bitter, hotness of flavour, strength of aftertaste, to establish if each sample was significantly different from the just about right score 3 (Hypothesis = 3).

2.3.3.4 Consumer Sample

A total of 111 consumer respondents were recruited, being evenly split over two locations, with 49% from Chester and 50% from Surrey. All respondents had eaten watercress within the last 12 months and all indicated that they would eat watercress in the future.

The majority of respondents were female, represented by 80% against 20% for male. The majority of respondents represented social class A/B/C1 (79%), with the remainder being C2/D/E (21%). Age ranged from 18 – 64. The full demographic results are shown in Appendix 1.

The statistical results are detailed in terms of a summary table showing significant differences and means. The letters in the table indicate where the samples are significantly different. Means sharing the same letter are not significantly different, whereas means that have different letters are significantly different to each other. The hedonic and Just about Right (JAR) full and summarised tabulations (count & %) are shown in Appendix 2.

3. Results

3.1 Stage 1 – Scoping trial

3.1.1 Agronomy results

Trial dates

Sulphur applications were made to a crop close to maturity (i.e. 4 weeks old) on May 27th 2005

Harvesting took place 4 days following the sulphur applications, on May 31st 2005

Samples

1	Untreated
2	Sulphomex (5l/ha)
3	Sulphomex (15l/ha)
4	Hortisul (20kg/ha)
5	Hortisul (40kg/ha)
6	Water-stressed

Sulphur analysis

Sample	Oven dry matter	Total nitrogen	Total sulphur	Total S at 7 % dry matter
Untreated	7.9	5.98	0.96	0.85
Sulphomex (5l/ha)	5.9	5.90	1.02	1.21
Sulphomex (15l/ha)	6.3	6.13	1.10	1.22
Hortisul 920kg/ha)	6.4	5.79	1.03	1.13
Hortisul (40kg/ha)	6.1	5.88	1.00	1.14

Table. 2 Results from S analysis (adjusted to 7% dry matter)

Sulphur analysis suggested that applications of Sulphomex at a concentration of 15l/ha had a greater effect on increasing the level of total sulphur in the plant tissue. The highest level of Hortisul (40kg/ha) had the next greatest effect on increasing the total sulphur content. There were therefore indications, that application of sulphur

compounds subsequently increased the level of sulphur in the leaf tissue of the growing crop.

3.1.2 Chemical analysis- Stage 1

Analysis of variance was carried out on all of the peaks chosen for examination (Appendix 2). These analyses showed significant differences in at least one of the treatments in the following peaks for 48 peaks. The most striking differences were detected between samples 5 (40kg/ha Hortisul) and 6 (waterstressed) and the remaining four treatments. However, without any comparable sensory data, it was not possible to determine the likely perceptual impact of the differences.

Ten sulphur-containing compounds (ethylthiophene, 4-methylpentyl isothiocyanate, hexyl isothiocyanate, n-heptyl isothiocyanate, 3-methylhexyl isothiocyanate, octyl isothiocyanate, methylheptyl isothiocyanate, nonyl isothiocyanate and 2-phenylethyl isothiocyanate) were present at significantly higher levels in treatment 4 (Hortisul at 40kg/ha) than in 1 (untreated), 2 (Sulphomex 5l/ha), 3 (sulphomex 15l/ha) and 4 (Hortisul 40kg/ha), and at significantly higher levels again in treatment 6 (waterstressed) than in 4 (Hortisul 40kg/ha). In addition, both samples 6 (waterstressed) and 4 (Hortisul 40kg/ha) had significantly higher levels of 1-hexanethiol compared to the other samples. 2-Phenylethyl isothiocyanate was by far the largest peak detected in the watercress chromatograms, with a peak area over 20 times larger than the next largest peak.

The following compounds were found at significantly lower levels in treatments 4 (Hortisul 40kg/ha) and 6 (waterstressed) than the other four treatments: a mixed peak of 1-penten-3-ol and 1-penten-3-one; benzenemethanol; 3-ethyl-4-methyl-1H-pyrrole-2,5-dione; 3-ethenyl-4-methyl-1H-pyrrole-2,5-dione; 4-ethoxybenzaldehyde; ethyl hydrocinnamate and 2,5-Dimethyl-1-phenylpyrrole. Of these compounds, 3-ethyl-4-methyl-1H-pyrrole-2,5-dione, 3-ethenyl-4-methyl-1H-pyrrole-2,5-dione and ethyl hydrocinnamate were also found at significantly higher levels in the untreated sample than in all the other treatments. The compound ethyl nicotinate followed the same trend (treatments 4 – Hortisul 40kg/ha, and 6 – waterstressed, lower than all other samples, and the untreated sample higher than all other samples), but pairwise differences were not found to be significant. Finally, treatments 4 (Hortisul 40kg/ha) and 6 (waterstressed) were significantly lower than treatments 2 (sulphomex 5l/ha) and 1 (untreated) for the compound 2-pentenal.

Hexanal, 2-hexenal and cis-3-hexenal were found at significantly higher levels in treatment 6 than in the other treatments. As the names suggest, these three compounds are extremely similar in structure. They all possess sensory properties described as 'green' in nature, although hexanal and 2-hexenal have also been described as 'fatty'. 2-Ethylfuran, 2,2,6,6-tetramethyl-3,5-heptanedione, methyl salicylate, 3-(methylthio)propyl isothiocyanate, 3-methylbutyl isothiocyanate, and cyclohexane methyl isothiocyanate (another sulphur-containing compound) were also found at higher levels in treatment 6 (waterstressed) than in the other treatments.

2,6-Nonadienal was found at a significantly lower level in treatment 6 (waterstressed) than in the other treatments. This compound possesses sensory characteristics described as 'oily', 'green', and 'cucumber' in nature.

It is apparent from the results of this trial that applying agronomic treatments to the watercress can affect its volatile composition. The two treatments that affected the volatile profiles the most were waterstress and high applications of Hortisul. Applying high levels of Hortisul to the watercress and subjecting it to waterstress were both found to lead to increases in the levels of the sulphur-containing isothiocyanates present. However, it is not possible to determine whether these differences would result in noticeable differences in the sensory properties of the watercress, or whether such differences, if present, would be desirable.

3.1.2 Sensory Analysis

Test No.	Sample	No. of Assessors	No. Correctly identifying the Different sample	Significance
1	Sulphomex 15l/ha	18	8	NSD
2	Hortisul 20kg/ha	18	5	NSD
3	Waterstress	18	9	NSD

Table. 3 Sample treatments and results from triangle test.

In terms of the triangle test, the samples of Sulphomex at 15l/ha, Hortisul at 20kg/ha and waterstressed sample were assessed against the control (untreated sample).

These represented the highest application rates of the scoping trial, where differences were most likely to have been detected. 18 assessors were used in each case. No significant differences were found between the samples in terms of sensory analysis. However, the waterstress sample was detected as the most different from the control, with 9 assessors identifying the sample as different. This was just under the minimum of 10 assessors needed for a significant difference, for a triangle test of this type.

The tables below list the descriptors of the three samples vs. the control. These describe the taste as perceived by the assessors in the triangle test.

Table 3: Descriptors of Samples

Test Reference No. AG/85493/1

AG/85493/1/1	Control	Hotter taste (1) Hotter, stronger (1) Milder, no acidic burn (1) Weaker, less hot (1)
AG/85493/2/2 Sulphomex 15l/ha	Test	Fummy (1) This sample seemed to have a weaker taste (1) Less hot/spicy (1) No peppery aftertaste (1)

Test Reference No. AG/85493/2

AG/85493/1/1	Control	Least peppery, limper texture (1) Tasted hotter (1) More bitter (1)
AG/85493/3/2 Hortisul 40kg/ha	Test	More peppery, hot (1) Hotter taste (1)

Test Reference No. AG/85493/3

AG/85493/1/1	Control	More peppery. The others are bland compared to this sample (1) More aromatic (1) Less hot (2) Less bitter (1) Weaker, less peppery (1)
AG/85493/4/1 waterstressed	Test	More peppery (2) No Difference (1)

3.2 Stage 2 replicated trial

Samples

4 high applications (50kg/ha)
4 low applications (30kg/ha)
2 high applications (50kg/ha)
2 low applications (30kg/ha)
Water-stressed
Control (untreated)

3.2.1 Agronomy results

The trial was established on July 8th 2005 and the replicated trial of 15 plots were harvested on July 29th. These samples underwent chemical analysis alone.

3.2.2 Stage 2 – Replicated trial: Chemical analysis

Results presented represent chemical analysis alone as no consumer work was carried out during this stage.

Analysis of variance was carried out on all the peaks chosen for examination (Appendix 4).

Waterstress treatment

The results show that the waterstressed treatment produces a very polarised sample, with many significant differences from the remaining five samples. The following peaks were detected at significantly higher levels in the waterstressed treatment than in the other treatments.

2-Ethylfuran

Hexanal

cis-3-Hexenal

2-Hexenal

3-Ethylthiophene

4-Heptenal

n-Heptanol

2,4-Hexadienal

Methylthiocyclopentane

1-Hexanethiol

2-Heptenal

3-Ethyl-2-hydroxy-2-cyclopenten-1-one

2,6-Dimethyl-5-hepten-1-ol

2,4-Heptadienal

Benzenemethanol

Benzeneacetaldehyde

(E)-2-Nonen-1-ol

n-Pentyl isothiocyanate

Carvacrol

Hexyl isothiocyanate

Cyclohexane methyl isothiocyanate

3-Methylhexyl isothiocyanate

4-Ethenyl-2-methoxyphenol

Methylheptyl isothiocyanate

The following peaks were detected at significantly lower levels in the waterstressed treatment than in the other treatments:

cis-3-Hexenal diethyl acetal

Benzeneethanol

2,2,6,6-Tetramethyl-3,5-heptanedione

Methyl salicylate

Ethyl nicotinate

Benzenepropanenitrile

3-(Methylthio)propyl isothiocyanate
 Ethyl hydrocinnamate
 94, 117, 142
3-methylbutyl isothiocyanate

Peaks highlighted in bold showed the same significant difference in Trial 1. Peaks highlighted in italics showed the opposite significant difference in Trial 1. Of the eleven sulphur-containing compounds referred to in Trial 1, six were found at significantly higher levels in the waterstressed samples than in the other treatments in trial 2. Two additional sulphur-containing compounds (methylthiocyclopentane and n-pentyl isothiocyanate) were also present at significantly higher levels, and one sulphur-containing compound (3-(methylthio)propyl isothiocyanate) was present at a significantly lower level. 2-Phenylethyl isothiocyanate was again by far the largest peak detected in the watercress samples, but in this trial no significant difference was detected between the results obtained for the different treatments. The waterstressed treatment samples actually had the lowest average peak area for 2-phenylethyl isothiocyanate, while the 4 high and 4 low application treatments had the highest average peak areas.

Sulphur treatments

The level of high and low volatile compounds associated with the five treatments in the replicated Sulphur treatments trial are shown in Table 4.

Table 4 . High and low levels of volatile compounds associated with each sample.

Treatment 2 HIGH APPLICATIONS Hortisul (2 x 50kg /ha)	
High levels	Low levels
CIS-3-HEXENAL-DIETHYL-ACETAL	77-105 *
2-2-6-6-TETRAMETHYL-3-5-HEPTANEDIONE	3-METHYL-3-BUTENYL-BENZENE *
ETHYL-HYDROCINNAMATE	CYCLOHEXANE-METHYL-ISOTHIOCYANATE
ISOAMYL-DECANOATE	
Treatment 2 LOW APPLICATIONS Hortisul (2 x 30kg/ha)	
High levels	Low levels
BENZENEPROPANENITRILE	2-ETHYLFURAN
	TOLUENE *
	HEXANAL
	CIS-3-HEXENAL
	2-HEXENAL
	N-HEPTANOL
	STYRENE *

	2-4-HEXADIENAL 1-HEXANETHIOL BENZALDEHYDE * 3-METHOXYPHENOL 3-5-OCTADIEN-2-ONE ETHYL-TRANS-4-HEPTENOATE N-PENTYL-ISOTHIOCYANATE 1-TERPINEOL HEXYL-ISOTHIOCYANATE 3-ETHYL-4-METHYL-1H-PYRROLE-2-5-DIONE * 3-METHYLHEXYL-ISOTHIOCYANATE 4-ETHOXYBENZALDEHYDE METHYLHEPTYL-ISOTHIOCYANATE GERANYL-ACETONE * 2-5-DIMETHYL-1-PHENYLPYRROLE
Treatment 4 HIGH APPLICATIONS Hortisul (4 x 50kg/ha)	
High levels	Low levels
THIACYCLOPENTANE BENZALDEHYDE * BENZENEETHANOL METHYL-SALICYLATE 3--METHYLTHIO-PROPYL-ISOTHIOCYANATE X94--117--142 2-PHENYLETHYLISOTHIOICYANATE *	2-PENTENAL 3-ETHYLTHIOPHENE 4-HEPTENAL METHYLTHIOCYCLOPENTANE 2-HEPTENAL 2-6-DIMETHYL-5-HEPTEN-1-OL 2-4-HEPTADIENAL
	BENZENEMETHANOL 2-2-6-TRIMETHYLCYCLOHEXANONE CARVACROL BETA-CYCLOCITRAL 4-ETHENYL-2-METHOXYPHENOL
Treatment 4 LOW APPLICATIONS Hortisul (2 x 30kg/ha)	
High levels	Low levels
1-PENTEN-3-OL---1-PENTEN-3-ONE 2-2-6-TRIMETHYLCYCLOHEXANONE 3-METHYLBUTYL-ISOTHIOCYANATE ETHYL-TRANS-4-HEPTENOATE 1-TERPINEOL 4-METHYLPENTYL-ISOTHIOCYANATE * 3-ETHYL-4-METHYL-1H-PYRROLE-2-5-DIO * BETA-CYCLOCITRAL 3-ETHENYL-4-METHYL-1H-PYRROLE-2-5-DIONE N-HEPTYL-ISOTHIOCYANATE * 4-ETHOXYBENZALDEHYDE OCTYL-ISOTHIOCYANATE * 2-5-DIMETHYL-1-PHENYLPYRROLE NONYL-ISOTHIOCYANATE *	THIACYCLOPENTANE 1-BROMOHEXANE * 3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-O BENZENEACETALDEHYDE 2-6-NONADIENAL *
Control	
ETHYL-NICOTINATE GERANYL-ACETONE *	E-2-NONEN-1-OL ISOAMYL-DECANOATE

* Denotes non-significant results at the 10% level of significance

Results show the waterstress treatment had a large impact on the volatile content compared to the remaining samples. However, significant differences in volatile content were also observed between the remaining samples as well. In particular, within the sulphur treated samples, there appeared to be a clear indication that the 4 high and 4 low applications increased the level of PEITC, albeit not significantly. In addition to both treatments (4 high and 4 low) appearing to play a role in the increase of PEITC levels, these two samples appear to have very different chemical profiles, with each sample being characterised by a different list of chemical volatiles. It was hoped that this difference in chemical profiles would translate to a difference in flavour profile, although this could not be confirmed at this stage. These results supported the inclusion of the 4 high and 4 low applications treatments in the final validation stage of the project.

Effects of shelf-life and cooking

In addition to the six different treatments compared, Trial 2 also investigated the effects of ageing and cooking on the volatile composition of watercress. A sub-sample of the watercress from the control treatment was stored for 4 days following its initial analysis, and further samples of this watercress were then analysed, both raw and cooked. Comparing the results obtained for the control and aged samples, it was found that every peak measured had a smaller average peak area for the aged samples than for the control. Statistical analysis of these showed the following twelve peaks to be significantly lower in the aged sample than in the control (at the 10% level of significance)

Toluene
Thiacyclopentane
Styrene
1-Bromohexane
2,6-Nonadienal
Methyl salicylate
Ethyl nicotinate
Cyclohexane methyl isothiocyanate
4-Ethenyl-2-methoxyphenol
3-(Methylthio)propyl isothiocyanate
94, 117, 142
2-Phenylethyl isothiocyanate

Conversely, the following seven peaks were shown to be significantly lower in the control sample than in the aged sample (at the 10% level of significance):

Mixed peak of 1-penten-3-ol and 1-Penten-3-one
Methylthiocyclopentane
2,6-Dimethyl-5-hepten-1-ol
Octyl isothiocyanate
2,5-Dimethyl-1-phenylpyrrole
Nonyl isothiocyanate
Isoamyl decanoate

Comparison of the aged and cooked samples, showed even more pronounced losses of volatiles due to cooking. Statistical analysis showed forty-four peaks to be significantly lower in the cooked sample than in the aged sample. All of the isothiocyanate compounds showed significant differences at the highest level of confidence (0.1%). The average peak area of 2-phenylethyl isothiocyanate in the cooked sample was less than 1% of the peak area in the aged sample. It is clear from both these results that the ageing and cooking of watercress both have a significant reductive effect on the levels of volatiles present.

3.3 Stage 3 – Validation trial

This represented the final phase of the work whereby 3 samples were generated for consumer and chemical analysis.

Samples

4 high applications Hortisul (50kg/ha)
4 low applications Hortisul (30kg/ha)
Control

3.3.1 Validation trial -Agronomy

Plots were harvested for both chemical and sensory analysis. There were three plots in total: 4 high applications of Hortisul (50kg/ha), 4 low applications of Hortisul (30kg/ha) and a control (untreated). These were analysed by both Chemical and Consumer and Sensory Science methods.

3.3.2 Validation trial – Chemical analysis

Analysis of variance was carried out on all the peaks chosen for examination (Appendix 4).

For each treatment, the following peaks were found at significantly different levels from the other two treatments:

Treatment - Control

Higher

n-Pentyl isothiocyanate
4-Methylpentyl isothiocyanate
Benzenepropanenitrile

Lower

Treatment - 4 Low applications

Higher	Lower
2-Ethylfuran	2-Phenylethyl isothiocyanate
2-Pentenal	
4-Heptenal	
Methylthiocyclopentane	
2,4-Heptadienal	
Benzenemethanol	
3,5-Octadien-2-one	
Carvacrol	
3-Ethyl-4-methyl-1H-pyrrole-2,5-dione	
2,5-Dimethyl-1-phenylpyrrole	

Treatment - 4 High applications

Higher	Lower
Thiacyclopentane	Hexanal
	cis-3-Hexenal
	2-Hexenal
	2,4-Hexadienal
	3-Methylbutyl isothiocyanate
	cis-3-Hexenal diethyl acetal
	4-Methylpentylisothiocyanate
	Methyl salicylate
	n-Heptyl isothiocyanate

	3-Methylhexyl isothiocyanate
--	------------------------------

In addition to these differences, the Control sample was found to be significantly higher than the 4 High Application treatment in 2,2,6,6-tetramethyl-3,5-heptanedione and hexyl isothiocyanate.

Based on the treatments analysed for Trial 3, and bearing in mind the results obtained for trial 1, it would have been reasonable to expect to see a trend of increasing peak areas for sulphur-containing compounds as the sulphur added to treatments increased. Therefore, such a trend would be expected to run across the samples from no extra sulphur (control), through low amounts of extra sulphur (4 low applications), to high amounts of extra sulphur (4 high applications). However, the results obtained do not appear to demonstrate such a trend. All three treatments have at least one sulphur-containing compound at significantly higher levels than in the other two treatments, and both the 4 low applications and 4 high applications treatment contain sulphur compounds at significantly lower levels than in the other two treatments.

The 4 low application treatment was found to contain significantly lower levels of 2-phenylethylisothiocyanate than the other two treatments. This is inconsistent with the 'trend' witnessed in trial 2, which showed higher levels (though not significant) of 2-phenylethylisothiocyanate for the 4 low application and 4 high application treatments compared to the control. As with the previous two trials, 2-phenylethyl isothiocyanate was once again by far the largest peak in all of the watercress chromatograms.

The treatment showing the greatest indication of increased sulphur levels is the control treatment, which has two sulphur-containing compounds at significantly higher levels, and none at significantly lower levels. However, these possibly increased levels are far less pronounced than the trend observed in the waterstressed and 15l/ha Hortisul treatments from trial 1. The reason for the absence of this expected trend is unknown.

3.3.3 Validation trial - Consumer acceptability

Table 5. HEDONIC – Summary Statistics, including one way ANOVA with Newman Keuls calculated multiple comparison

Variable	Sample	N	Mean	Median	StDev	P value	Sig	NK 5%
Overall	4 x Low	111	6.8	7.0	1.49	0.609	NS	A
	4 x High	111	6.8	7.0	1.66			A
	Control	111	6.6	7.0	1.75			A
Flavour	4 x High	111	6.7	7.0	1.68	0.615	NS	A
	4 x Low	111	6.6	7.0	1.60			A
	Control	111	6.5	7.0	1.82			A
Aftertaste	4 x High	111	6.3	7.0	1.72	0.324	NS	A
	4 x Low	111	6.2	7.0	1.61			A
	Control	111	5.9	6.0	1.81			A

Table of significance

P Value		Significance Level
≤ 0.001	0.1%	Significant at 0.1% level of significance
≤ 0.010	1%	Significant at 1% level of significance
≤ 0.050	5%	Significant at 5% level of significance
> 0.050	NS	Not significant

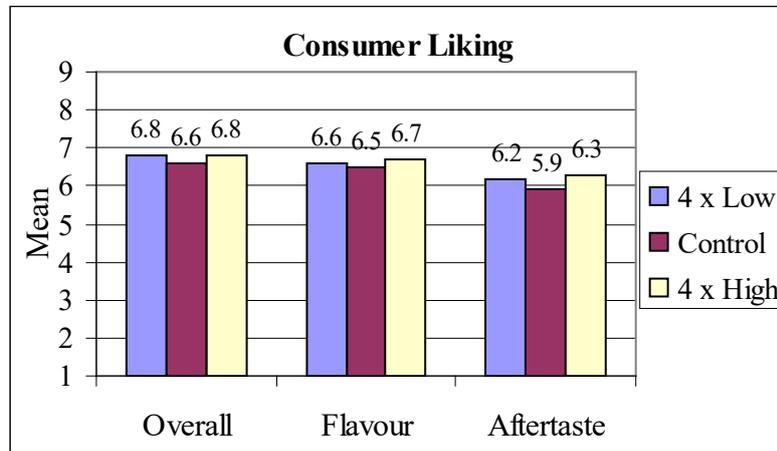
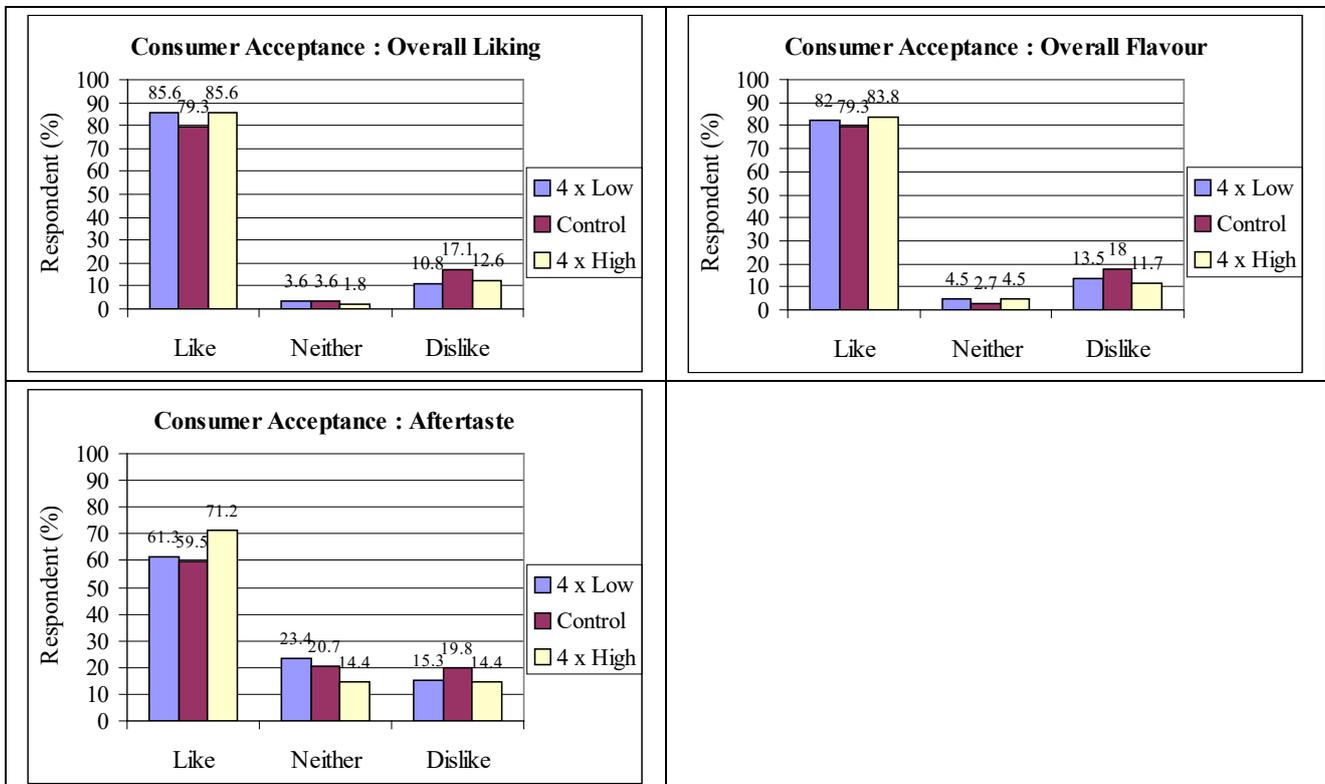


Fig. 4 Graph of consumer liking for sulphur treatments and control

Fig. 5 Hedonic – Graphs of summarised percentages



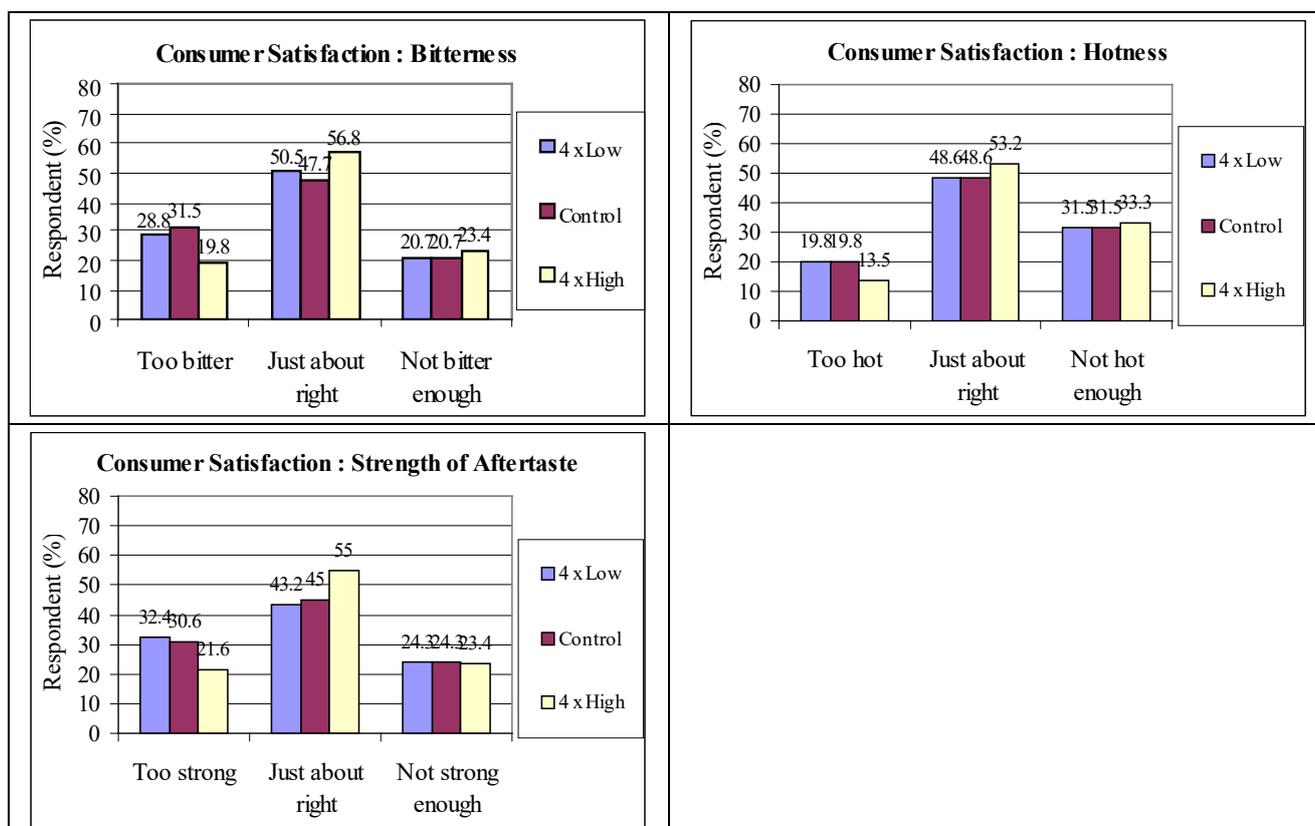
Just About Right Summary Statistics, including T-Test (3)

Variable	Sample	N	Mean	Median	StDev	P. value	Sig
Bitterness	4 x Low	111	3.1	3.0	0.84	0.313	NS
	Control	111	3.1	3.0	0.95	0.320	NS
	4 x High	111	3.0	3.0	0.81	1.000	NS
Hotness of Flavour	4 x Low	111	2.9	3.0	0.83	0.070	NS
	Control	111	2.8	3.0	0.93	0.056	NS
	4 x High	111	2.8	3.0	0.84	0.014	5%
Strength of Aftertaste	4 x Low	111	3.1	3.0	0.90	0.294	NS
	Control	111	3.1	3.0	0.98	0.440	NS
	4 x High	111	3.0	3.0	0.80	0.724	NS

Table of significance

P Value		Significance Level
≤ 0.001	0.1%	Significant at 0.1% level of significance
≤ 0.010	1%	Significant at 1% level of significance
≤ 0.050	5%	Significant at 5% level of significance
> 0.050	NS	Not significant

Fig. 6 Just about Right – Graphs of summarised percentages



No significant differences between the samples were recorded for any of the hedonic attributes. The Control sample recorded the lowest mean values across all hedonic attributes, although these slightly lower acceptability levels were not statistically significant.

For overall liking all samples recorded acceptable levels of liking, recording similar mean scores. Both the 4 x Low and 4 x High samples recorded mean scores of 6.8 with liking to some degree expressed by 86% of respondents. The Control sample recorded a slightly lower mean score of 6.6 with liking to some degree expressed by 79% of respondents.

For overall flavour all samples recorded acceptable levels of liking, recording similar mean scores of between 6.5 and 6.7. High levels of liking acceptability were recorded, with liking to some degree expressed by between 79-84% of respondents.

For aftertaste slightly lower acceptability levels were shown for all samples, with means of between 5.9 and 6.3 being recorded. Across all samples liking to some degree was expressed by between 59-71% of respondents.

None of the samples recorded particularly high levels of consumer satisfaction for the diagnostic attributes, bitterness, hotness of flavour and strength of aftertaste.

For bitterness consumer acceptability was recorded by between 48 – 57% of respondents. For all samples respondents were split fairly evenly between the sample being too bitter to some degree and not bitter enough. The Control sample recorded the lowest acceptability level for bitter, with consumer satisfaction indicated by 48%, with 31% indicating the sample to be too bitter to some degree.

For hotness of flavour all samples recorded similar values, with consumer acceptability indicated by between 49 – 53% of respondents. All samples recorded a fairly high percentage of respondents indicating the sample to be not hot enough to some degree, indicated by between 31-33% of respondents.

For strength of aftertaste all samples recorded similar values, with consumer acceptability indicated by between 43 – 55% of respondents. For all samples respondents were split fairly evenly

between the sample being too strong to some degree and not strong enough.

APPENDICES

APPENDIX 1

CONSUMER AND SENSORY DATA

Demographic Tabulations

Gender		Age					Total
		18-24	25-34	35-44	45-54	55-64	
Male	Count	1	3	6	8	4	22
	% of Total	0.9	2.7	5.4	7.2	3.6	19.8
Female	Count	14	9	28	21	17	89
	% of Total	12.6	8.1	25.2	18.9	15.3	80.2
Total	Count	15	12	34	29	21	111
	% of Total	13.5	10.8	30.6	26.1	18.9	100

Social Class		Age					Total
		18-24	25-34	35-44	45-54	55-64	
A/B/C1	Count	12	9	26	23	18	88
	% of Total	10.8	8.1	23.4	20.7	16.2	79.3
C2/D/E	Count	3	3	8	6	3	23
	% of Total	2.7	2.7	7.2	5.4	2.7	20.7
Total	Count	15	12	34	29	21	111
	% of Total	13.5	10.8	30.6	26.1	18.9	100

Gender		Social Class		
		A/B/C1	C2/D/E	Total
Male	Count	19	3	22
	% of Total	17.1	2.7	19.8
Female	Count	69	20	89
	% of Total	62.2	18.0	80.2
Total	Count	88	23	111
	% of Total	79.3	20.7	100

Purchase - counts

Have you eaten any of the following types of fresh uncooked salad leaves in the last 12 months

	Count	%
Lettuce	110	99.1
Spinach	94	84.7
Watercress	111	100
Rocket	92	82.9
Mustard and cress	69	62.2

Which of the following types of fresh uncooked salad leaves would you be willing to eat in the future

	Count	%
Lettuce	109	98.2
Spinach	99	89.2
Watercress	111	100
Rocket	95	85.6
Mustard and cress	80	72.1

Site	Count	Percent
North - Chester	55	49.5
South - Surrey	56	50.5
Total	111	100

Summarised Hedonic Counts & Percentages

Overall	Count	Count	Count	Mean	%	%	%
Sample	Like	Neither	Dislike		Like	Neither	Dislike
4 x Low	95	4	12	6.8	85.6	3.6	10.8
Control	88	4	19	6.6	79.3	3.6	17.1
4 x High	95	2	14	6.8	85.6	1.8	12.6

Flavour	Count	Count	Count	Mean	%	%	%
Sample	Like	Neither	Dislike		Like	Neither	Dislike
4 x Low	91	5	15	6.6	82.0	4.5	13.5
Control	88	3	20	6.5	79.3	2.7	18.0
4 x High	93	5	13	6.7	83.8	4.5	11.7

Aftertaste	Count	Count	Count	Mean	%	%	%
Sample	Like	Neither	Dislike		Like	Neither	Dislike
4 x Low	68	26	17	6.2	61.3	23.4	15.3
Control	66	23	22	5.9	59.5	20.7	19.8
4 x High	79	16	16	6.3	71.2	14.4	14.4

Sample Assessment Tabulations – Full Tabulations

Hedonic – Full Counts

Overall	4 x Low	Control	4 x High	4 x Low	Control	4 x High
	Count	Count	Count	Percent	Percent	Percent
Like extremely	6	7	5	5.4	6.3	4.5
Like very much	32	31	37	28.8	27.9	33.3
Like moderately	39	34	37	35.1	30.6	33.3
Like slightly	18	16	16	16.2	14.4	14.4
Neither like or dislike	4	4	2	3.6	3.6	1.8
Dislike slightly	7	14	9	6.3	12.6	8.1
Dislike moderately	3	1	1	2.7	0.9	0.9
Dislike very much	2	2	1	1.8	1.8	0.9
Dislike extremely	0	2	3	0.0	1.8	2.7
Total	111	111	111	100	100	100

Flavour	4 x Low	Control	4 x High	4 x Low	Control	4 x High
	Count	Count	Count	Percent	Percent	Percent
Like extremely	6	5	5	5.4	4.5	4.5
Like very much	30	34	35	27.0	30.6	31.5
Like moderately	38	29	37	34.2	26.1	33.3
Like slightly	17	20	16	15.3	18.0	14.4
Neither like or dislike	5	3	5	4.5	2.7	4.5
Dislike slightly	9	13	7	8.1	11.7	6.3
Dislike moderately	3	2	2	2.7	1.8	1.8
Dislike very much	3	2	1	2.7	1.8	0.9
Dislike extremely	0	3	3	0.0	2.7	2.7
Total	111	111	111	100	100	100

Aftertaste	4 x Low	Control	4 x High	4 x Low	Control	4 x High
	Count	Count	Count	Percent	Percent	Percent
Like extremely	3	3	3	2.7	2.7	2.7
Like very much	23	19	26	20.7	17.1	23.4
Like moderately	30	31	32	27.0	27.9	28.8
Like slightly	12	13	18	10.8	11.7	16.2
Neither like or dislike	26	23	16	23.4	20.7	14.4
Dislike slightly	12	13	10	10.8	11.7	9.0
Dislike moderately	2	3	1	1.8	2.7	0.9
Dislike very much	3	3	2	2.7	2.7	1.8
Dislike extremely	0	3	3	0.0	2.7	2.7
Total	111	111	111	100	100	100

Just about Right – Summarised Counts & percentages

Bitterness	4 x Low	Control	4 x High	4 x Low	Control	4 x High
	Count	Count	Count	Percent	Percent	Percent
Too bitter	32	35	22	28.8	31.5	19.8
Just about right	56	53	63	50.5	47.7	56.8
Not bitter enough	23	23	26	20.7	20.7	23.4
Total	111	111	111	100	100	100

Hotness of Flavour	4 x Low	Control	4 x High	4 x Low	Control	4 x High
	Count	Count	Count	Percent	Percent	Percent
Too hot	22	22	15	19.8	19.8	13.5
Just about right	54	54	59	48.6	48.6	53.2
Not hot enough	35	35	37	31.5	31.5	33.3
Total	111	111	111	100	100	100

Strength of Aftertaste	4 x Low	Control	4 x High	4 x Low	Control	4 x High
	Count	Count	Count	Percent	Percent	Percent
Too strong	36	34	24	32.4	30.6	21.6
Just about right	48	50	61	43.2	45.0	55.0
Not strong enough	27	27	26	24.3	24.3	23.4
Total	111	111	111	100	100	100

Just about Right – Full Counts

Bitterness	4 x Low	Control	4 x High	4 x Low	Control	4 x High
	Count	Count	Count	Percent	Percent	Percent
Much too bitter	4	6	6	3.6	5.4	5.4
A little too bitter	28	29	16	25.2	26.1	14.4
Just about right	56	53	63	50.5	47.7	56.8
Not quite bitter enough	19	15	24	17.1	13.5	21.6
Not at all bitter enough	4	8	2	3.6	7.2	1.8
Total	111	111	111	100	100	100

Hotness of Flavour	4 x Low	Control	4 x High	4 x Low	Control	4 x High
	Count	Count	Count	Percent	Percent	Percent
Much too hot	2	4	5	1.8	3.6	4.5
A little too hot	20	18	10	18.0	16.2	9.0
Just about right	54	54	59	48.6	48.6	53.2
Not quite hot enough	30	25	32	27.0	22.5	28.8
Not at all hot enough	5	10	5	4.5	9.0	4.5
Total	111	111	111	100	100	100

Strength of Aftertaste	4 x Low	Control	4 x High	4 x Low	Control	4 x High
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	Count	Count	Count	Percent	Percent	Percent
Much too strong	5	8	3	4.5	7.2	2.7
A little too strong	31	26	21	27.9	23.4	18.9
Just about right	48	50	61	43.2	45.0	55.0
A little too mild	23	20	22	20.7	18.0	19.8
Much too mild	4	7	4	3.6	6.3	3.6
Total	111	111	111	100	100	100

Cross Tabulations

Demographics V Hedonic Acceptability

		Social Grade				Gender			
		A/B/C1		C2/D/E		Male		Female	
	Sample	Mean	Median	Mean	Median	Mean	Median	Mean	Median
Overall	4 x Low	6.8	7.0	6.7	7.0	6.7	7.0	6.8	7.0
	Control	6.6	7.0	6.5	7.0	6.5	7.0	6.6	7.0
	4 x High	6.8	7.0	6.5	7.0	6.6	7.0	6.8	7.0
Flavour	4 x Low	6.7	7.0	6.3	7.0	6.5	7.0	6.7	7.0
	Control	6.5	7.0	6.4	7.0	6.3	6.5	6.5	7.0
	4 x High	6.8	7.0	6.5	7.0	6.6	7.0	6.7	7.0
Aftertaste	4 x Low	6.2	6.0	6.1	7.0	5.9	6.0	6.2	7.0
	Control	5.9	6.0	5.9	7.0	5.8	6.0	6.0	6.0
	4 x High	6.3	7.0	6.1	7.0	6.0	6.0	6.3	7.0
Count		88		23		22		89	

		Age									
		18-24y		25-34y		35-44y		45-54y		55-64y	
	Sample	Mean	Median								
Overall	4 x Low	6.7	7.0	7.0	7.0	6.6	7.0	7.0	7.0	6.7	7.0
	Control	6.6	7.0	6.7	7.0	6.1	6.0	6.9	7.0	7.0	7.0
	4 x High	6.9	7.0	6.8	7.5	6.5	7.0	7.0	7.0	6.7	7.0
Flavour	4 x Low	6.3	6.0	6.9	7.0	6.6	7.0	6.8	7.0	6.6	7.0
	Control	6.2	6.0	6.9	8.0	5.9	6.0	6.8	7.0	7.0	7.0
	4 x High	6.6	7.0	6.8	7.5	6.5	7.0	6.8	7.0	6.9	7.0
Aftertaste	4 x Low	5.7	5.0	6.3	7.0	6.0	6.0	6.3	7.0	6.3	7.0
	Control	5.5	5.0	5.8	6.0	5.3	5.0	6.7	7.0	6.3	7.0
	4 x High	6.6	7.0	6.6	7.0	5.7	6.0	6.6	7.0	6.4	7.0
Count		15		12		34		29		21	

	Site	Tasting Order
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Sample		North		South		Tasted 1st		Tasted 2nd		Tasted 3rd	
		Mean	Median	Mean	Median	Mean	Median	Mean	Median	Mean	Median
Overall	4 x Low	6.9	7.0	6.7	7.0	7.2	7.5	6.7	7.0	6.4	7.0
	Control	6.8	7.0	6.4	7.0	7.1	7.0	6.2	7.0	6.4	7.0
	4 x High	6.5	7.0	7.0	7.0	7.0	7.0	6.7	7.0	6.6	7.0
Flavour	4 x Low	6.7	7.0	6.6	7.0	7.2	7.0	6.6	7.0	6.2	6.0
	Control	6.7	7.0	6.3	7.0	7.1	8.0	6.1	7.0	6.4	7.0
	4 x High	6.5	7.0	6.9	7.0	6.8	7.0	6.7	7.0	6.6	7.0
Aftertaste	4 x Low	6.1	6.0	6.2	7.0	6.4	7.0	6.3	7.0	5.8	6.0
	Control	6.3	7.0	5.6	6.0	6.3	7.0	5.8	6.5	5.7	6.0
	4 x High	6.1	7.0	6.4	7.0	6.4	7.0	6.0	6.0	6.4	7.0
Count		55		56		36-38		36-38		36-38	

Appendix 2

Chemistry stage 1

Attrs	Sample	Mean	Stdev	PVal	Sig	Groupings (NK at 5%)
1-PENTEN-3-OL / 1-PENTEN-3-ONE	SULPHOMEX (5L/HA)	79838	31563.71	<0.001	0.10	A
1-PENTEN-3-OL / 1-PENTEN-3-ONE	UNTREATED	66214	4640.664			AB
1-PENTEN-3-OL / 1-PENTEN-3-ONE	HORTISUL (5L/HA)	51554.7	3237.722			AB
1-PENTEN-3-OL / 1-PENTEN-3-ONE	SULPHOMEX (15L/HA)	46260	7792			B
1-PENTEN-3-OL / 1-PENTEN-3-ONE	WATERSTRESSED	12889	1020.19			C
1-PENTEN-3-OL / 1-PENTEN-3-ONE	HORTISUL (15L/HA)	10039	568.493			C
2-ETHYLFURAN	WATERSTRESSED	14676.7	991.032	<0.001	0.10	A
2-ETHYLFURAN	HORTISUL (15L/HA)	10543.3	570.942			B
2-ETHYLFURAN	UNTREATED	9894.7	488.314			B
2-ETHYLFURAN	SULPHOMEX (5L/HA)	9223.3	1397.188			B
2-ETHYLFURAN	SULPHOMEX (15L/HA)	6952.3	524.048			C
2-ETHYLFURAN	HORTISUL (5L/HA)	6524.7	1408.871			C
77, 105	SULPHOMEX (15L/HA)	57872.7	5433.62	0.149	NS	
77, 105	HORTISUL (15L/HA)	57208	221.881			
77, 105	WATERSTRESSED	56885	3138.232			
77, 105	SULPHOMEX (5L/HA)	53983.7	667.371			
77, 105	UNTREATED	52113	2345.576			
77, 105	HORTISUL (5L/HA)	50198.3	6457.435			
2-PENTENAL	SULPHOMEX (5L/HA)	21095.3	9882.826	0.002	1%	A
2-PENTENAL	UNTREATED	15881.7	4200.694			AB
2-PENTENAL	HORTISUL (5L/HA)	10915.3	1379.588			BC
2-PENTENAL	SULPHOMEX (15L/HA)	8751.3	569.354			BC
2-PENTENAL	WATERSTRESSED	3989.7	890.517			C

2-PENTENAL	HORTISUL (15L/HA)	3003.3	520.56			C
			2			
TOLUENE	HORTISUL (15L/HA)	7326	523.76	0.11	NS	
			8			
TOLUENE	WATERSTRESSED	6401	492.39			
			4			
TOLUENE	SULPHOMEX (15L/HA)	5938	58.275			
TOLUENE	HORTISUL (5L/HA)	5800.3	534.00			
			8			
TOLUENE	UNTREATED	5288.7	1106.3			
			51			
TOLUENE	SULPHOMEX (5L/HA)	4927.3	1898.5			
			03			
HEXANAL	WATERSTRESSED	15980.3	5413.8	0.001	0.10	A
			98		%	
HEXANAL	HORTISUL (15L/HA)	6725.7	1602.9			B
			46			
HEXANAL	UNTREATED	5835.3	1329.7			B
			96			
HEXANAL	SULPHOMEX (5L/HA)	5558.3	1123.1			B
			46			
HEXANAL	SULPHOMEX (15L/HA)	5198.3	1186.0			B
			09			
HEXANAL	HORTISUL (5L/HA)	4505.3	1066.3			B
			43			
THIACYCLOPENTANE	WATERSTRESSED	254.7	80.208	0.558	NS	
THIACYCLOPENTANE	SULPHOMEX (15L/HA)	210	85.563			
THIACYCLOPENTANE	HORTISUL (5L/HA)	197	39.95			
THIACYCLOPENTANE	HORTISUL (15L/HA)	191	26.514			
THIACYCLOPENTANE	SULPHOMEX (5L/HA)	185	108.89			
			4			
THIACYCLOPENTANE	UNTREATED	149.7	38.501			
CIS-3-HEXENAL	WATERSTRESSED	2887.3	225.95	<0.00	0.10	A
			2	1	%	
CIS-3-HEXENAL	SULPHOMEX (5L/HA)	1534.7	627.76			B
			2			
CIS-3-HEXENAL	UNTREATED	1363	311.46			B
			7			
CIS-3-HEXENAL	HORTISUL (5L/HA)	1287.7	155.06			B
			9			
CIS-3-HEXENAL	SULPHOMEX (15L/HA)	915.7	99.219			B
CIS-3-HEXENAL	HORTISUL (15L/HA)	882.3	267.29			B
			1			
2-HEXENAL	WATERSTRESSED	307283.7	39591.	<0.00	0.10	A
			6	1	%	
2-HEXENAL	SULPHOMEX (5L/HA)	112139.7	70063.			B
			9			
2-HEXENAL	UNTREATED	75555.7	24792.			B
			69			
2-HEXENAL	HORTISUL (5L/HA)	69617.3	11953.			B
			66			
2-HEXENAL	HORTISUL (15L/HA)	53721	7958.4			B

2-HEXENAL	SULPHOMEX (15L/HA)	36778.7	4484.2	06		B
3-ETHYLTHIOPHENE	WATERSTRESSED	2588	179.51	<0.00	0.10	A
3-ETHYLTHIOPHENE	HORTISUL (15L/HA)	734	62.554	9 1	%	B
3-ETHYLTHIOPHENE	HORTISUL (5L/HA)	450.3	30.892			C
3-ETHYLTHIOPHENE	SULPHOMEX (5L/HA)	447.7	34.122			C
3-ETHYLTHIOPHENE	UNTREATED	366.7	29.28			C
3-ETHYLTHIOPHENE	SULPHOMEX (15L/HA)	351.3	15.144			C
4-HEPTENAL	SULPHOMEX (5L/HA)	378.7	87.956	0.003	1%	A
4-HEPTENAL	UNTREATED	292.7	29.28			AB
4-HEPTENAL	SULPHOMEX (15L/HA)	232.7	38.734			BC
4-HEPTENAL	HORTISUL (5L/HA)	232.3	52.205			BC
4-HEPTENAL	HORTISUL (15L/HA)	177.7	22.679			BC
4-HEPTENAL	WATERSTRESSED	144.3	69.867			C
N-HEPTANOL	WATERSTRESSED	627.3	97.516	0.011	5%	A
N-HEPTANOL	HORTISUL (15L/HA)	576	171.76			AB
N-HEPTANOL	HORTISUL (5L/HA)	416.7	37.581	4		B
N-HEPTANOL	SULPHOMEX (5L/HA)	394.7	60.699			B
N-HEPTANOL	UNTREATED	384.7	56.048			B
N-HEPTANOL	SULPHOMEX (15L/HA)	352.3	10.408			B
STYRENE	WATERSTRESSED	26069.7	7047.7	0.079	NS	
STYRENE	HORTISUL (15L/HA)	23920	3225.5	14		
STYRENE	UNTREATED	20237.7	2434.3	31		
STYRENE	SULPHOMEX (5L/HA)	20032.7	1577.7	79		
STYRENE	SULPHOMEX (15L/HA)	17946.3	3170.4	43		
STYRENE	HORTISUL (5L/HA)	17158.3	1768.5	46		
2,4-HEXADIENAL	SULPHOMEX (5L/HA)	9818.3	4583.6	12	0.052	NS
2,4-HEXADIENAL	WATERSTRESSED	8785.3	1333.0	8		
2,4-HEXADIENAL	UNTREATED	8134.3	2177.0	03		
2,4-HEXADIENAL	HORTISUL (5L/HA)	6579.3	477	33		
2,4-HEXADIENAL	SULPHOMEX (15L/HA)	4645	263.18	1		
2,4-HEXADIENAL	HORTISUL (15L/HA)	4484	910.57	8		
METHYLTHIOCYCLOPENTANE	WATERSTRESSED	254.3	60.863	0.025	5%	A
METHYLTHIOCYCLOPENTANE	HORTISUL (5L/HA)	220	95.645			AB

ANE							
METHYLTHIOCYCLOPENTANE	SULPHOMEX (15L/HA)	210.3	65.919				AB
METHYLTHIOCYCLOPENTANE	HORTISUL (15L/HA)	164.3	50.639				AB
METHYLTHIOCYCLOPENTANE	UNTREATED	83.7	77.501				AB
METHYLTHIOCYCLOPENTANE	SULPHOMEX (5L/HA)	65.7	39.068				B
1-HEXANETHIOL	WATERSTRESSED	100.3	6.658	0.002		1%	A
1-HEXANETHIOL	HORTISUL (15L/HA)	86	33.151				A
1-HEXANETHIOL	HORTISUL (5L/HA)	31.7	32.532				B
1-HEXANETHIOL	SULPHOMEX (5L/HA)	24.7	42.724				B
1-HEXANETHIOL	SULPHOMEX (15L/HA)	5.7	9.815				B
1-HEXANETHIOL	UNTREATED	0	0				B
1-BROMOHEXANE	HORTISUL (15L/HA)	85302.7	6756.6	0.002		1%	A
1-BROMOHEXANE	WATERSTRESSED	77972.7	2743.9				A
1-BROMOHEXANE	SULPHOMEX (15L/HA)	40393.7	3923.3				B
1-BROMOHEXANE	HORTISUL (5L/HA)	40238.3	8036.4				B
1-BROMOHEXANE	UNTREATED	36708.7	13188.01				B
1-BROMOHEXANE	SULPHOMEX (5L/HA)	35542	29350.4				B
2-HEPTENAL	SULPHOMEX (5L/HA)	3619.7	1789.0	0.012		5%	A
2-HEPTENAL	UNTREATED	3249	1217.4				A
2-HEPTENAL	SULPHOMEX (15L/HA)	2179.3	613.90				AB
2-HEPTENAL	HORTISUL (5L/HA)	1949.7	532.83				AB
2-HEPTENAL	WATERSTRESSED	917	403.92				B
2-HEPTENAL	HORTISUL (15L/HA)	571.7	70.868				B
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	SULPHOMEX (5L/HA)	931.3	279.78	0.001		0.10%	A
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	UNTREATED	874.7	48.232				AB
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	WATERSTRESSED	792.7	56.959				AB
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	HORTISUL (5L/HA)	647	47.791				AB
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	SULPHOMEX (15L/HA)	592	65.506				B
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	HORTISUL (15L/HA)	325.7	30.039				C
BENZALDEHYDE	WATERSTRESSED	31061.3	4121.8	0.025		5%	A
BENZALDEHYDE	UNTREATED	26985	3692.8				AB

BENZALDEHYDE	SULPHOMEX (5L/HA)	26972	2299.9 72			AB
BENZALDEHYDE	HORTISUL (5L/HA)	26738.3	1291.1 05			AB
BENZALDEHYDE	SULPHOMEX (15L/HA)	25179.3	1834.4 8			AB
BENZALDEHYDE	HORTISUL (15L/HA)	21614.7	1556.7 1			B
2,6-DIMETHYL-5-HEPTEN-1-OL	SULPHOMEX (5L/HA)	22350.7	16808.19	0.078	NS	
2,6-DIMETHYL-5-HEPTEN-1-OL	UNTREATED	19924.3	6779.3 16			
2,6-DIMETHYL-5-HEPTEN-1-OL	HORTISUL (5L/HA)	17484.3	3762.0 86			
2,6-DIMETHYL-5-HEPTEN-1-OL	SULPHOMEX (15L/HA)	13709.3	2612.3 2			
2,6-DIMETHYL-5-HEPTEN-1-OL	WATERSTRESSED	10417	1504.1 39			
2,6-DIMETHYL-5-HEPTEN-1-OL	HORTISUL (15L/HA)	2606	728.43 5			
2,4-HEPTADIENAL	SULPHOMEX (5L/HA)	86063.3	28186.23	0.001	0.10 A %	
2,4-HEPTADIENAL	UNTREATED	73612	16056.08			AB
2,4-HEPTADIENAL	HORTISUL (5L/HA)	60948.7	4607.9 51			AB
2,4-HEPTADIENAL	SULPHOMEX (15L/HA)	51181.3	1575.7 41			BC
2,4-HEPTADIENAL	WATERSTRESSED	29065.7	3289.5 89			C
2,4-HEPTADIENAL	HORTISUL (15L/HA)	22961	3009.3 41			C
BENZENEMETHANOL	SULPHOMEX (5L/HA)	1768	559.95 4	<0.00 1	0.10 A %	
BENZENEMETHANOL	UNTREATED	1566.3	329.36 7			AB
BENZENEMETHANOL	HORTISUL (5L/HA)	1340	168.32 1			AB
BENZENEMETHANOL	SULPHOMEX (15L/HA)	1065.3	63.129			B
BENZENEMETHANOL	WATERSTRESSED	534.3	135.07 9			C
BENZENEMETHANOL	HORTISUL (15L/HA)	405.3	107.77 9			C
3-METHOXYPHENOL	SULPHOMEX (5L/HA)	1762.7	703.43 2	0.025	5% A	
3-METHOXYPHENOL	UNTREATED	1374.7	295.40 2			AB
3-METHOXYPHENOL	HORTISUL (5L/HA)	1308	154.7			AB
3-METHOXYPHENOL	HORTISUL (15L/HA)	1218.3	171.79 7			AB
3-METHOXYPHENOL	SULPHOMEX (15L/HA)	865.7	139.73 3			B
3-METHOXYPHENOL	WATERSTRESSED	711.3	67.515			B
2,2,6-	WATERSTRESSED	2844	51.264	0.069	NS	

TRIMETHYLCYCLOHEXAN ONE						
2,2,6- TRIMETHYLCYCLOHEXAN ONE	SULPHOMEX (5L/HA)	2837	938.10			
				2		
2,2,6- TRIMETHYLCYCLOHEXAN ONE	HORTISUL (15L/HA)	2732.7	130.31			
				6		
2,2,6- TRIMETHYLCYCLOHEXAN ONE	UNTREATED	2334.3	337.36			
				4		
2,2,6- TRIMETHYLCYCLOHEXAN ONE	HORTISUL (5L/HA)	2321	19.975			
2,2,6- TRIMETHYLCYCLOHEXAN ONE	SULPHOMEX (15L/HA)	1778.7	330.53			
				3		
BENZENEACETALDEHYD E	WATERSTRESSED	25696.7	4914.6	0.143	NS	
				9		
BENZENEACETALDEHYD E	HORTISUL (15L/HA)	22951	4003.1			
				98		
BENZENEACETALDEHYD E	SULPHOMEX (5L/HA)	20450.7	1682.1			
				72		
BENZENEACETALDEHYD E	SULPHOMEX (15L/HA)	20206.7	3585.5			
BENZENEACETALDEHYD E	UNTREATED	19576.7	2121.7			
				17		
BENZENEACETALDEHYD E	HORTISUL (5L/HA)	18244	1789.2			
				15		
3-METHYLBUTYL ISOTHIOCYANATE	WATERSTRESSED	7628.3	678.55	<0.00	0.10	A
				8	1	%
3-METHYLBUTYL ISOTHIOCYANATE	HORTISUL (15L/HA)	3436	285.73			B
				2		
3-METHYLBUTYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	2163.7	338.57			C
				1		
3-METHYLBUTYL ISOTHIOCYANATE	HORTISUL (5L/HA)	2014.3	86.234			C
3-METHYLBUTYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	1924.7	755.32			C
				9		
3-METHYLBUTYL ISOTHIOCYANATE	UNTREATED	1919.7	270.14			C
				3		
3,5-OCTADIEN-2-ONE	UNTREATED	2820.7	94.384	0.002	1%	A
3,5-OCTADIEN-2-ONE	SULPHOMEX (5L/HA)	2599.3	1290.0			A
				92		
3,5-OCTADIEN-2-ONE	HORTISUL (5L/HA)	1955.3	269.83			AB
				8		
3,5-OCTADIEN-2-ONE	SULPHOMEX (15L/HA)	1275.7	116.92			B
3,5-OCTADIEN-2-ONE	HORTISUL (15L/HA)	874.3	142.00			B
				1		
3,5-OCTADIEN-2-ONE	WATERSTRESSED	769.7	73.921			B
CIS-3-HEXENAL DIETHYL ACETAL	SULPHOMEX (5L/HA)	13595.3	5063.5	0.003	1%	A
				7		
CIS-3-HEXENAL DIETHYL ACETAL	WATERSTRESSED	13190	1690.5			A
				4		

CIS-3-HEXENAL DIETHYL ACETAL	UNTREATED	12361.7	1522.8			A
CIS-3-HEXENAL DIETHYL ACETAL	HORTISUL (5L/HA)	8902	273.08			AB
CIS-3-HEXENAL DIETHYL ACETAL	SULPHOMEX (15L/HA)	8768.3	861.42			AB
CIS-3-HEXENAL DIETHYL ACETAL	HORTISUL (15L/HA)	4490.3	215.28			B
ETHYL-TRANS-4-HEPTENOATE	HORTISUL (15L/HA)	5265.7	699.80	0.007	1%	A
ETHYL-TRANS-4-HEPTENOATE	SULPHOMEX (5L/HA)	3710.3	1396.2			B
ETHYL-TRANS-4-HEPTENOATE	WATERSTRESSED	3451.7	820.23			B
ETHYL-TRANS-4-HEPTENOATE	UNTREATED	2849.3	605.93			B
ETHYL-TRANS-4-HEPTENOATE	HORTISUL (5L/HA)	2688.3	300.76			B
ETHYL-TRANS-4-HEPTENOATE	SULPHOMEX (15L/HA)	2260	359.58			B
(E)-2-NONEN-1-OL	WATERSTRESSED	5943	481.87	0.285	NS	
(E)-2-NONEN-1-OL	HORTISUL (15L/HA)	5558.7	661.10			
(E)-2-NONEN-1-OL	UNTREATED	5378.3	739.55			
(E)-2-NONEN-1-OL	SULPHOMEX (5L/HA)	5212.7	1397.6			
(E)-2-NONEN-1-OL	HORTISUL (5L/HA)	4848.3	361.71			
(E)-2-NONEN-1-OL	SULPHOMEX (15L/HA)	4498.7	200.56			
N-PENTYL ISOTHIOCYANATE	HORTISUL (15L/HA)	8749.7	1296.9	0.903	NS	
N-PENTYL ISOTHIOCYANATE	UNTREATED	8521.3	2005.9			
N-PENTYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	8346.7	2881.4			
N-PENTYL ISOTHIOCYANATE	WATERSTRESSED	8226.7	1033.5			
N-PENTYL ISOTHIOCYANATE	HORTISUL (5L/HA)	7820.3	392.70			
N-PENTYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	7347	452.88			
CARVACROL	SULPHOMEX (5L/HA)	894.7	28.746	0.003	1%	A
CARVACROL	UNTREATED	840.3	110.12			AB
CARVACROL	HORTISUL (5L/HA)	682	154.26			BC
CARVACROL	HORTISUL (15L/HA)	656	79.228			BC
CARVACROL	WATERSTRESSED	622	19.672			C
CARVACROL	SULPHOMEX (15L/HA)	553	58.404			C
1-TERPINEOL	SULPHOMEX (5L/HA)	658	245.92	0.016	5%	A

1-TERPINEOL	HORTISUL (5L/HA)	436	23.431			AB
1-TERPINEOL	UNTREATED	434.3	85.002			AB
1-TERPINEOL	HORTISUL (15L/HA)	329.7	48.563			B
1-TERPINEOL	WATERSTRESSED	314.3	27.465			B
1-TERPINEOL	SULPHOMEX (15L/HA)	307	36.166			B
BENZENEETHANOL	HORTISUL (5L/HA)	10007	264.05	<0.00	0.10	A
				1	1	%
BENZENEETHANOL	WATERSTRESSED	8246	1676.8			B
				21		
BENZENEETHANOL	HORTISUL (15L/HA)	7134.3	857.56			B
				9		
BENZENEETHANOL	SULPHOMEX (15L/HA)	5190	550.61			C
				3		
BENZENEETHANOL	SULPHOMEX (5L/HA)	3889.7	470.03			C
				1		
BENZENEETHANOL	UNTREATED	3883	725.97			C
				6		
2,2,6,6-TETRAMETHYL- 3,5-HEPTANEDIONE	WATERSTRESSED	2785	210.94	<0.00	0.10	A
				1	1	%
2,2,6,6-TETRAMETHYL- 3,5-HEPTANEDIONE	HORTISUL (5L/HA)	1441	70.064			B
2,2,6,6-TETRAMETHYL- 3,5-HEPTANEDIONE	UNTREATED	1282.3	221.34			B
				2		
2,2,6,6-TETRAMETHYL- 3,5-HEPTANEDIONE	SULPHOMEX (15L/HA)	1183	77.698			B
2,2,6,6-TETRAMETHYL- 3,5-HEPTANEDIONE	SULPHOMEX (5L/HA)	1132.7	164.44			B
				6		
2,2,6,6-TETRAMETHYL- 3,5-HEPTANEDIONE	HORTISUL (15L/HA)	620	20			C
2,6-NONADIENAL	SULPHOMEX (5L/HA)	2427.7	213.93	<0.00	0.10	A
				1	1	%
2,6-NONADIENAL	UNTREATED	2259.7	260.62			A
				5		
2,6-NONADIENAL	HORTISUL (5L/HA)	2254	176.55			A
				3		
2,6-NONADIENAL	HORTISUL (15L/HA)	2193.3	181.75			A
				1		
2,6-NONADIENAL	SULPHOMEX (15L/HA)	1945	79.956			A
2,6-NONADIENAL	WATERSTRESSED	1331.7	196.04			B
				2		
4-METHYLPENTYL ISOTHIOCYANATE	WATERSTRESSED	31219	2114.8	<0.00	0.10	A
				8	1	%
4-METHYLPENTYL ISOTHIOCYANATE	HORTISUL (15L/HA)	16767	873.37			B
				1		
4-METHYLPENTYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	7582	1008.9			C
				85		
4-METHYLPENTYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	7524.3	2798.5			C
				93		
4-METHYLPENTYL ISOTHIOCYANATE	HORTISUL (5L/HA)	6746.3	216.48			C
				4		
4-METHYLPENTYL ISOTHIOCYANATE	UNTREATED	6279.3	890.57			C
				9		
HEXYL ISOTHIOCYANATE	WATERSTRESSED	4121.3	147.03	<0.00	0.10	A

HEXYL ISOTHIOCYANATE	HORTISUL (15L/HA)	3238.3	487.10	9 1	%	B
HEXYL ISOTHIOCYANATE	HORTISUL (5L/HA)	2246.3	378.36	4		C
HEXYL ISOTHIOCYANATE	UNTREATED	2034.3	674.28	5		C
HEXYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	1923	397.43	1		C
HEXYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	1833	578.81	2		C
METHYL SALICYLATE	WATERSTRESSED	9416.3	247.01	<0.00	0.10	A
METHYL SALICYLATE	SULPHOMEX (5L/HA)	6593	388.15	5 1	%	B
METHYL SALICYLATE	HORTISUL (5L/HA)	6324.7	344.01	3		B
METHYL SALICYLATE	HORTISUL (15L/HA)	5941.3	240.43	5		B
METHYL SALICYLATE	SULPHOMEX (15L/HA)	5824.7	355.40	4		B
METHYL SALICYLATE	UNTREATED	5677.7	1003.3	2		B
ETHYL NICOTINATE	UNTREATED	25353	8054.3	74	0.028	5% A
ETHYL NICOTINATE	SULPHOMEX (5L/HA)	22181.7	8169.4	78		A
ETHYL NICOTINATE	HORTISUL (5L/HA)	21420.7	7301.0	14		A
ETHYL NICOTINATE	SULPHOMEX (15L/HA)	17989.3	8361.8	37		A
ETHYL NICOTINATE	HORTISUL (15L/HA)	8475	2548.8	71		A
ETHYL NICOTINATE	WATERSTRESSED	7006	3975.3	85		A
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	UNTREATED	22324.3	2685.6	96	<0.00	0.10 A
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	SULPHOMEX (15L/HA)	10141.7	752.15	58 1	%	B
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	SULPHOMEX (5L/HA)	9725.3	4264.4	51		B
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	HORTISUL (5L/HA)	8825.7	2927.3	57		B
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	HORTISUL (15L/HA)	2312.3	168.71	7		C
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	WATERSTRESSED	2242.7	709.05	5		C
(3-METHYL-3-BUTENYL)BENZENE	WATERSTRESSED	686041.3	289044	0.053	NS	
(3-METHYL-3-BUTENYL)BENZENE	HORTISUL (15L/HA)	527764	103430	.2		
(3-METHYL-3-BUTENYL)BENZENE	UNTREATED	368193.7	74596	.1		
(3-METHYL-3-BUTENYL)BENZENE	SULPHOMEX (5L/HA)	365689	45417	28		
				01		

(3-METHYL-3-BUTENYL)BENZENE	SULPHOMEX (15L/HA)	360961	137750.6		
(3-METHYL-3-BUTENYL)BENZENE	HORTISUL (5L/HA)	301446	45614.89		
BETA-CYCLOCITRAL	SULPHOMEX (5L/HA)	13116.3	3963.783	0.023	5% A
BETA-CYCLOCITRAL	UNTREATED	10820.3	2014.983		AB
BETA-CYCLOCITRAL	HORTISUL (5L/HA)	9392	348.901		AB
BETA-CYCLOCITRAL	HORTISUL (15L/HA)	8713	492.685		AB
BETA-CYCLOCITRAL	WATERSTRESSED	8393.7	69.529		AB
BETA-CYCLOCITRAL	SULPHOMEX (15L/HA)	7059.7	471.706		B
BENZENEPROPANENITRILE	HORTISUL (5L/HA)	554047.7	66759.05	0.032	5% A
BENZENEPROPANENITRILE	UNTREATED	464492.3	327991.5		AB
BENZENEPROPANENITRILE	SULPHOMEX (15L/HA)	449646.3	236848.9		AB
BENZENEPROPANENITRILE	SULPHOMEX (5L/HA)	244644	45505.45		AB
BENZENEPROPANENITRILE	WATERSTRESSED	189831.3	2445.738		AB
BENZENEPROPANENITRILE	HORTISUL (15L/HA)	83270	4018.966		B
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	UNTREATED	16867.3	1577.204	<0.001	0.10 A %
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	SULPHOMEX (5L/HA)	8010.7	3067.719		B
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	SULPHOMEX (15L/HA)	7621.3	833.694		B
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	HORTISUL (5L/HA)	6720	2163.03		B
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	HORTISUL (15L/HA)	2424	71.106		C
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	WATERSTRESSED	2098	558.587		C
N-HEPTYL ISOTHIOCYANATE	WATERSTRESSED	68499	3362.392	<0.001	0.10 A %
N-HEPTYL ISOTHIOCYANATE	HORTISUL (15L/HA)	39315.7	1580.552		B
N-HEPTYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	22524.3	2196.323		C
N-HEPTYL ISOTHIOCYANATE	HORTISUL (5L/HA)	21150.7	1180.014		C
N-HEPTYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	20963.7	6094.657		C
N-HEPTYL ISOTHIOCYANATE	UNTREATED	18553.3	1179.249		C
CYCLOHEXANE METHYL ISOTHIOCYANATE	WATERSTRESSED	18577.7	1544.966	<0.001	0.10 A %
CYCLOHEXANE METHYL ISOTHIOCYANATE	HORTISUL (15L/HA)	11059.7	735.898		B

CYCLOHEXANE METHYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	8315.3	1195.1			BC
CYCLOHEXANE METHYL ISOTHIOCYANATE	HORTISUL (5L/HA)	7778.7	656.33			BC
CYCLOHEXANE METHYL ISOTHIOCYANATE	UNTREATED	5737	462.70			C
CYCLOHEXANE METHYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	4758	4700.1			C
3-METHYLHEXYL ISOTHIOCYANATE	WATERSTRESSED	5847.7	430.01	<0.00	0.10	A
3-METHYLHEXYL ISOTHIOCYANATE	HORTISUL (15L/HA)	3883	291.15	7 1	%	B
3-METHYLHEXYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	2476	681.47			C
3-METHYLHEXYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	2411.3	197.56			C
3-METHYLHEXYL ISOTHIOCYANATE	HORTISUL (5L/HA)	2321.7	113.77			C
3-METHYLHEXYL ISOTHIOCYANATE	UNTREATED	2195.3	250.01			C
4-ETHENYL-2-METHOXYPHENOL	SULPHOMEX (5L/HA)	4198	581.70	0.067	NS	
4-ETHENYL-2-METHOXYPHENOL	UNTREATED	3809.3	814.65			
4-ETHENYL-2-METHOXYPHENOL	SULPHOMEX (15L/HA)	3715.3	342.20			
4-ETHENYL-2-METHOXYPHENOL	WATERSTRESSED	3254	399.18			
4-ETHENYL-2-METHOXYPHENOL	HORTISUL (5L/HA)	3111.3	377.15			
4-ETHENYL-2-METHOXYPHENOL	HORTISUL (15L/HA)	2950.3	226.32			
4-ETHOXYBENZALDEHYDE	UNTREATED	2155.7	376.06	<0.00	0.10	A
4-ETHOXYBENZALDEHYDE	SULPHOMEX (5L/HA)	1651.3	571.00	4 1	%	AB
4-ETHOXYBENZALDEHYDE	SULPHOMEX (15L/HA)	1215.3	178.08			B
4-ETHOXYBENZALDEHYDE	HORTISUL (5L/HA)	1174	356.73			B
4-ETHOXYBENZALDEHYDE	WATERSTRESSED	282.3	89.79			C
4-ETHOXYBENZALDEHYDE	HORTISUL (15L/HA)	85.3	79.387			C
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	WATERSTRESSED	4410.3	567.02	<0.00	0.10	A
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	HORTISUL (15L/HA)	3026	287.09	9 1	%	B
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	2721.7	638.32			BC
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	HORTISUL (5L/HA)	2245.3	290.97			BC
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	1648.3	918.15			C
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	UNTREATED	1425	313.51			C

ISOTHIOCYANATE			7			
94, 117, 142	WATERSTRESSED	3099.7	912.36	0.009	1% A	
			7			
94, 117, 142	SULPHOMEX	2135.3	398.61		AB	
	(15L/HA)		1			
94, 117, 142	HORTISUL (5L/HA)	2091	356.25		AB	
			7			
94, 117, 142	HORTISUL (15L/HA)	1438	275.10		B	
			2			
94, 117, 142	UNTREATED	1255.7	571.77		B	
			5			
94, 117, 142	SULPHOMEX	1054.3	655.21		B	
	(5L/HA)		6			
ETHYL	UNTREATED	11010.7	1187.5	<0.00	0.10 A	
HYDROCINNAMATE			92	1	%	
ETHYL	SULPHOMEX	7696.7	2322.2		B	
HYDROCINNAMATE	(5L/HA)		7			
ETHYL	SULPHOMEX	6238.7	3257.4		B	
HYDROCINNAMATE	(15L/HA)		15			
ETHYL	HORTISUL (5L/HA)	6090.7	1709.2		B	
HYDROCINNAMATE			71			
ETHYL	WATERSTRESSED	1350.3	355.39		C	
HYDROCINNAMATE			5			
ETHYL	HORTISUL (15L/HA)	535.7	48.542		C	
HYDROCINNAMATE						
OCTYL ISOTHIOCYANATE	WATERSTRESSED	35607.7	1988.5	<0.00	0.10 A	
			64	1	%	
OCTYL ISOTHIOCYANATE	HORTISUL (15L/HA)	22895	335.54		B	
			1			
OCTYL ISOTHIOCYANATE	SULPHOMEX	11728.3	1056.7		C	
	(15L/HA)		64			
OCTYL ISOTHIOCYANATE	SULPHOMEX	11629.3	3042.5		C	
	(5L/HA)		56			
OCTYL ISOTHIOCYANATE	HORTISUL (5L/HA)	9826	599.42		C	
			3			
OCTYL ISOTHIOCYANATE	UNTREATED	8358	590.54		C	
			3			
METHYLHEPTYL	WATERSTRESSED	6003	370.67	<0.00	0.10 A	
ISOTHIOCYANATE			1	1	%	
METHYLHEPTYL	HORTISUL (15L/HA)	4405.3	204.79		B	
ISOTHIOCYANATE			3			
METHYLHEPTYL	SULPHOMEX	2762.3	714.43		C	
ISOTHIOCYANATE	(5L/HA)		5			
METHYLHEPTYL	SULPHOMEX	2555.3	175.74		C	
ISOTHIOCYANATE	(15L/HA)		2			
METHYLHEPTYL	HORTISUL (5L/HA)	2366.3	207.85		C	
ISOTHIOCYANATE			2			
METHYLHEPTYL	UNTREATED	2168.3	126.80		C	
ISOTHIOCYANATE			8			
GERANYL ACETONE	UNTREATED	19972.3	7122.3	0.124	NS	
			95			
GERANYL ACETONE	SULPHOMEX	16241.3	6445.5			
	(5L/HA)		14			
GERANYL ACETONE	HORTISUL (15L/HA)	12155.3	6203.0			
			76			

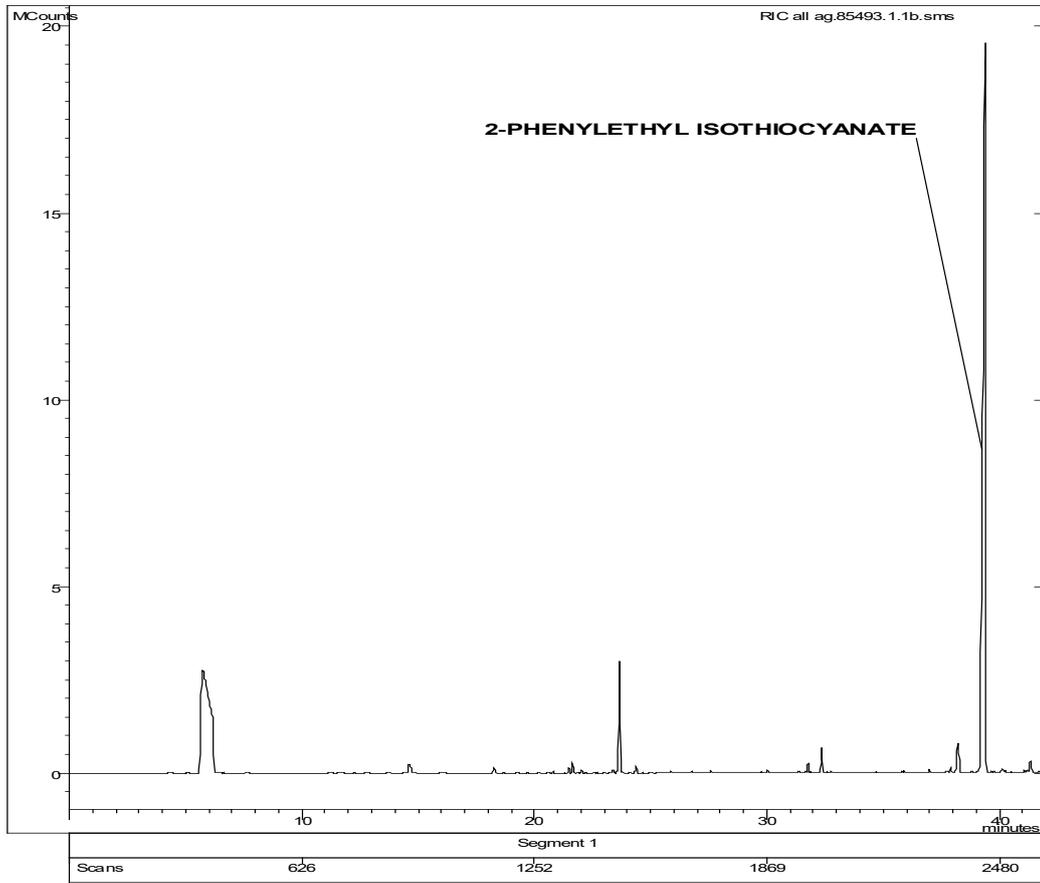
GERANYL ACETONE	HORTISUL (5L/HA)	11461.7	3663.9			
			25			
GERANYL ACETONE	SULPHOMEX (15L/HA)	11344.7	4620.3			
			68			
GERANYL ACETONE	WATERSTRESSED	6912.7	1528.1			
			98			
2,5-DIMETHYL-1-PHENYLPYRROLE	UNTREATED	8988	2008.8	0.001	0.10	A
			86		%	
2,5-DIMETHYL-1-PHENYLPYRROLE	SULPHOMEX (5L/HA)	8452.3	1615.7			A
			87			
2,5-DIMETHYL-1-PHENYLPYRROLE	HORTISUL (5L/HA)	7335	1599.0			A
			74			
2,5-DIMETHYL-1-PHENYLPYRROLE	SULPHOMEX (15L/HA)	6647	2147.2			A
			93			
2,5-DIMETHYL-1-PHENYLPYRROLE	WATERSTRESSED	2941	1296.9			B
			82			
2,5-DIMETHYL-1-PHENYLPYRROLE	HORTISUL (15L/HA)	2581.3	561.60			B
			2			
NONYL ISOTHIOCYANATE	WATERSTRESSED	6429.3	195.98	<0.00	0.10	A
			6	1	%	
NONYL ISOTHIOCYANATE	HORTISUL (15L/HA)	4114.7	178.35			B
			2			
NONYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	2033.3	75.976			C
NONYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	1982.7	617.51			C
			1			
NONYL ISOTHIOCYANATE	HORTISUL (5L/HA)	1552.7	176.41			C
			5			
NONYL ISOTHIOCYANATE	UNTREATED	1372.7	186.35			C
ISOAMYL DECANOATE	UNTREATED	191416.7	40900.	<0.00	0.10	A
			32	1	%	
ISOAMYL DECANOATE	HORTISUL (15L/HA)	148374.7	8116.9			B
			99			
ISOAMYL DECANOATE	WATERSTRESSED	131784	10986.			BC
			94			
ISOAMYL DECANOATE	SULPHOMEX (5L/HA)	99390.3	27140.			C
			47			
ISOAMYL DECANOATE	HORTISUL (5L/HA)	87690.3	7270.8			C
			26			
ISOAMYL DECANOATE	SULPHOMEX (15L/HA)	80948.7	5858.5			C
			27			
2-PHENYLETHYL ISOTHIOCYANATE	WATERSTRESSED	92690189	242987	<0.00	0.10	A
			9	1	%	
2-PHENYLETHYL ISOTHIOCYANATE	HORTISUL (15L/HA)	82634539	333525			B
			9			
2-PHENYLETHYL ISOTHIOCYANATE	SULPHOMEX (5L/HA)	58208380	137937			C
			6			
2-PHENYLETHYL ISOTHIOCYANATE	SULPHOMEX (15L/HA)	53710541	527296			CD
			8			
2-PHENYLETHYL ISOTHIOCYANATE	UNTREATED	53078163	764636			CD
			3			
2-PHENYLETHYL ISOTHIOCYANATE	HORTISUL (5L/HA)	47482351	126114			D
			2			

APPENDIX 3
CHEMICAL ANALYSIS FROM STAGE 2

Chromatogram Plot

File: d:\85493 watercress 010605\ag.85493.1.1b.sms
Sample: ag.85493.1.1b
Scan Range: 1 - 2601 Time Range: 0.00 - 41.98 min.

Operator: JP
Date: 6/2/05 1:45 AM



Typical Watercress Chromatogram

Chemical analysis (results from trial 2)

ANOVA results

2-way ANOVA (Sample & Analysis Group, Full factorial)

		N
Samprname	2HighAppl	8
	2LowAppl	8
	4HighAppl	9
	4LowAppl	7
	Contrl	8
	Waterstr	3
	Analysis Group	1
2		12
3		12
4		7

Attribute/Volatile	SampleName (p-value)
1-PENTEN-3-OL / 1-PENTEN-3-ONE	0.001
2-ETHYLFURAN	0.000
77, 105	0.360
2-PENTENAL	0.000
TOLUENE	0.277
HEXANAL	0.000
THIACYCLOPENTANE	0.008
CIS-3-HEXENAL	0.000
2-HEXENAL	0.000
3-ETHYLTHIOPHENE	0.000
4-HEPTENAL	0.000
N-HEPTANOL	0.001
STYRENE	0.212
2,4-HEXADIENAL	0.000
METHYLTHIOCYCLOPENTANE	0.000
1-HEXANETHIOL	0.002
1-BROMOHEXANE	0.306
2-HEPTENAL	0.000
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	0.000
BENZALDEHYDE	0.197
2,6-DIMETHYL-5-HEPTEN-1-OL	0.000
2,4-HEPTADIENAL	0.000
BENZENEMETHANOL	0.000
3-METHOXYPHENOL	0.030

2,2,6-TRIMETHYLCYCLOHEXANONE	0.005
BENZENEACETALDEHYDE	0.000
3-METHYLBUTYL ISOTHIOCYANATE	0.058
3 5-OCTADIEN-2-ONE	0.006
CIS-3-HEXENAL DIETHYL ACETAL	0.000
ETHYL-TRANS-4-HEPTENOATE	0.001
(E)-2-NONEN-1-OL	0.010
N-PENTYL ISOTHIOCYANATE	0.000
CARVACROL	0.000
1-TERPINEOL	0.019
BENZENEETHANOL	0.000
2,2,6,6-TETRAMETHYL-3 5- HEPTANEDIONE	0.000
2 6-NONADIENAL	0.656
4-METHYLPENTYL ISOTHIOCYANATE	0.174
HEXYL ISOTHIOCYANATE	0.000
METHYL SALICYLATE	0.000
ETHYL NICOTINATE	0.051
3-ETHYL-4-METHYL-1H-PYRROLE-2,5- DIONE	0.121
(3-METHYL-3-BUTENYL)BENZENE	0.380
BETA-CYCLOCITRAL	0.001
BENZENEPROPANENITRILE	0.000
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5- DIONE	0.078
N-HEPTYL ISOTHIOCYANATE	0.213
CYCLOHEXANE METHYL ISOTHIOCYANATE	0.000
3-METHYLHEXYL ISOTHIOCYANATE	0.000
4-ETHENYL-2-METHOXYPHENOL	0.000
4-ETHOXYBENZALDEHYDE	0.036
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	0.000
94, 117, 142	0.000
ETHYL HYDROCINNAMATE	0.000
OCTYL ISOTHIOCYANATE	0.192
METHYLHEPTYL ISOTHIOCYANATE	0.000
GERANYL ACETONE	0.917
2,5-DIMETHYL-1-PHENYLPYRROLE	0.001
NONYL ISOTHIOCYANATE	0.159
ISOAMYL DECANOATE	0.045
2-PHENYLETHYLISOTHOICYANATE	0.167

NK at 10% - Chemistry data Trial 2 Groupings
(NK at 10%)

1-PENTEN-3-OL / 1-PENTEN-3-ONE

SampleName

4 LOW APPLICATIONS CONTROL	410492 a
2 LOW APPLICATIONS	362018 a
2 HIGH APPLICATIONS	247455 b
4 HIGH APPLICATIONS	195904 b
WATERSTRESSED	160487 b
	151143 b

2-ETHYLFURAN

SampleName

WATERSTRESSED	431429 a
4 LOW APPLICATIONS CONTROL	231962 b
2 HIGH APPLICATIONS	139673 c
4 HIGH APPLICATIONS	111920 c
2 LOW APPLICATIONS	68756 c
	56730 c

77, 105

SampleName

WATERSTRESSED	45960 NSD
2 LOW APPLICATIONS	34315 NSD
4 HIGH APPLICATIONS	32148 NSD
4 LOW APPLICATIONS	28887 NSD
CONTROL	24145 NSD
2 HIGH APPLICATIONS	18843 NSD

2-PENTENAL

SampleName

WATERSTRESSED	166184 a
4 LOW APPLICATIONS CONTROL	150954 a
2 LOW APPLICATIONS	134882 a
2 HIGH APPLICATIONS	75590 b
4 HIGH APPLICATIONS	74341 b
	60180 b

TOLUENE

SampleName

WATERSTRESSED	83525 NSD
4 HIGH APPLICATIONS CONTROL	50528 NSD
4 LOW APPLICATIONS	48941 NSD
2 HIGH APPLICATIONS	45330 NSD
2 LOW APPLICATIONS	44222 NSD
	43113 NSD

HEXANAL

SampleName

WATERSTRESSED	279409 a
4 LOW APPLICATIONS	126590 b
2 HIGH APPLICATIONS	93389 bc
4 HIGH APPLICATIONS	88842 bc
CONTROL	87745 bc
2 LOW APPLICATIONS	56331 c

THIACYCLOPENTANE

SampleName

4 HIGH APPLICATIONS	3063 a
2 LOW APPLICATIONS	2972 ab
WATERSTRESSED	2832 ab
2 HIGH	2655 ab

APPLICATIONS	
CONTROL	2423 bc
4 LOW	2094 c
APPLICATIONS	

CIS-3-HEXENAL

SampleName	4
WATERSTRESSED	53132 a
4 LOW	25806 b
APPLICATIONS	
CONTROL	22808 bc
4 HIGH	17181 cd
APPLICATIONS	
2 HIGH	16851 cd
APPLICATIONS	
2 LOW	12780 d
APPLICATIONS	

2-HEXENAL

SampleName	
WATERSTRESSED	6399151 a
4 LOW	2401564 b
APPLICATIONS	
CONTROL	1889730 bc
2 HIGH	1204892 c
APPLICATIONS	
4 HIGH	1095717 c
APPLICATIONS	
2 LOW	680225 c
APPLICATIONS	

3-ETHYLTHIOPHENE

SampleName	4
WATERSTRESSED	22134 a
4 LOW	13374 b
APPLICATIONS	
CONTROL	10740 c
2 HIGH	8163 d
APPLICATIONS	
2 LOW	7656 d
APPLICATIONS	
4 HIGH	6680 d
APPLICATIONS	

4-HEPTENAL

SampleName

WATERSTRESSED	4597 a
4 LOW APPLICATIONS	3282 b
CONTROL	2427 c
2 HIGH APPLICATIONS	2049 c
2 LOW APPLICATIONS	1537 c
4 HIGH APPLICATIONS	1493 c

N-HEPTANOL

SampleName

WATERSTRESSED	6753 a
4 LOW APPLICATIONS	4244 b
4 HIGH APPLICATIONS	3603 b
2 HIGH APPLICATIONS	3544 b
CONTROL	3307 b
2 LOW APPLICATIONS	2675 b

STYRENE

SampleName

WATERSTRESSED	316180 NSD
4 HIGH APPLICATIONS	244060 NSD
4 LOW APPLICATIONS	234306 NSD
CONTROL	225626 NSD
2 HIGH APPLICATIONS	222040 NSD
2 LOW APPLICATIONS	217864 NSD

2,4-HEXADIENAL

SampleName

	4
WATERSTRESSED	241586 a
4 LOW APPLICATIONS	133116 b
CONTROL	107531 bc

2 HIGH APPLICATIONS	84210 cd
4 HIGH APPLICATIONS	77240 cd
2 LOW APPLICATIONS	57403 d

METHYLTHIOCYCLO
PENTANE

SampleName

WATERSTRESSED	9109 a
4 LOW APPLICATIONS	4716 b
CONTROL	4229 bc
2 LOW APPLICATIONS	4057 bc
2 HIGH APPLICATIONS	3549 bc
4 HIGH APPLICATIONS	3249 c

1-HEXANETHIOL

SampleName

WATERSTRESSED	2859 a
CONTROL	1644 b
4 HIGH APPLICATIONS	1589 b
2 HIGH APPLICATIONS	1457 b
4 LOW APPLICATIONS	1296 b
2 LOW APPLICATIONS	1267 b

1-BROMOHEXANE

SampleName

WATERSTRESSED	2753800 NSD
4 HIGH APPLICATIONS	1749631 NSD
CONTROL	1727153 NSD
2 HIGH APPLICATIONS	1600898 NSD
2 LOW APPLICATIONS	1475196 NSD
4 LOW APPLICATIONS	1382051 NSD

2-HEPTENAL

SampleName

WATERSTRESSED	28204 a
4 LOW APPLICATIONS	21756 b
CONTROL	18222 b
2 HIGH APPLICATIONS	12389 c
2 LOW APPLICATIONS	11342 c
4 HIGH APPLICATIONS	10889 c

3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE

SampleName

WATERSTRESSED	2756 a
2 HIGH APPLICATIONS	1611 b
4 HIGH APPLICATIONS	1405 bc
CONTROL	1404 bc
2 LOW APPLICATIONS	1078 c
4 LOW APPLICATIONS	1067 c

BENZALDEHYDE

SampleName

4 HIGH APPLICATIONS	324731 NSD
4 LOW APPLICATIONS	313787 NSD
CONTROL	300233 NSD
WATERSTRESSED	299040 NSD
2 HIGH APPLICATIONS	298196 NSD
2 LOW APPLICATIONS	274043 NSD

2,6-DIMETHYL-5-HEPTEN-1-OL

SampleName

WATERSTRESSED	381287 a
4 LOW APPLICATIONS	92784 b
CONTROL	78521 b
2 LOW APPLICATIONS	44698 c
2 HIGH APPLICATIONS	35151 c
4 HIGH APPLICATIONS	29284 c

2,4-HEPTADIENAL

SampleName

WATERSTRESSED	693072 a
4 LOW APPLICATIONS	571621 b
CONTROL	534120 b
2 LOW APPLICATIONS	383747 c
2 HIGH APPLICATIONS	357538 c
4 HIGH APPLICATIONS	337979 c

BENZENEMETHANOL

SampleName

WATERSTRESSED	17697 a
4 LOW APPLICATIONS	10645 b
CONTROL	10293 b
2 LOW APPLICATIONS	7411 c
2 HIGH APPLICATIONS	7126 c
4 HIGH APPLICATIONS	6688 c

3-METHOXYPHENOL

SampleName

WATERSTRESSED	10061 a
4 LOW APPLICATIONS	8878 a
2 HIGH APPLICATIONS	7148 ab
CONTROL	7106 ab

4 HIGH APPLICATIONS	7099 ab
2 LOW APPLICATIONS	4769 b

2,2,6-TRIMETHYLCYCLOHEXANONE

SampleName

4 LOW APPLICATIONS	21002 a
CONTROL	17536 b
2 HIGH APPLICATIONS	16942 bc
2 LOW APPLICATIONS	15685 bc
WATERSTRESSED	13307 c
4 HIGH APPLICATIONS	13091 c

BENZENEACETALDEHYDE

SampleName

WATERSTRESSED	393228 a
4 HIGH APPLICATIONS	197880 b
CONTROL	188420 b
2 HIGH APPLICATIONS	188230 b
2 LOW APPLICATIONS	174460 b
4 LOW APPLICATIONS	164662 b

3-METHYLBUTYL ISOTHIOCYANATE

SampleName

4 LOW APPLICATIONS	106849 a
4 HIGH APPLICATIONS	97506 a
CONTROL	97106 a
2 HIGH APPLICATIONS	94754 a
2 LOW APPLICATIONS	87684 a
WATERSTRESSED	64114 b

3 5-OCTADIEN-2-ONE

SampleName

WATERSTRESSED	10466 a
4 LOW APPLICATIONS	10159 a
CONTROL	7849 ab
2 HIGH APPLICATIONS	6274 b
4 HIGH APPLICATIONS	5744 b
2 LOW APPLICATIONS	5022 b

CIS-3-HEXENAL DIETHYL ACETAL

SampleName

2 HIGH APPLICATIONS	24458 a
CONTROL	20059 ab
4 HIGH APPLICATIONS	18952 ab
4 LOW APPLICATIONS	17091 b
2 LOW APPLICATIONS	16475 b
WATERSTRESSED	9341 c

ETHYL-TRANS-4-HEPTENOATE

SampleName

4 LOW APPLICATIONS	18254 a
2 HIGH APPLICATIONS	16659 ab
CONTROL	13326 abc
4 HIGH APPLICATIONS	12488 abc
WATERSTRESSED	10553 bc
2 LOW APPLICATIONS	8523 c

(E)-2-NONEN-1-OL

SampleName

WATERSTRESSED	33534 a
2 HIGH APPLICATIONS	24511 b
4 HIGH APPLICATIONS	22743 b
2 LOW APPLICATIONS	20838 b
4 LOW APPLICATIONS	20592 b
CONTROL	19707 b

N-PENTYL ISOTHIOCYANATE

SampleName

WATERSTRESSED	38123 a
4 LOW APPLICATIONS	24755 b
CONTROL	24301 b
4 HIGH APPLICATIONS	22862 bc
2 HIGH APPLICATIONS	20980 bc
2 LOW APPLICATIONS	19660 c

CARVACROL

SampleName

WATERSTRESSED	8354 a
4 LOW APPLICATIONS	5992 b
CONTROL	4889 b
2 HIGH APPLICATIONS	3378 c
2 LOW APPLICATIONS	2905 c
4 HIGH APPLICATIONS	2830 c

1-TERPINEOL

SampleName

4 LOW APPLICATIONS	3105 a
CONTROL	2617 ab
2 HIGH APPLICATIONS	1863 b
WATERSTRESSED	1856 b

4 HIGH APPLICATIONS	1775 b
2 LOW APPLICATIONS	1718 b

BENZENEETHANOL

SampleName

4 HIGH APPLICATIONS	74544 a
CONTROL	61636 a
2 LOW APPLICATIONS	57887 a
2 HIGH APPLICATIONS	56943 a
4 LOW APPLICATIONS	55211 a
WATERSTRESSED	22941 b

2,2,6,6-TETRAMETHYL-3 5-HEPTANEDIONE

SampleName

	4
2 HIGH APPLICATIONS	5026 a
4 HIGH APPLICATIONS	4512 ab
CONTROL	3684 bc
2 LOW APPLICATIONS	3458 bc
4 LOW APPLICATIONS	3196 c
WATERSTRESSED	1639 d

2 6-NONADIENAL

SampleName

WATERSTRESSED	24627 NSD
2 HIGH APPLICATIONS	21155 NSD
CONTROL	20754 NSD
4 HIGH APPLICATIONS	20440 NSD
2 LOW APPLICATIONS	20290 NSD
4 LOW APPLICATIONS	20199 NSD

4-METHYLPENTYL
ISOTHIOCYANATE

SampleName

4 LOW APPLICATIONS	321046 NSD
2 HIGH APPLICATIONS	298803 NSD
4 HIGH APPLICATIONS	294070 NSD
CONTROL	286677 NSD
2 LOW APPLICATIONS	262695 NSD
WATERSTRESSED	210277 NSD

HEXYL
ISOTHIOCYANATE

SampleName

WATERSTRESSED	62091 a
CONTROL	42474 b
4 HIGH APPLICATIONS	42144 b
4 LOW APPLICATIONS	42134 b
2 HIGH APPLICATIONS	38131 b
2 LOW APPLICATIONS	36458 b

METHYL SALICYLATE

SampleName

4 HIGH APPLICATIONS	163231 a
CONTROL	158454 ab
4 LOW APPLICATIONS	150034 b
2 LOW APPLICATIONS	149011 b
2 HIGH APPLICATIONS	145416 b
WATERSTRESSED	102331 c

ETHYL NICOTINATE

SampleName

CONTROL	37057 a
---------	---------

2 LOW APPLICATIONS	35960 a
4 LOW APPLICATIONS	35301 a
4 HIGH APPLICATIONS	34777 a
2 HIGH APPLICATIONS	33387 a
WATERSTRESSED	4982 b

3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE

SampleName

4 LOW APPLICATIONS	71790 NSD
CONTROL	63822 NSD
2 HIGH APPLICATIONS	49910 NSD
4 HIGH APPLICATIONS	45885 NSD
WATERSTRESSED	41019 NSD
2 LOW APPLICATIONS	39150 NSD

(3-METHYL-3-BUTENYL)BENZENE

SampleName

WATERSTRESSED	7374699 NSD
4 HIGH APPLICATIONS	4792071 NSD
CONTROL	4548250 NSD
4 LOW APPLICATIONS	4166786 NSD
2 LOW APPLICATIONS	3982812 NSD
2 HIGH APPLICATIONS	3981588 NSD

BETA-CYCLOCITRAL

SampleName

4 LOW APPLICATIONS	74041 a
WATERSTRESSED	60264 ab
CONTROL	60229 ab
2 HIGH APPLICATIONS	51840 bc
2 LOW	45589 bc

APPLICATIONS 4 HIGH APPLICATIONS	41802 c
----------------------------------------	---------

BENZENEPROPANEN
ITRILE

SampleName

2 LOW APPLICATIONS	3221418 a
2 HIGH APPLICATIONS	3098780 a
CONTROL	2571337 ab
4 HIGH APPLICATIONS	2401654 ab
4 LOW APPLICATIONS	1827214 b
WATERSTRESSED	835720 c

3-ETHENYL-4-METHYL-1H-
PYRROLE-2,5-DIONE

SampleName

4 LOW APPLICATIONS	73781 a
CONTROL	62630 ab
2 HIGH APPLICATIONS	52770 ab
4 HIGH APPLICATIONS	44257 b
2 LOW APPLICATIONS	38249 b
WATERSTRESSED	35941 b

N-HEPTYL
ISOTHIOCYANATE

SampleName

4 LOW APPLICATIONS	561870 NSD
4 HIGH APPLICATIONS	536648 NSD
CONTROL	528376 NSD
2 HIGH APPLICATIONS	513222 NSD
2 LOW APPLICATIONS	467113 NSD
WATERSTRESSED	457986 NSD

CYCLOHEXANE METHYL
ISOTHIOCYANATE

SampleName

WATERSTRESSED	197157 a
4 HIGH APPLICATIONS	175935 b
4 LOW APPLICATIONS	168369 b
CONTROL	167344 b
2 LOW APPLICATIONS	148744 c
2 HIGH APPLICATIONS	146926 c

3-METHYLHEXYL
ISOTHIOCYANATE

SampleName

WATERSTRESSED	63312 a
CONTROL	49927 b
4 LOW APPLICATIONS	49826 b
4 HIGH APPLICATIONS	49288 b
2 HIGH APPLICATIONS	45319 bc
2 LOW APPLICATIONS	41798 c

4-ETHENYL-2-
METHOXYPHENOL

SampleName

WATERSTRESSED	93208 a
CONTROL	51991 b
4 LOW APPLICATIONS	47744 b
2 LOW APPLICATIONS	44204 b
2 HIGH APPLICATIONS	43031 b
4 HIGH APPLICATIONS	42003 b

4-
ETHOXYBENZALDEH
YDE

SampleName

4 LOW APPLICATIONS CONTROL	9483 a
2 HIGH APPLICATIONS	8589 a
4 HIGH APPLICATIONS	5472 a
4 HIGH APPLICATIONS	5006 a
WATERSTRESSED	4572 a
2 LOW APPLICATIONS	4204 a

3-(METHYLTHIO)PROPYL ISOTHIOCYANATE

SampleName

4 HIGH APPLICATIONS	72461 a
2 LOW APPLICATIONS	69207 a
2 HIGH APPLICATIONS	69168 a
CONTROL	63333 ab
4 LOW APPLICATIONS	54935 b
WATERSTRESSED	38517 c

94, 117, 142

SampleName

	4
4 HIGH APPLICATIONS	44619 a
2 HIGH APPLICATIONS	37893 ab
2 LOW APPLICATIONS	35602 abc
CONTROL	31230 bc
4 LOW APPLICATIONS	26785 c
WATERSTRESSED	17958 d

ETHYL HYDROCINNAMATE

SampleName

2 HIGH APPLICATIONS	11345 a
---------------------	---------

CONTROL	11216 a
2 LOW APPLICATIONS	10478 a
4 HIGH APPLICATIONS	6673 b
4 LOW APPLICATIONS	5514 b
WATERSTRESSED	2688 c

OCTYL ISOTHIOCYANATE

SampleName

4 LOW APPLICATIONS	281527 NSD
CONTROL	265944 NSD
2 HIGH APPLICATIONS	260363 NSD
4 HIGH APPLICATIONS	256872 NSD
2 LOW APPLICATIONS	223553 NSD
WATERSTRESSED	215002 NSD

METHYLHEPTYL ISOTHIOCYANATE

SampleName

WATERSTRESSED	52925 a
CONTROL	40521 b
4 LOW APPLICATIONS	39737 b
4 HIGH APPLICATIONS	39431 b
2 HIGH APPLICATIONS	35812 bc
2 LOW APPLICATIONS	32418 c

GERANYL ACETONE

SampleName

CONTROL	43031 NSD
4 LOW APPLICATIONS	41839 NSD
WATERSTRESSED	41791 NSD
4 HIGH APPLICATIONS	39723 NSD
2 HIGH	39398 NSD

APPLICATIONS
 2 LOW 38999 NSD
 APPLICATIONS

2,5-DIMETHYL-1-PHENYLPYRROLE

SampleName

4 LOW 95812 a
 APPLICATIONS
 CONTROL 81162 a
 WATERSTRESSED 78700 a
 4 HIGH 52700 b
 APPLICATIONS
 2 HIGH 50854 b
 APPLICATIONS
 2 LOW 48039 b
 APPLICATIONS

NONYL ISOTHIOCYANATE

SampleName

4 LOW 50265 NSD
 APPLICATIONS
 CONTROL 46594 NSD
 2 HIGH 46234 NSD
 APPLICATIONS
 4 HIGH 45229 NSD
 APPLICATIONS
 2 LOW 38132 NSD
 APPLICATIONS
 WATERSTRESSED 34777 NSD

ISOAMYL DECANOATE

SampleName

2 HIGH 500286 a
 APPLICATIONS
 WATERSTRESSED 496536 a
 4 HIGH 470581 a
 APPLICATIONS
 2 LOW 424634 ab
 APPLICATIONS
 4 LOW 391299 ab
 APPLICATIONS
 CONTROL 336112 b

2-
PHENYLETHYLISOTHOICYANATE

SampleName

4 HIGH APPLICATIONS	501572900 NSD
4 LOW APPLICATIONS	499378491 NSD
CONTROL	496369164 NSD
2 HIGH APPLICATIONS	488515860 NSD
2 LOW APPLICATIONS	479545822 NSD
WATERSTRESSED	473106965 NSD

APPENDIX 4 – Chemical analysis stage 3

Attrs	Sample	Mean	Media n	Stdev	N	PVal	Sig	Groupings (NK at 5%)	Groupings (NK at 10%)
1-PENTEN-3-OL / 1-PENTEN-3-ONE	4 LOW	246932.7	210945	80580.62	3	0.201	NS		
1-PENTEN-3-OL / 1-PENTEN-3-ONE	CONTR OL	174739.7	159528	58718.36	3				
1-PENTEN-3-OL / 1-PENTEN-3-ONE	4 HIGH	153885.7	155462	13032.2	3				
2-ETHYLFURAN	4 LOW	65287.3	66959	20919.65	3	0.065	10%		A
2-ETHYLFURAN	CONTR OL	40501.7	42333	6128.763	3				B
2-ETHYLFURAN	4 HIGH	36305.3	36518	4654.645	3				B
77, 105	CONTR OL	24611	27635	16771.73	3	0.983	NS		
77, 105	4 LOW	24123.3	23253	1676.489	3				
77, 105	4 HIGH	23149.7	22673	864.875	3				
2-PENTENAL	4 LOW	95199	92156	17196.63	3	0.018	5% A		A
2-PENTENAL	4 HIGH	71685.7	73593	3375.733	3			B	B
2-PENTENAL	CONTR OL	61659.3	60945	3280.361	3			B	B
TOLUENE	CONTR OL	9995.7	9585	2501.412	3	0.488	NS		
TOLUENE	4 LOW	9869.3	9188	1366.011	3				
TOLUENE	4 HIGH	8453.7	8498	106.651	3				
HEXANAL	4 LOW	50730.3	50422	3610.388	3	0.003	1% A		A
HEXANAL	CONTR OL	46604	44808	8369.79	3			A	A
HEXANAL	4 HIGH	26748	26765	1722.563	3			B	B
THIACYCLOPENTANE	4 HIGH	3237	3277	80.802	3	0.063	10%		A
THIACYCLOPENTANE	CONTR OL	2609.7	2640	367.44	3				B
THIACYCLOPENTANE	4 LOW	2418	2529	470.426	3				B
CIS-3-HEXENAL	4 LOW	8166.7	7402	1774.219	3	0.071	10%		A
CIS-3-HEXENAL	CONTR OL	8041.7	8763	1770.845	3				A
CIS-3-HEXENAL	4 HIGH	5112	5155	166.712	3				B
2-HEXENAL	CONTR OL	877338.3	798764	160109.4	3	0.02	5% A		A
2-HEXENAL	4 LOW	786914.7	653357	256992.3	3			A	A

2-HEXENAL	4 HIGH	338238	32849	34023.	3			B	B
		.7	3	93					
3-ETHYLTHIOPHENE	CONTR	3243	3387	837.33	3	0.111	NS		
	OL			9					
3-ETHYLTHIOPHENE	4 LOW	2820.7	2396	914.23	3				
				5					
3-ETHYLTHIOPHENE	4 HIGH	1787.7	1718	133.86	3				
				7					
4-HEPTENAL	4 LOW	3812.7	3624	609.31	3	0.018	5% A		A
				5					
4-HEPTENAL	4 HIGH	2989	2859	230.38	3			AB	B
				2					
4-HEPTENAL	CONTR	2369	2445	372.85	3			B	B
	OL			5					
N-HEPTANOL	4 LOW	5139.3	5122	241.46	3	0.436	NS		
				7					
N-HEPTANOL	CONTR	5074	4322	1527.7	3				
	OL			6					
N-HEPTANOL	4 HIGH	4181	4250	555.72	3				
				2					
STYRENE	CONTR	110113	11603	14468.	3	0.592	NS		
	OL			3					
STYRENE	4 LOW	107035	10671	4624.8	3				
				4					
STYRENE	4 HIGH	102336	10155	3170.3	3				
		.7	1	73					
2,4-HEXADIENAL	4 LOW	39235	37527	9146.4	3	0.033	5% A		A
2,4-HEXADIENAL	CONTR	35157.	33317	4349.0	3			A	A
	OL	3		55					
2,4-HEXADIENAL	4 HIGH	22766	23324	1407.5	3			B	B
				54					
METHYLTHIOCYCLOPEN	4 LOW	3972	4094	560.05	3	0.007	1% A		A
TANE				6					
METHYLTHIOCYCLOPEN	CONTR	2094.7	2004	783.94	3			B	B
TANE	OL			2					
METHYLTHIOCYCLOPEN	4 HIGH	1878.7	1880	129.00	3			B	B
TANE				5					
1-HEXANETHIOL	CONTR	9131.3	7035	3811.6	3	0.722	NS		
	OL			29					
1-HEXANETHIOL	4 LOW	8905.7	7358	3125.4	3				
				77					
1-HEXANETHIOL	4 HIGH	7358	7315	197.05	3				
				1					
1-BROMOHEXANE	4 LOW	440210	46923	646049	3	0.142	NS		
		3	45	.2					
1-BROMOHEXANE	CONTR	371516	37706	446287	3				
	OL	3	78	.2					
1-BROMOHEXANE	4 HIGH	356502	35454	184021	3				
		6	13	.5					
2-HEPTENAL	4 LOW	15589.	12661	7142.8	3	0.105	NS		
		3		54					
2-HEPTENAL	CONTR	9245	8794	1737.9	3				
	OL			57					
2-HEPTENAL	4 HIGH	6818.7	7070	893.90	3				
				5					

3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	4 LOW	1291.3	1389	187.64	3	0.222 NS		
				4				
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	CONTR	803	898	759.96	3			
	OL			6				
3-ETHYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE	4 HIGH	576.3	556	53.482	3			
BENZALDEHYDE	CONTR	109645	80723	53615.	3	0.289 NS		
	OL	.7		53				
BENZALDEHYDE	4 LOW	87626.	82807	19205.	3			
		7		55				
BENZALDEHYDE	4 HIGH	62571.	62796	1388.6	3			
		3		98				
2,6-DIMETHYL-5-HEPTEN-1-OL	4 LOW	43875.	28759	28604.	3	0.341 NS		
		3		02				
2,6-DIMETHYL-5-HEPTEN-1-OL	CONTR	29189	28073	4238.6	3			
	OL			58				
2,6-DIMETHYL-5-HEPTEN-1-OL	4 HIGH	22398	22298	1239.0	3			
				3				
2,4-HEPTADIENAL	4 LOW	293499	29496	15250.	3	0.014	5% A	A
		.3	4	84				
2,4-HEPTADIENAL	4 HIGH	263011	26370	8428.7	3		B	B
			2	7				
2,4-HEPTADIENAL	CONTR	249815	24843	13333.	3		B	B
	OL	.7	7	56				
BENZENEMETHANOL	4 LOW	8209.3	8020	845.06	3	0.019	5% A	A
BENZENEMETHANOL	4 HIGH	6737.7	6764	262.49	3		B	B
				3				
BENZENEMETHANOL	CONTR	6116	6249	690.17	3		B	B
	OL			9				
3-METHOXYPHENOL	4 LOW	6310.7	4462	3232.3	3	0.167 NS		
				43				
3-METHOXYPHENOL	CONTR	4733	3915	1725.1	3			
	OL			59				
3-METHOXYPHENOL	4 HIGH	2494.7	2340	277.47	3			
				1				
2,2,6-TRIMETHYLCYCLOHEXANONE	CONTR	4387.7	3636	2136.1	3	0.338 NS		
	OL			04				
2,2,6-TRIMETHYLCYCLOHEXANONE	4 LOW	4176.7	3512	1310.2	3			
				16				
2,2,6-TRIMETHYLCYCLOHEXANONE	4 HIGH	2632.7	2688	230.04	3			
				6				
BENZENEACETALDEHYDE	CONTR	123313	79940	82653.	3	0.587 NS		
	OL	.3		34				
BENZENEACETALDEHYDE	4 LOW	113076	86144	61928.	3			
		.7		3				
BENZENEACETALDEHYDE	4 HIGH	73547	74471	3478.2	3			
				98				
3-METHYLBUTYL ISOTHIOCYANATE	CONTR	34207.	32812	4284.5	3	0.022	5% A	A
	OL	7		21				
3-METHYLBUTYL ISOTHIOCYANATE	4 LOW	30087.	30478	1694.5	3		AB	A
		7		59				
3-METHYLBUTYL ISOTHIOCYANATE	4 HIGH	25235	24434	1451.9	3		B	B

ISOTHIOCYANATE					3				
3,5-OCTADIEN-2-ONE	4 LOW	11843	9581	4563.8	3	0.023	5% A	A	
				11					
3,5-OCTADIEN-2-ONE	CONTR	4727.3	5207	942.03	3		B	B	
	OL			5					
3,5-OCTADIEN-2-ONE	4 HIGH	4049	3951	668.41	3		B	B	
CIS-3-HEXENAL DIETHYL	CONTR	5706	5357	3027.6	3	0.062	10%	A	
ACETAL	OL			24					
CIS-3-HEXENAL DIETHYL	4 LOW	5154.7	4673	1187.1	3			A	
ACETAL				96					
CIS-3-HEXENAL DIETHYL	4 HIGH	1415.3	1359	346.94	3			B	
ACETAL				7					
ETHYL-TRANS-4-HEPTENOATE	4 LOW	8296	4813	7282.5	3	0.376	NS		
				46					
ETHYL-TRANS-4-HEPTENOATE	CONTR	5044	4653	2739.5	3				
	OL			08					
ETHYL-TRANS-4-HEPTENOATE	4 HIGH	2733	2947	386.35	3				
				2					
(E)-2-NONEN-1-OL	4 HIGH	23708.	23854	458.60	3	0.555	NS		
		7		9					
(E)-2-NONEN-1-OL	4 LOW	21601.	22086	3143.6	3				
		7		08					
(E)-2-NONEN-1-OL	CONTR	21026.	19151	4187.4	3				
	OL	7		02					
N-PENTYL ISOTHIOCYANATE	CONTR	10780.	11329	1254.8	3	0.025	5% A	A	
	OL	7		24					
N-PENTYL ISOTHIOCYANATE	4 HIGH	8403	8320	378.39	3		B	B	
N-PENTYL ISOTHIOCYANATE	4 LOW	8125	7916	954.81	3		B	B	
				3					
CARVACROL	4 LOW	1614	1475	254.73	3	0.005	1% A	A	
				7					
CARVACROL	CONTR	1052	1105	101.47	3		B	B	
	OL			4					
CARVACROL	4 HIGH	921	922	87.504	3		B	B	
1-TERPINEOL	4 LOW	1130.3	925	361.72	3	0.362	NS		
				7					
1-TERPINEOL	CONTR	865.3	818	243.47	3				
	OL			6					
1-TERPINEOL	4 HIGH	821.7	842	132.67	3				
				4					
BENZENEETHANOL	4 LOW	39280.	20623	32729.	3	0.203	NS		
		3		41					
BENZENEETHANOL	CONTR	17894.	11481	11656.	3				
	OL	3		31					
BENZENEETHANOL	4 HIGH	6157.7	6354	818.35	3				
				8					
2,2,6,6-TETRAMETHYL-3,5-HEPTANEDIONE	CONTR	1529.3	1708	595.45	3	0.089	10%	A	
	OL			5					
2,2,6,6-TETRAMETHYL-3,5-HEPTANEDIONE	4 LOW	1251.7	1264	206.77	3			AB	
				6					
2,2,6,6-TETRAMETHYL-3,5-HEPTANEDIONE	4 HIGH	722	668	103.20	3			B	
				4					
2,6-NONADIENAL	4 LOW	7725	6750	1769.9	3	0.199	NS		
				01					

2,6-NONADIENAL	4 HIGH	5530	5628	394.24	3			
				4				
2,6-NONADIENAL	CONTR	5483.7	6539	1901.1	3			
	OL			01				
4-METHYLPENTYL ISOTHIOCYANATE	CONTR	88940	91318	4201.3	3	0.013	5% A	A
	OL			58				
4-METHYLPENTYL ISOTHIOCYANATE	4 LOW	77995.	77389	7370.2	3		AB	B
		3		29				
4-METHYLPENTYL ISOTHIOCYANATE	4 HIGH	66176	63655	6992.0	3		B	C
				95				
HEXYL ISOTHIOCYANATE	CONTR	14680	14271	1569.0	3	0.081	10%	A
	OL			04				
HEXYL ISOTHIOCYANATE	4 LOW	13096.	13187	626.93	3			AB
		3		6				
HEXYL ISOTHIOCYANATE	4 HIGH	12403	12523	503.83	3			B
				4				
METHYL SALICYLATE	4 LOW	11954	10880	2185.7	3	0.002	1% A	A
				7				
METHYL SALICYLATE	CONTR	10412	10696	588.82	3		A	A
	OL			7				
METHYL SALICYLATE	4 HIGH	5370.7	5343	58.62	3		B	B
ETHYL NICOTINATE	4 LOW	17317.	10463	15814.	3	0.49	NS	
		7		45				
ETHYL NICOTINATE	CONTR	12314.	15034	7810.4	3			
	OL	7		99				
ETHYL NICOTINATE	4 HIGH	6740.3	7100	1489.4	3			
				34				
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	4 LOW	24227.	17369	13172.	3	0.086	10%	A
		7		25				
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	CONTR	10501.	8568	5526.7	3			B
	OL	3		19				
3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	4 HIGH	6210.3	5102	2406.2	3			B
				3				
(3-METHYL-3-BUTENYL)BENZENE	CONTR	914063	10047	179458	3	0.476	NS	
	OL	.3	31	.2				
(3-METHYL-3-BUTENYL)BENZENE	4 LOW	849426	79231	104679	3			
		.7	6	.3				
(3-METHYL-3-BUTENYL)BENZENE	4 HIGH	786369	78235	20254.	3			
		.7	9	04				
BETA-CYCLOCITRAL	4 LOW	21914.	18409	6357.5	3	0.148	NS	
		3		87				
BETA-CYCLOCITRAL	CONTR	15943.	16039	2289	3			
	OL	3						
BETA-CYCLOCITRAL	4 HIGH	15149.	15502	696.53	3			
		3		2				
BENZENEPROPANENITRILE	CONTR	767531	64674	328714	3	0.066	10%	A
	OL	.3	8	.9				
BENZENEPROPANENITRILE	4 LOW	363483	30177	138764	3			B
		.7	6	.6				
BENZENEPROPANENITRILE	4 HIGH	310386	30481	9771.0	3			B
		.7	8	56				
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	4 LOW	16165.	13979	4677.4	3	0.07	10%	A
		7		85				
3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	CONTR	10376	7028	6667.4	3			AB
	OL			47				

3-ETHENYL-4-METHYL-1H-PYRROLE-2,5-DIONE	4 HIGH	4747.7	4179	1574.0	3				B
N-HEPTYL ISOTHIOCYANATE	CONTR OL	135567.3	13431	7062.8	3	0.052	10%		A
N-HEPTYL ISOTHIOCYANATE	4 LOW	128862	11780	24116.53	3				A
N-HEPTYL ISOTHIOCYANATE	4 HIGH	98990.3	96298	6656.2	3				B
CYCLOHEXANE METHYL ISOTHIOCYANATE	CONTR OL	100245.3	85442	28571.65	3	0.317	NS		
CYCLOHEXANE METHYL ISOTHIOCYANATE	4 LOW	79783	80282	11603.55	3				
CYCLOHEXANE METHYL ISOTHIOCYANATE	4 HIGH	78522.7	79312	2564.7	3				
3-METHYLHEXYL ISOTHIOCYANATE	CONTR OL	11638.7	11524	218.82	3	0.059	10%		A
3-METHYLHEXYL ISOTHIOCYANATE	4 LOW	10740	9745	1939.4	3				A
3-METHYLHEXYL ISOTHIOCYANATE	4 HIGH	8854.3	8777	198.63	3				B
4-ETHENYL-2-METHOXYPHENOL	4 LOW	11045.3	6843	8298.1	3	0.916	NS		
4-ETHENYL-2-METHOXYPHENOL	CONTR OL	10698.7	6311	9048.9	3				
4-ETHENYL-2-METHOXYPHENOL	4 HIGH	8773	8494	982.66	3				
4-ETHOXYBENZALDEHYDE	CONTR OL	7663.7	1182	11408.05	3	0.512	NS		
4-ETHOXYBENZALDEHYDE	4 HIGH	1921.3	2062	279.00	3				
4-ETHOXYBENZALDEHYDE	4 LOW	1871.3	2359	1681.4	3				
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	4 HIGH	20980	20712	1010.0	3	0.174	NS		
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	CONTR OL	18217.3	17864	3259.3	3				
3-(METHYLTHIO)PROPYL ISOTHIOCYANATE	4 LOW	15549.3	16969	4045.8	3				
94, 117, 142	CONTR OL	8305.7	7836	2416.9	3	0.235	NS		
94, 117, 142	4 HIGH	6161.7	5984	974.72	3				
94, 117, 142	4 LOW	6046	5540	1017.2	3				
ETHYL HYDROCINNAMATE	4 LOW	7144.3	5096	6028.4	3	0.432	NS		
ETHYL HYDROCINNAMATE	CONTR OL	4406	2783	4219.4	3				
ETHYL HYDROCINNAMATE	4 HIGH	2327	2462	278.25	3				
OCTYL ISOTHIOCYANATE	4 LOW	54397.3	45367	19809.55	3	0.289	NS		

OCTYL ISOTHIOCYANATE	CONTR OL	51944.3	52882.92	6908.3	3			
OCTYL ISOTHIOCYANATE	4 HIGH	38175.7	37044.03	2608.6	3			
METHYLHEPTYL ISOTHIOCYANATE	4 LOW	6445	5355	2130.5	3	0.198	NS	
METHYLHEPTYL ISOTHIOCYANATE	CONTR OL	6353.7	6200	450.6	3			
METHYLHEPTYL ISOTHIOCYANATE	4 HIGH	4550.7	4485	184.48	3			
GERANYL ACETONE	4 LOW	20463.7	15639.76	10039.	3	0.282	NS	
GERANYL ACETONE	4 HIGH	16486.7	16529.8	864.27	3			
GERANYL ACETONE	CONTR OL	12001	11934	933.30	3			
2,5-DIMETHYL-1-PHENYLPYRROLE	4 LOW	43664.3	44502.61	5041.9	3	<0.001	0.10 A	A
2,5-DIMETHYL-1-PHENYLPYRROLE	4 HIGH	24876.7	24594.92	2590.5	3		B	B
2,5-DIMETHYL-1-PHENYLPYRROLE	CONTR OL	19366.3	20185.73	2616.8	3		B	B
NONYL ISOTHIOCYANATE	CONTR OL	8759	7222	4518.9	3	0.355	NS	
NONYL ISOTHIOCYANATE	4 LOW	7666.3	6509	2812.6	3			
NONYL ISOTHIOCYANATE	4 HIGH	4924.3	4897	300.93	3			
ISOAMYL DECANOATE	4 LOW	513714.3	52408.6	45045.11	3	0.38	NS	
ISOAMYL DECANOATE	4 HIGH	502406.3	51156.3	29645.28	3			
ISOAMYL DECANOATE	CONTR OL	453892	41692	71107.8	3			
2-PHENYLETHYL ISOTHIOCYANATE	CONTR OL	1.49E+08	1.53E+08	999127	3	0.052	10%	A



A
A
B

