The Influence of Yeasts on the Aroma of Stilton cheese

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ii. Contents

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iii. Abbreviations

ANOVA – Analysis of variance

BHI - Brain heart infusion agar

BS – British Standards

CFU – Colony forming units

CV – Coefficient of variation

FCP – Free choice profiling

FP – Flash Profile

GC – Gas Chromatogaphy

GPA – Generalised Procrustes Analysis

ISO – International Standards Organisation

MFA – Multiple Factor Analysis

MS –Mass Spectrometry

NIST - National Institute of Standards and Technology

PBS - Phosphate buffered saline

PCA – Principal Component Analaysis

PC1 –Principal Component 1

PC2 – Principal Component 2

PDO - Protected Designation of Origin

PFTE- Polytetrafluoroethylene

RBCA - Rose bengal chloramphenicol agar

REF – reference (sample)

RI – Retention Indices

SD – Standard Deviation

SDA - Sabouraud dextrose agar

SPME – Solid phase microextraction

TIC - Total Ion Current

UHT – Ultra heat treated

iv. Abstract

Blue cheeses comprise secondary microbial flora which is not controlled during production. The secondary flora of Stilton comprises distinct yeast communities in each section of the cheese (blue veins, white core, outer crust). Previous work has identified yeasts species-specific effects on aroma development. However, large variation between replicates was observed and this emulates the problem faced by the industry in achieving product consistency. Stilton shows variation in aroma between and within batches produced.

In the present study factors influencing yeasts' impact on aroma variation were investigated by incubating Stilton yeast isolates in milk-based models, with and without the mould *Penicillium roqueforti,* which is the major contributor to blue cheese aroma development.

Resultant aroma profiles of models were analysed via Solid-Phase Microextraction Gas Chromatography-Mass Spectrometry (SPME GC-MS) and Principal Component Analysis (PCA). Sensory studies (Flash Profile, Napping®, Triangle, Paired Comparison and Constant Reference ranking tests) were conducted to determine whether findings were perceivable by humans.

The concentration of yeasts and growth conditions of the models influenced aroma generation. The production of ketones, major contributors to blue cheese aroma, increased as the concentration of *Yarrowia lipolytica,* inoculated into models containing *P. rouqeforti,* increased. Variation in the aroma profiles of replicate samples decreased as the concentration of *Kluyveromyces lactis,* inoculated into models containing *P. roqueforti,* decreased. Sensory analysis indicated the effects of *Y. lipoltyica* and *K. lactis* on aroma profiles observed instrumentally may not be perceivable by humans.

The results of this study suggest that yeasts could be used as adjuncts in Stilton production to manipulate the production of aroma compounds and limit variation in aroma profiles.

1. INTRODUCTION

1.1 BLUE CHEESES IN THE EAST MIDLANDS

Stilton is a cows' milk, semi-soft blue cheese. Unique amongst British cheese, Stilton was granted an assurance trademark in 1966 for sales within Britain and in 1996 was bestowed Protected Designation of Origin (PDO) status from the EU commission. As such, Stilton is protected and can only be produced in three English counties: Derbyshire, Leicestershire and Nottinghamshire.

High quality mould-ripened Stilton has long been admired as the finest of all British cheese, commonly revered as 'King' amongst English cheeses (Avarvarei & Nistor, 2011) and Stilton sales account for 38% of all blue cheese sold in the UK (Mintel, 2007). Worth an estimated £50 million per annum, Stilton is of economic importance both regionally and nationally (Trott, 1994), yet within the global blue cheese market foreign cheese varieties dominate (Hopkins, 2006).

Stichelton is a cheese produced in a single dairy in Nottingham by the same production methods as Stilton, except for the use of raw milk. Until the 1980s Stilton was produced from raw milk but following multiple health scares concerning *Listeria* contamination, a move to pasteurised milk was made. Since coming to market in 2006, Stichelton has garnered favourable reviews, praised for its deeper and more complex flavour characteristics (Naley, 2008; Aslet, 2007; Haynes, 2007). Stilcheton shows variation between batches with the use of raw milk introducing further complexities during production (Haynes, 2007).

1.1.1 Stilton production

Stilton cheese production begins with the addition of starter cultures and rennet to pasteurised milk. Stater cultures are microbial cultures which carry out fermentation. In cheese stater cultures typically comprises lactic acid bacteria which acidify the milk, promoting clotting via the enzymatic activity of rennet, forming curds and whey. Stilton starter culture also contains spores of the mould species *Penicillium roqueforti* whose development promotes ripening (Fox *et al.*, 2000). Following formation of the curds and whey, the whey is removed and the curds left to drain overnight. The next day the curds are cut into blocks allowing further drainage, then milled and salt added. Salted curd is placed into cylindrical moulds and put onto boards, being turned daily over the next five to six days for further drainage. Stilton is not pressed giving the cheese its semi-soft interior. After further drainage the cylindrical moulds are removed and the outer coat of Stilton is smoothed through a technique known as 'rubbing-up', creating an airtight seal. Sealed cheeses are then stored in a ripening room (approximately 10°C / 85% humidity) for around six weeks to form a hard brown crust, being turned regularly. 'Needling' the cheese after six weeks breaks the airtight seal and involves piercing the cheese with steel needles. The introduction of air in the cheese core promotes *P. roqueforti's* spore germination, forming mycelia, which grow and elongate throughout the cheese. Maturation of *P. roqueforti* leads to sporulation, with spores produced at the growing tips of mycelium, giving rise to the blue veins of the cheese. Following needling blue veins develop over the three to four weeks storage in the ripening room. At nine to ten weeks old Stilton is a final product ready for sale, unless further maturation is desired.

1.1.2 Micro-organisms of Stilton

Penicillium species are the visual dominance of many blue cheeses and the role they play throughout ripening is well studied (Law, 2010; Chávez *et al.*, 2009); often being hailed the sole contributor to blue cheese flavour (Hiscox *et al.*, 1951). *P. roqueforti* sporulation gives rise to the blue veins characteristic of many blue cheese varieties (Bockelmann, 2010) and also contributes to the generation of aroma compounds (McSweeney & Sousa, 2000; Anderson & Day, 1966); notably the ketones 2-nonanone and 2-heptanone, which are the major contributors to blue cheese aroma (Frank *et al.*, 2004; Qian *et al.*, 2002; Urbach, 1997).

In Stilton production addition of spores into the milk gives uniform dispersal of spores throughout the curds but for some varieties *P. roqueforti* spores are added into the cheese later at the needling stages.

Salt concentration and temperature have been shown to influence the germination, growth rate and sporulation of *P. roqueforti* (Cuppers *et al.*, 1997) and enzymatic activity of strains (Larsen & Jensen, 1999; Kinsella *et al.*, 1976). Enzymatic activity of both the mycelia and spores of *P. roqueforti* contribute to formation of blue cheese flavour compounds (Fox *et al.*, 2004). Even distribution of blue veins is linked to the commercial quality of Stilton (Law & Tamine, 2010) and the secondary flora of cheese has been suggested to be responsible for poor blue vein formation (Whitley, 2002). Mycelial growth, sporulation and the enzymatic activity of *P. roqueforti* has been shown to be inhibited by some strains of yeast (Tempel & Jakobsen, 2000; Tempel & Nielsen, 2000).

Mould-ripened cheese manufacturing is complex and following ripening the secondary microflora are the predominant microbial presence (Addis *et. al*, 2001). The secondary flora of cheeses can comprise bacteria and fungi which are naturally present in the dairy environment (Flórez & Mayo, 2006). Present on cheese-maker's skin and manufacturing equipment within the ripening room along with being airborne, these microorganisms are spontaneously introduced into Stilton throughout the whole manufacturing and ripening process (Viljoen *et al.*, 2003).

Stilton's secondary flora is far less studied than that of other blue varieties, but research has shown that the bacterial community within Stilton displays differential local distributions between different zones of cheese (Ercolini *et al.*, 2003). Also different yeast communities (species and quantities) populate each of the cheese sections i.e. blue veins, white core and outer crust (Gkatzionis, 2010). The metabolic activity of this secondary flora has been highlighted as key variable factors which influence ripening and sensory characteristics of the final product

(Sousa *et al.*, 2001; Roostita, 1996), yet knowledge upon mechanisms of flavour production is lacking (Marilley & Casey, 2004).

1.1.3 Yeast flora

Yeasts are abundant within Stilton's secondary flora (Fox *et al.*, 2004) and the influence of yeast species upon the flavour and texture of blue cheese has been noted as of great importance (Wojtatowicz *et al.*, 2001; Fleet, 1990).

In 2002, Whitley examined the microflora of Stilton cheeses showing poor blue vein development. Isolation of species using culture dependent techniques found *Debaryomyces hansenii* and *Kluyveromyces lactis* to be most abundant with *Yarrowia lipolytica* and various other *Candida* species also identified. Relating each species to the quality of cheese however proved challenging and species specific impact remained inconclusive. Gkatzionis (2010) later applied molecular analysis alongside culture dependent techniques to study the flora composition of different sections of Stilton. Differing yeast communities were identified across the outer crust, blue veins and white core. The outer crust of the cheese showed the most complex flora and counts 10-fold greater than other sections. Species diversity was found to be greater within the white core than blue veins, but lower counts were observed. *K. lactis* was the greatest presence in the blue veins with *D. hansenii* dominating the white core and outer crust, thus being the most abundant species of the whole cheese. *K. lactis* was not present in the outer crust whereas *D. hansenii* and *Y. lipolytica* were both absent from the blue veins. *Trichosporon beigelii* was occasionally identified within the blue sections. Mould presence was greater in the blue veins than white core and absent from the outer crust.

1.2 FLAVOUR DEVELOPMENT

1.2.1 Aroma of blue cheese

The flavour of matured cheese results from interaction between starter bacteria, enzymes from the milk, enzymes from the rennet and accompanying lipases, and secondary flora (Urbach, 1997). Cheese flavour compounds are primarily derived from the breakdown of casein proteins, triglyceride fats and the metabolism of lactose and citrate of the milk. Lactose is metabolised to lactate by the starter culture, acidifying the milk. Acidification aids the activity of the milk clotting agent, rennet. The caseins proteins aggregate and with the fat forms curds. The liquid whey protein, water and remaining lactose are drained. The protein and fat in the curds, provides the substrates for residual enzymes and metabolism of microbial flora and the products of lipolytic and proteolytic reactions are then futher metabolised to many important cheese flavour compounds (Marilley & Casey, 2004; Collins *et al.*, 2003). For Stilton and other blue cheeses, lipolysis is considered most important, as free fatty acids are not only aroma compounds themselves but also precursors for methyl ketones, alcohols and esters (McSweeney & Sousa, 2000).

The microflora present within cheeses is extremely diverse and this microbial consortium makes a key contribution to all organoleptic aspects of cheese and is specific to each cheese variety (Beresford *et al.*, 2001; Jakobsen & Narvhus, 1996). Whilst the major flavour producing biochemical pathways: proteolysis (Sousa *et al.*, 2001), glycolysis and lipolysis (Collins *et al.*, 2003) have been defined (Marilley & Casey, 2004; McSweeney & Sousa, 2000), cheese ripening is complex. Factors governing the enzymology, and the origins of reactions are not well understood (Wilkinson & Kilcawley, 2005).

The sensory characteristics of blue cheeses vary (Mintel, 2007; Flórez *et al.*, 2005; Kupiec & Revell, 1998) yet despite recognizing large product variation there is limited scientific understanding about how the characteristics of blue cheeses develop. Flavour perception is also influenced by textural and visual characteristics resulting from complex interactions between manufacturing method, volatile composition and the gross composition of cheese (Lawlor *et al.*, 2001).

Aroma is a key factor of consumer preference for cheeses (Jaillais *et al.*, 1999), and along with taste comprises the flavour of product. The aroma of Stilton shows a large degree of variation between producers and variation is noted between sections (white core, outer crust and blue veins) of a single cheese (Gkatzionis *et al.*, 2009).

Ketones, especially 2-heptanone and 2-nonanone have long been identified as the principal contributors to blue cheese flavour (Dartey & Kinsella, 1971; Hiscox *et al.*, 1951). These compounds are the major presence (Qian *et al.*, 2002) but ketone levels are highly variable in blue cheeses (Anderson, 1965). No difference in the level of ketones were found between Roquefort and other blue cheeses (Anderson & Day, 1966). 'Component balance theory' (McSweeney & Sousa, 2000) has received attention and the need to analyse the composition of the aroma profile as a whole, along with concentrations and ratios of compounds, has been realised.

Qian *et al.* (2002) found 18 compounds which contributed to blue cheese aroma and showed that compounds such as methional and butanoic acid had higher flavour dilution values than 2-heptanone and 2-nonanone. When samples of aroma extract from the Blue Moon Cheese (Thorp, WI) were sniffed, methional and butanoic acid were more easily detectable that the two methyl ketones commonly hailed as most important. Wolf *et al.* (2011) suggested that low concentration compounds, such as esters, impart a fruitiness which reduces the pungency of methyl ketones and compounds, such as alcohols and acids, augment cheese aroma. In synthetic mixtures 2-phenylethanol, ethyl butanoate, methyl hexanoate and methyl octanoate (Anderson, 1965) plus 1-octen-3-ol (Ney *et al.*, 1975) greatly improved the blue cheese flavour and aroma. The fact that a large proportion of volatile compounds are common to all foods (Maarse, 1991) suggests that unique aroma of each cheese variety is influenced largely by the composition of esters, aldehydes and alcohols though these are less studied than ketones (Urbach, 1997).

1.2.2 Yeasts' influence upon aroma

Production of compounds which dominate blue cheese aromas mostly derives from the mould *Penicillium roqueforti*, yet contribution from additional microflora has been highlighted as crucial (Marilley & Casey, 2004). Yeasts native to blue cheeses were shown to be capable of reducing methyl ketones to secondary alcohols which are further metabolised to other alcohols and esters (Anderson & Day, 1966), thus having a potential role in flavour development of blue cheeses. The specific role yeasts play during cheese ripening has been noted as being difficult to distinguish (Lanciotti *et al.*, 2005).

Gkatzionis (2010) studied yeast-*P.roqueforti* interaction by incubating combinations of yeasts, with and without *P. roqueforti* spores, in a model dairy system. The resultant aroma profiles showed species specific trends and promoted further investigation into the impact that yeasts have on aroma profiles of Stilton cheese. Yeasts isolated from different sections of commercial Stilton cheeses demonstrated strain-specific properties (aroma production, lipolytic, proteolytic activity, mould inhibition). For example, production of blue cheese aroma compounds increased when *P. roqueforti* was incubated in the dairy model with the yeast *Y. lipolytica*, compared to incubating *P. roqeuforti* alone. This showed a synergistic like effect and suggested that yeasts may influence the quality (both positively and negatively) of Stilton aroma. Whilst initial statistical analysis identified the same trends in aroma profile produced for each microbial combination, the absolute values obtained for individual flavour compounds varied greatly between the four replicate samples for any one microbial combination (unpublished data, Food and Drink iNET project, 2011). Reasons for the significant degree of variation between replicates are not known yet it emulates the variation within the same batches of cheese in real manufacture (Madkor *et al.*, 1987).

1.2.3 Relationship of aroma compounds and sensory characteristics

There is limited knowledge about the composition of Stilton aroma. Whilst instrumental measurement of the aroma compounds of Stilton allows statistical analysis of the aroma profile, data does not necessarily relate to the sensory characteristics of the cheese (Molimard & Spinnler, 1996). Sensory analysis of Stilton aroma offers insight into consumer perception.

Aroma perception is complex and not well understood. Humans cannot distinguish specific compounds from mixtures (Laing & Jinks, 2001; Laing & Francis, 1989) and aroma compounds are context specific (Lawless *et al.,* 1991). This means that perception of aroma mixtures do not relate to the individual components within them (Cook *et al.,* 2005). Instrumental analysis does not show how aroma compounds interact within mixtures and as sensory perception is multimodal (Verhagen & Engelen, 2006) the interaction of textural, visual and flavour characteristics further complicates the linking of instrumental and sensory analysis.

1.3 AIM AND OBJECTIVES

The aim of this study is to understand reasons for variation in aroma production of yeasts incubated in a dairy model system. Possible ways to limit the variation between replicates will also be investigated. The work addresses the problems faced in the industry to maintain consistency of product batch to batch. To achieve the aim the following objectives have been set:

1. To investigate the impact of yeast inoculum concentration on the production of aroma compounds from incubating yeasts, with and without Stilton stater mould, in a model dairy system.

2. To investigate the impact that incubation temperature has on the production of aroma compounds resulting from incubating yeasts with and without Stilton stater mould, in a model dairy system.

3. To investigate whether differences observed in the aroma profiles found in Aims 1 and 2 impacts on the perception of a model dairy system.

Sensory investigations (Aim 3) are presented separately in Section 3. This is because experimental design of this work was decided based on the results from the investigations in Section 2.

By analysing the aroma profile qualitatively as a whole and the absolute amounts of individual flavour compounds produced, the factors which govern differences between replicate models can be investigated. To investigate variation between replicate samples, the effect of altering the yeast inoculation concentration and incubation temperature of a dairy model will be studied. Gathering further understanding about the model system would aid later refinement and for this reason the growth of organisms during the model incubation period will be studied. Sensory analysis will be undertaken to relate statistical data collected from the model to the impact upon human perception of the blue cheese aroma.

The yeast composition of many blue cheeses has been studied (Viljoen *et al.*, 2003; Addis *et al.*, 2001; Wojtatowicz *et al.*, 2001; Roostita, 1996), including Stilton (Gkatzionis, 2010). However, the influence each particular species may play upon aroma generation has not been linked to the amounts present. The aroma profiles of models inoculated at different yeast concentrations was studied to understand the significance of the amount of yeasts during ripening. Temperature affects microbial growth and therefore the effect of altering the model's incubation temperature upon the aroma profiles generated was investigated. The production of volatiles was analysed instrumentally, using Solid-phase Microextraction Gas Chromatography-Mass Spectrometry. A separate study testing the effect of salt and salt substitutes upon yeast growth in the model was conducted. Yeasts were enumerated in models with and without salt and two commercial salt substitutes: Sub4salt® and seaweed (Appendix 1).

2. STUDY OF THE YEAST MICROFLORA OF STILTON USING A DAIRY MODEL SYSTEM

2.1 Model development

Previous studies of flavour profiles from cheeses have shown results to be dependent upon both the type of cheese and methods of study (Vitova *et al.*, 2006). Gkatzionis (2010) used a UHT-based blue cheese model as means to study the effects interaction between yeasts and moulds had upon aroma, through incubating yeasts isolated from different regions of Stilton in the model system, both individually and with *P. roqueforti.* Modelling Stilton using a dairy model allows yeasts impact upon cheese aroma to be studied in isolation. Knowledge of this pre-defined model allows easier development and alteration of model parameters to investigate key factors influencing variation.

Milk is the main component of cheese, typically used in raw form or pasteurised. Ultra heat treated (UHT) milk, having a similar composition to raw milk, creates a suitable medium for modelling dairy systems (Rosenthal, 1991), with the advantage of being commercially available. Roostita & Fleet (1996) showed several yeast species from cheeses grow well within UHT milk, and also how the medium is not selective for particular species. UHT-milk has been used as growth media for studies investigating the influence of the microbial consortium relevant to cheese production inclusive of lactic acid bacteria (Gadaga *et al.*, 2001), yeasts (Viljoen, 2001), and for studies of contamination risks from the pathogen *Listeria monocytogenes* (Murphy *et al.*, 1996).

Previous work standardised the yeast inoculum concentration at $1x10^5$ cells mL^{-1}, with *P. roqueforti* spores inoculated to $1x10^5$ spores mL^{-1}. Incubation of the model was also standardised at 25°C for 10 days (unpublished data, Food and Drink iNET project, 2011). Growth of some yeasts in milk is documented (Roostita & Fleet, 1996), but data is limited. Enumerating growth of yeasts throughout incubation may give insight into possible reasons for variation between model samples. Growth of yeasts within the dairy model is not well defined because models are sealed for the incubation period prior to sampling for aroma analysis and counting yeasts would require models to be opened during the incubation period. Aroma analysis could not be conducted on models which have been disrupted. For this reason microbiological and aroma analysis must be conducted on replicate models. The influence that the concentration of each particular species may have on aroma generation has not been studied. Yeasts of blue cheese are present in the dairy environment (Viljoen *et al.*, 2003) and their growth in cheeses is uncontrolled. Studying aroma profiles of models across different yeast concentrations may allow some understanding of the significance that the level of yeast presence has during ripening. Temperature is a key factor for microbial growth and thus aroma development. Within industry ripening rooms are controlled at around 10°C yet the effect temperature may have upon aroma generation is undefined.

2.1.1 Solid Phase Micro Extraction Gas Chromatography-Mass Spectrometry (SPME GC-MS)

SPME allows collection of volatile compounds directly from samples by absorbing to a coated fused-silica fibre. The fibre can either be immersed into a liquid sample or exposed to the vaporous headspace above a sample in any physical state (Kataoka *et al.*, 2000). The fibres' coating material is chosen according to the type of compounds wanted to be extracted. Most aroma compounds are highly volatile, yet present only in low concentrations (Frank *et al.*, 2004). SPME GC-MS is highly sensitive ideally suited to complex volatile mixtures, exhibiting lower background and a higher degree of reproducibility when compared to other headspace techniques (Kataoka *et al.*, 2000). The robustness of SPME is limited as the technique only extracts a limited range of compounds and quantification can be difficult (Marilley & Casey, 2004; Alewijn *et al.*, 2003). Page & Lacroix (2000) also argued how samples with a high lipid content reduce the efficiency of SPME extraction and Stashenko & Martínez (2007) tell of how compounds with similar volatilities are in effect directly competing to be adsorbed and that this can then lead to analysis which does not accurately represent the samples aroma profile.

SPME GC-MS analysis has been conducted to analyse the aroma upon many dairy products including cheese samples in recent years (Croissant *et al.*, 2011; Wolf *et al.*, 2011; Hayaloglu *et al.*, 2008; Berezińska *et al.*, 2007; Hermansen *et al.*, 2006; Vitova *et al.*, 2006; Chin *et al.*, 1996). Gkatzionis *et al.* (2009) compared the method to other extraction techniques when analysing Stilton cheese and used the technique for cost-effective analysis of model's headspace (Gkatzionis, 2010).

2.1.2 Effect of salt concentration on yeast growth in Stilton

Salting cheese has multiple roles. It is primarily used to halt or slow acidification of curds through inducing stress upon the lactic acid bacteria of the starter cultures and also expels moisture (Guinee, 2004). As Stilton is not pressed, controlling moisture content is vitally important for attaining the proper texture and development of the crust (Law & Tamine, 2010).

During production of Stilton the curds are salted after milling. Salt is typically added at 5.4%, with approximately 2.5% in the final product, almost double the UK guidelines (1.5g per 100g)(Daniels, 2009). High salt intake has been associated with many adverse health effects such as elevated blood pressure which in turn increasing risk of heart attack and strokes (He & MacGregor, 2009 ; Alderman *et al.*, 1998). Following an advisory report on *Salt and Health* (Scientific Advisory Committee on Nutrition, 2003) the UK government began a public health initiative to lower consumption of salt (Food Standards Agency, 2009). Reducing sodium chloride in foods, including cheeses, is an area which has been widely researched (American Dairy Science Association, 2010) and alternative compounds that can be used as substitutes for salt without detracting from the sensory qualities of the cheese (Cruz *et al.*, 2011) has been a major focus. Most of the commercial salt substitutes replace some part of the sodium chloride with potassium chloride. Also, natural products such as seaweed (*Ascophyllum nodosum*) have been marketed as potential salt substitutes. Seaweed is claimed to reduce growth of micro-ogranisms and extend the shelf life of products (www.seaweedhealthfoundation.org.uk).

Salt is a natural preservative and prevents spoilage of the curds. Salt levels aid development of *P. roqueforti* and influence the growth of microflora. Halotolerant organisms have a competitive growth advantage. The concentration of salt and using salt substitutes may influence the balance of the secondary flora and the growth or suppression of pathogens.

2.2 MATERIALS AND METHODS

2.2.1 Models undergoing SPME GC-MS analysis

2.2.1.1 Micro-organisms

From a collection of yeasts and *P. roqueforti* previously isolated from Stilton cheese (Appendix 2) a representative isolate each of *Debaryomyces hansenii; Kluyveromyces lactis*; *Trichosporon beigelii* and *Yarrowia lipolytica* were selected for incubation in models undergoing aroma analysis (Table 2.1). Isolates selected have previously been shown to have enzymatic activity (proteolytic and lipolytic) which suggests they could influence the aroma quality of Stilton (Viljoen, 2001; Jakobsen & Narvhus, 1996).

Yeasts were grown on Rose Bengal Chloramphenicol Agar [RBCA] (Oxoid, Basingstoke, UK) at 25°C for five days. Pure cultures were stored at 4°C and re-cultured twice before use. *P. roqueforti* spores were harvested onto Sabouraud Dextrose Agar [SDA] (Oxoid) at 25°C and grown for seven days each subculture. Subcultures were stored at room temperature and spores harvested for re-culturing once a month. Before use in models, pure cultures were re-streaked twice.

Table 2.1: Yeast strains selected for microbial and aroma analysis in the model.

Yeast species	Microbial analysis – Enumeration[1]		Aroma analysis*
	Growth +/- *P. roqueforti*	Salt supplementation	
Kluyveromyces lactis	DB09	Y44	Y24
Yarrowia lipolytica	SB04	SO10	SB11
Debaryomyces hansenii	DO04	n/a	Y5
Trichosporon beigelii	Y19	n/a	Y17

* The same isolates were used for aroma analysis and sensory analysis.

[1] Isolates selected showed proteolytic and lipolytic activity (data not shown, Food and Drink iNET project).

2.2.1.2 Preparation of models for SPME GC-MS analysis

Yeasts and spores of *P. roqueforti* were harvested using sterile swabs and suspended in Phosphate Buffered Saline [PBS] (Oxoid). The concentration of cells or conidia in the PBS suspension was standardised using a haemocytometer (Weber Scientific International, Teddington, UK).

Models were prepared using UHT-treated milk (3.6% fat, pH 6.65 at 21°C) purchased from a local retailer. Milk (100 mL) was aseptically dispensed into sterilised 250 mL borosilicate glass bottles (Fischerbrand, Fischer Scientific, Loughborough, UK) containing a magnetic stirrer (PTFE 40 mm x 8 mm, Fischerbrand). The ratio of liquid to headspace in the model was the same as previous work to allow the data to be comparable. Replicate models were prepared from the same batch of milk. The milk was inoculated with cells/spores suspensions in PBS to the desired concentration of cells mL^{-1} and/or spores mL^{-1} by adding 1mL of suspension to a final concentration of $1x10^2$, $1x10^5$ and $1x10^8$ cells and/or spores mL^{-1}.

Yeasts were inoculated at $1x10^2$, $1x10^5$ and $1x10^8$ cells mL^{-1}. *P. roqueforti* was inoculated at $1x10^5$ spores mL^{-1}. Models were incubated at 5°C, 15°C and 25°C. The choice of 5°C and 15°C was to give a range around the industrial ripening temperature and allowing the model to better represent the actual Stilton production process.

Models were stirred on days 3, 7 and 10. pH was measured on day 0 and the day of trial termination. Three replicates were prepared for each model and samples (10 mL), taken on the termination day, transferred in 20 mL Headspace vials (22.5 mm x 75.5 mm; Grace Alltech, UK). Vials were sealed with a magnetic cap (20 mm diameter, 8 mm centre, PTFE / Silicone Liner; Grace Alltech) stored at -80°C until SPME GC-MS analysis.

The termination of models incubating at 25°C was day 10. This was selected to allow the data to be comparable to those of previous work which also used the same time-frame. Models incubated at 5°C or 15°C were terminated on day 20. Yeasts were eumerated in replicate samples prepared in parallel to those undergoing SPME GC-MS analysis and termination was decided when yeasts in replicate models inoculated at $1x10^2$ cell mL^{-1} achieved a minimum of $1x10^8$ CFU mL^{-1}.

2.2.1.3 SPME GC-MS

2.2.1.3.1 Chemicals

All the chemicals used as standards were GC grade (≥99.5%) purchased from Sigma-Aldrich (Gillingham, UK).

2.2.1.3.2 SPME GC-MS procedure

The SPME vials with the models were defrosted overnight at 4°C and left to equilibrate at 22°C for 30 min before analysis.

A 1-cm Stableflex fibre coated with 50/30 μm divinylbenzene-carboxen on polydimethylsiloxane bonded to a flexible fused silica core (Supelco, Bellefonte, PA, USA) was used for the extraction of the volatiles. Prior to use, the fibre was conditioned for 90 min in the injection port (300°C) in split mode. An extraction time of 20 min at room temperature was used, with desorption time set to 10 min at 230°C.

GC-MS was carried out using a Trace GC Ultra gas chromatograph (Thermo Scientific, Hemel Hemstead, UK) and DSQ mass spectrometer (Thermo Scientific). A BP5 capillary column (30 m x 0.25 mm I.D.; film thickness: 1 μm) from SGE analytical science (Milton Keynes, UK) was used. Helium was the carrier gas, at a constant pressure of 17 psi.

The GC-MS oven temperature programme was as follows:

An initial temperature of 40°C was maintained for 2 min, increasing at a rate of 8°C/min to a final temperature of 220°C. The transfer line from the gas chromatograph to the mass spectrometer was held at 250°C.

The mass spectrometer was operating under positive ionisation electron impact mode [EI+] at 70 eV. The detector was operated in scan mode (2 scans/s) scanning from m/z 20 to 250. Source temperature was 200°C.

The SPME GC-MS procedure followed that of Gkatzionis, 2010.

Compounds were identified by comparing their retention times and mass spectra with those of standards or their retention indexes [RI] with those published in databases and their mass spectra with the National Institute of Standards and Technology [NIST] mass spectral library. The Total Ion Current [TIC] signal intensity for each compound was expressed relative to the chromatograph peak area observed when the headspace above a 5 μgL^{-1} 2-nonanone was sampled.

All data were processed with Xcalibur v1.0 (Thermo Scientific) software.

2.2.1.3.3 Data analysis of data collected from SPME GC-MS

The relationship between the model samples and their volatiles (variables) detected with SPME GC-MS analysis was evaluated by Principal Component Analysis [PCA] using XLSTAT PRO 2011 (Addinsoft, New York, USA) and The Unscrambler v9.0 (CAMO Software AS, Oslo, Norway).

All data were centered and standardised (1/standard deviation) prior to analysis so that each variable is weighted equally. Thus each variable was given a mean of 0 and a standard deviation of 1 and the PCA is an eigenanalysis of the correlation matrix. Analysis of variance [ANOVA] was performed with SPSS Statistics 17.0

(IBM, Portsmouth, UK) or XLSTAT PRO 2011 (Addinsoft) in order to examine the significance of the differences between the quantities of the aroma compounds in the replicates.

2.2.2 Models undergoing micobiological analysis

2.2.2.1 Micro-ogranisms

An isolate each of *D. hansenii; K. lactis; T. beigelii* and *Y. lipolytica* were selected to undergo enumeration in the model with and *without P. roqueforti* present and a different isolate of each species chosen for enumeration in models supplemented with salt or salt substitutes (Table 2.1). Yeasts were subcultured following methods in Section 2.3.1.1.

Yeasts were inoculated at $1x10^5$ cells mL^{-1} and *P. roqueforti* at $1x10^5$ spores mL^{-1} following the same methods as in Section 2.3.1.2. Models were incubated at 25°C over 10 days. Samples were stirred on days 3, 6 and the pH was measured on day 0 and 10. Models were prepared in duplicate.

2.2.2.2 Enumeration of yeasts

Samples (1 mL) were aseptically taken from each model on days 0, 3, 6 or 7 and 10, serially diluted in PBS and viable surface counts taken following the Miles-Misra method (Miles *et al.*, 1938):

3 x 20μl spots of original sample and each dilution were plated onto respective media plates corresponding to organism wanting to be counted. The dilution with highest number of discrete colonies for all 3 spots was used to calculate the CFU mL^{-1} / conidia mL^{-1} in the respective model.

2.2.2.3 Enumeration of yeasts in models with salt supplements

Models were prepared as in section 2.3.2.1 but with the addition of salt supplements. NaCl (Oxoid), Sub4salt (Jungbunzlauer, Basel, Switzerland) and *Ascophyllum nodosum* [seaweed] (Appendix 1) were autoclaved and added into the model at 4% w/v. Yeasts were inoculated at $1x10^5$ cells mL^{-1} and *P. roqueforti* at $1x10^5$ spores mL^{-1}. Models were prepared in duplicate. Incubation of the models, stirring, pH recording, sampling and enumeration followed the methods discussed in section 2.3.2.2.

Milk samples of yeasts and yeasts co-present with *P. roqueforti* were plated onto SDA, RBCA and Brain Heart Infusion Agar [BHI] (Oxoid). Yeasts were co-suspended in PBS and streaked onto BHI, RBCA and SDA. Plates were incubated at 25°C.

2.3 RESULTS

2.3.1 MICROBIAL ANALYSIS

2.3.1.1 Yeast growth with and without *P. roqueforti* presence

Based on the findings from co-plating yeasts and *P. roqueforti* on selective media (data not shown) RBCA was chosen to enumerate yeasts after 4-5 days incubation. Plates were stored to 8 days incubation to assess *P. roqueforti* presence.

Following incubation for 10 days at 25°C all yeasts achieved a minimum of $1x10^8$ CFU mL^{-1}, irrespective of *P. roqueforti* presence (Figure 2.1). From ANOVA of counts at day 10, the only model to present growth significantly different ($p<0.05$) from all other yeasts was that of *K. lactis* with *P.roqueforti* which attained $1.3x10^{10}$ CFU mL^{-1} (Appendix 3 and Appendix 4).

Following 10 days incubation, *D. hansenii* with *P. roqueforti* present attained the lowest concentration with an average of $1.0x10^8$ CFU mL^{-1} whilst *T. beigelii* incubated individually and co-present with *P. roqueforti* attained $1.3x10^8$ and $4.0x10^8$ CFU mL^{-1} respectively (Figure 2.1). Growth within these models was at least 0.5 log lower than for other inoculums. *D. hansenii* alone achieved $1.6x10^9$ CFU mL^{-1} whilst *K. lactis* reached a maximum of $3.3x10^9$ CFU mL^{-1} at Day 6, decreasing to $2.1x10^9$ CFU mL^{-1} by day 10. *Y. lipoltyica,* both with and without *P. roqueforti,* also achieved peak concentrations at Day 6: $3.1x10^9$ and $3.3x10^9$ CFU mL^{-1} respectively with levels dropping to $2.9x10^9$ and $2.1x10^9$ CFU mL^{-1} during the following 4 days. *P. roqueforti* alone achieved an average of $3.4x10^5$ conidia mL^{-1}.

The 10 day incubation period has been deemed suitable for flavour analysis to represent the impact yeast growth has upon aroma profile generated as yeasts inoculated to $1x10^5$ CFU mL^{-1} all achieved at least $1x10^8$ CFU mL^1 in the model irrespective of *P. roqueforti* presence and previous work has used an inoculum concentration of $1x10^5$ CFU mL^{-1} for samples undergoing flavour analysis.

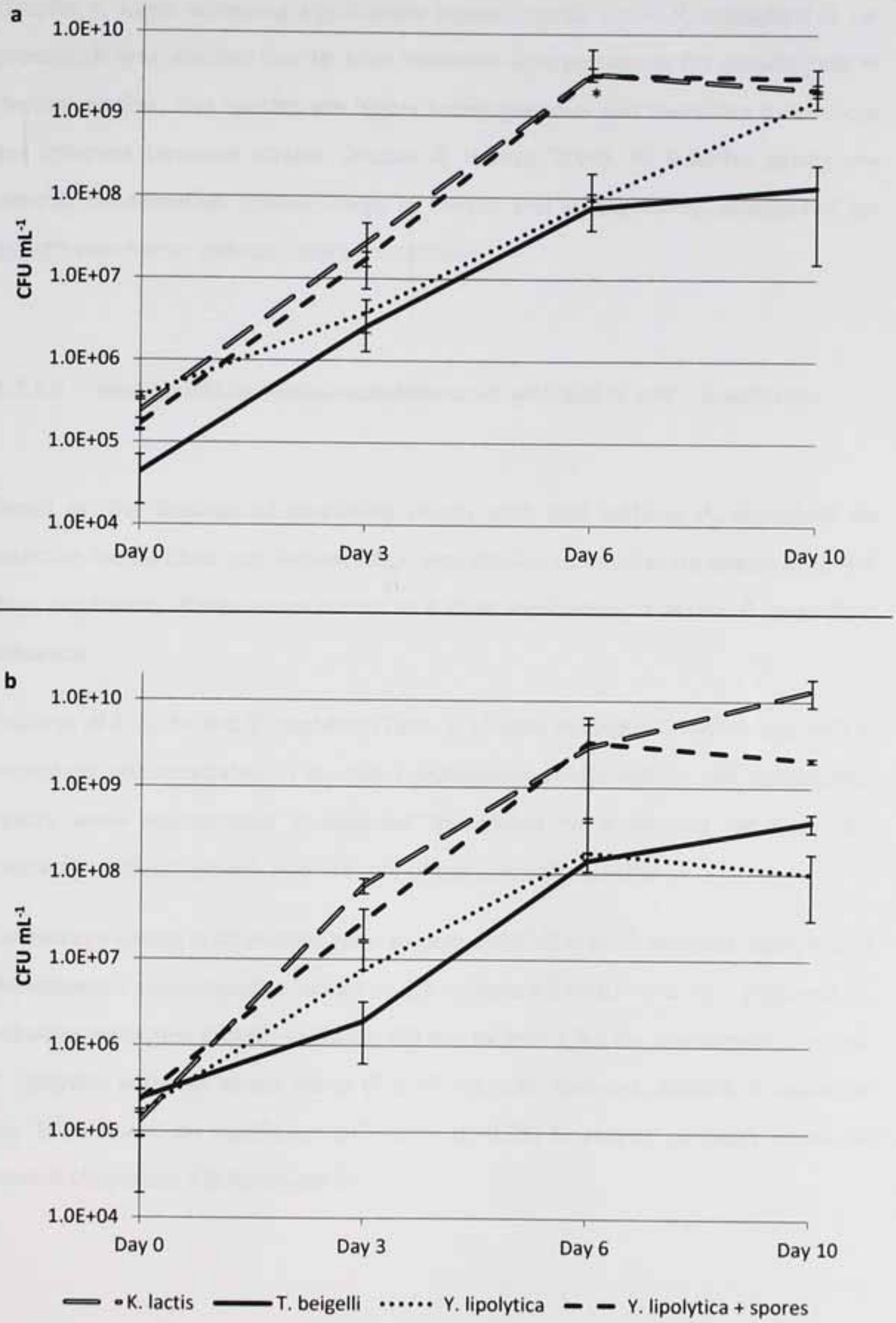


Figure 2.1: Mean counts$^{(\pm SD)}$ of yeast species inoculated at 1x10^5 cells mL^{-1} and incubated at 25°C over 10 days (a) without *P.roqueforti*; (b) with *P. roqueforti* inoculated at 1x10^5 spores mL^{-1}.

* Error bars show 1 stadard deviation about the mean. Negative error bars are not shown on logarithmic scale.

Despite *K. lactis* achieving significantly higher counts when *P. roqueforti* is co-present, it was decided not to alter inoculum concentrations for growth rate in flavour models. The species are highly heterogeneous and therefore differences are inherent between strains (Breuer & Harms, 2006). In industry yeasts are natural, uncontrolled, contaminants in cheese and so the model unadjusted for growth rate better reflects natural conditions.

2.3.1.2 Yeast counts in models supplemented with salt or salt substitutes

Based on the findings of co-plating yeasts with and without *P. roqueforti* on selective media (data not shown) RBCA was chosen to enumerate yeasts after 4-5 days incubation. Plates were stored to 8 days incubation to assess *P. roqueforti* presence.

Cultures of *K. lactis* and *Y. lipolytica* (Table 2.1) were individually inoculated with *P. roqueforti* and incubated in models supplemented with salt or salt substitutes. Yeasts were enumerated throughout incubation to determine whether any interaction affects growth and the role of salt and salt substitutes.

On average yeasts in all models grew to over $1x10^8$ CFU mL^{-1}, except *Y. lipolytica* in the seaweed supplemented model which achieved $5.0x10^7$ CFU mL^{-1} (Figure 2.2). Between replicates growth variation did not exceed 1 log for any samples, except *Y. lipolytica* with salt where range of a 2.5 log was observed. ANOVA of counts at day 10, showed no significant difference ($p>0.05$) in growth of yeast across all models (Appendix 5 & Appendix 6).

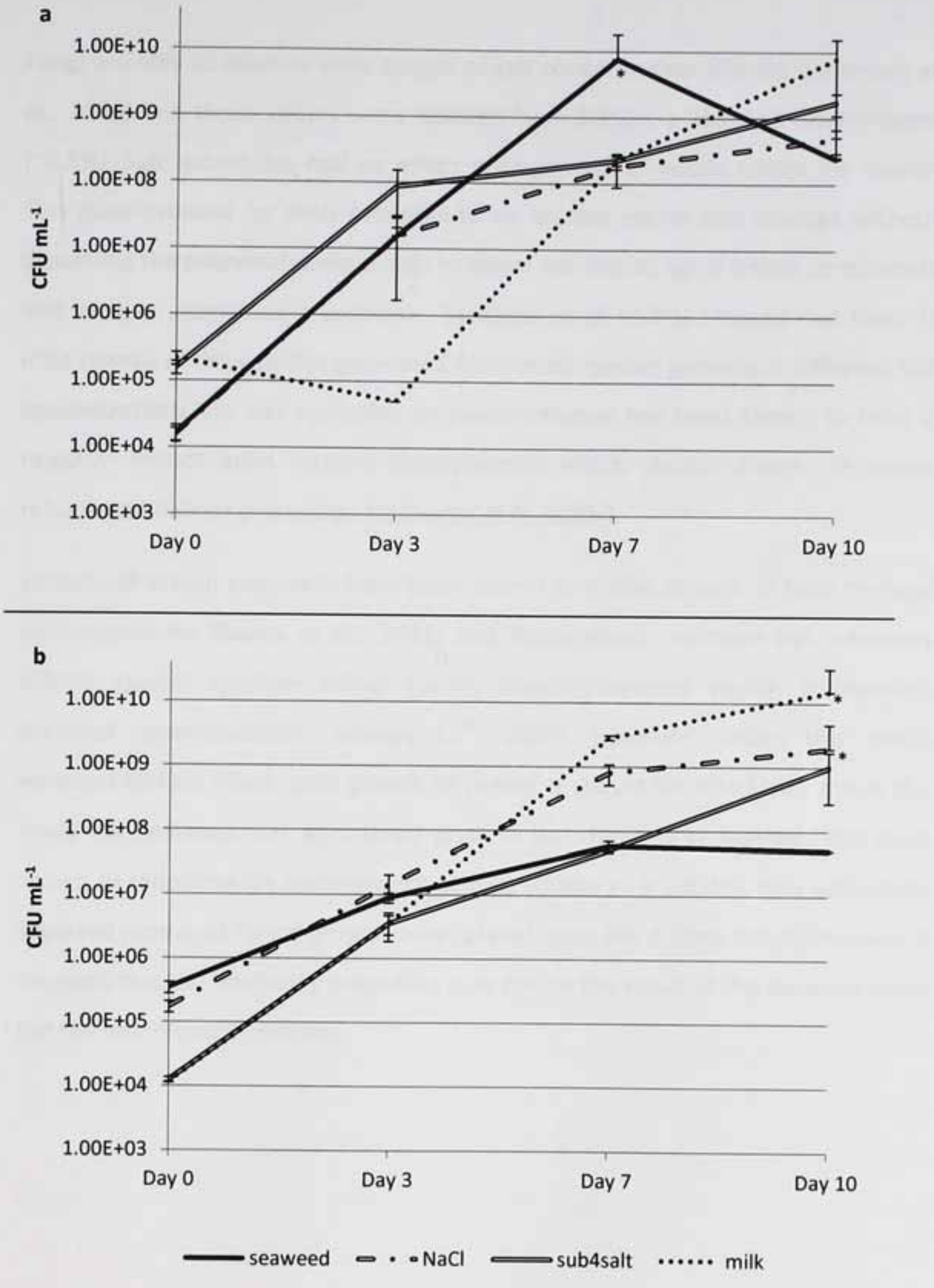


Figure 2.2: Mean counts $^{(\pm SD)}$ of (a) *Kluyveromyces lactis* and (b) *Yarrowia lipolytica* over 10 days incubation at 25°C in models[1] containing salt supplements, at $1x10^5$ cells mL^{-1} present.

* Error bars show 1 standard deviation about the mean. Negative error bars are not shown on logarithmic scale.

[1] *P. roqueforti* inoculated into all model at $1x10^5$ spores mL^{-1}.

Fungi are able to tolerate wide ranges of salt concentration (Gunde-Cimerman *et al.*, 2009) and these strains were isolated from Stilton, a high salt environment (~2.5%). Salt substitutes had no effect upon growth of yeasts within the model. This gives promise for their potential to be applied within real cheeses without disturbing the microbial composition however the impact upon aroma compounds and sensory properties is unknown. Guerzoni *et al.* (2001) showed that there is little change in the volatiles generated from yeast species growing at different salt concentrations but salt reduction in model cheeses has been shown to have a negative impact upon textural characteristics which causes changes in aroma release and flavour perception (Lauverjat *et al.*, 2009).

Extracts of brown seaweeds have been shown to inhibit growth of food spoilage microogranisms (Gupta *et al.*, 2011) and *Ascophyllum nodosum* has inhibitory effects against spoilage within bakery goods (Seaweed Health Foundation, personal communication, January 11th, 2012). However, within this model seaweed had no effect upon growth of yeasts. It should be noted that within this study the seaweed was autoclaved prior to use. Heating of seaweed has been shown to reduction it's antimicrobial activity (Gupta *et al.*, 2010). Non autoclaved seaweed produced fungal growth when plated upon RBCA (data not shown) which suggests that the inhibitory properties may not be the result of the seaweed itself, but the microflora it contains.

2.3.2 AROMA ANALYSIS

2.3.2.1 Reviewing previous data of aroma production by yeasts in models

Previous research investigated the aroma of Stilton, Stichelton and the aroma production of yeast isolates in a dairy model (unpublished data, Food and Drink iNET project, 2011). Each yeast species generated a distinct aroma profile by SPME GC-MS analysis; however, data showed large variation in the absolute amounts of aroma compounds between replicate model samples. In the present project the raw data from that study was reviewed and analysed in order to identify if the variation observed in the model was similar to that for real cheese. Also, trends that could be subject of further study in the present project were investigated.

Reprocessing data from previous work has shown that replicate variation is greater in the model than real cheese (data not shown). The reasons for this this are not understood.

There was no significant difference in the average %CV for replicate models prepared from the same or different batch of milk (data not shown). Geater variation was observed for the amounts of aroma compounds recorded between replicate models inoculated with both yeast and *P. roqueforti,* compared to models only containing yeasts (data not shown). Some compounds presented higher variance ([Sum of each compounds standard deviation from the mean signal intensity recorded for the model] ^{2}/ number of compounds -1); for example ethanol, 2-heptanone, 2- nonanone and 2-pentanone. These compounds along with acetone, methyl-butanol, ethyl butyrate, hexanoic acid and ethyl acetate showed the highest frequency of a high CV (>100%) and range (>1x10^{8}, signal intensity relative to standard) over replicate readings (data not shown).

Stilton final product showed an average CV of 60% and 64% from two different producers. Stichelton final product showed a far higher average CV of 136% across 12 replicate samples. Ketones, especially 2-heptanone, 2-nonanone and 2-

pentanone, showed greatest variance in amounts measured for replicate samples of Stilton and Stichelton (data not shown).

Following reviewing of the previous data it has been decided in the present study to create replicates from a single batch of milk in order to investigate how differences in the growth conditions of the model influence the generation of aroma compounds and the aroma variation within replicates.

2.3.2.2 The effect of the yeast inoculum concentration on the amounts of aroma compounds generated in a dairy model

The role of the yeast inoculum concentration on the aroma production was the first parameter of the blue cheese model to be investigated. Representative isolates of each yeast species (Table 2.1) were inoculated into the model at a range of concentrations ($1x10^2$ $1x10^5$ and $1x10^8$ cells mL^{-1}), both with and without *P. roqueforti*. The results of SPME GC-MS analysis (Appendix 7) are summarised in Table 2.2 to focus upon the overall amount of aroma compounds generated and specifically the level of ketones produced in models inoculated with each yeast species, with and without *P. roqueforti* present.

Comparing models containing yeasts alone with the milk only controls shows the direct aroma production of yeasts. Comparison between models inoculated with yeasts and spores to those of solely *P. roqueforti* represents the impact yeasts may have on the aroma production of Stilton. By comparing the aroma production of yeasts directly with the impact yeasts have when co-present with *P. roqueforti* allows the influence of *P. roqueforti*-yeast interaction to be investigated.

Models inoculated with *K. lactis* at $1x10^5$ and $1x10^2$ cells mL^{-1} with *P. roqueforti* significantly increased aroma production compared to that of *P. roqueforti* alone (Table 2.2). However, models containing *K.lactis* and *P. roqueforti* did not shows significantly greater aroma production compared to respective models of yeast alone, suggesting that the *K. lactis* directly contributes to the generation of aroma compounds. At all three concentrations the aroma production of models containing *T. beigelli* with *P. roqueforti* was significantly lower than models of solely *P. roqueforti* (Table 2.2). Models inoculated at $1x10^8$ and $1x10^5$ cells mL^{-1} of *T. beigelli* showed no significant differences in aroma production with and without *P. roqueforti* co-present suggesting that *T. beigelii* inhibits the aroma generation of *P. roqueforti.*

Ketone production was increased when *Y. lipolytica* at $1x10^8$ and $1x10^5$ cells mL^{-1} and K. lactis at $1x10^2$ cells mL^{-1} were co-inoculated with *P. roqueforti,* however following ANOVA the increases were not significant (Table 2.2). Co-inoculating *T. beigelii* with *P. roqueforti* singicantly decreased the production of ketones when compared to models containing *P. roqueforti* alone and this reduction was significant at all inoculum concentrations.

By normalising the data of models containing yeasts and *P. roqueforti* against those inoculated with solely *P. roqueforti,* the infleunce that yeasts have on the aroma generation during *P. roqueforti* can be shown. Models containing *K. lactis* diverge from models containing other yeast species and *P. roqueforti* alone on Principal Component 1 (PC1, Figure 2.3), tending towards ester production and showing distinct aroma profiles dependent upon the inoculum concentration. Principal Component 2 (PC2, Figure 2.2) appears to separate models depending on ketone production. Co-inoculating *Y. lipolytica* with *P. roqueforti* increases the proportion of most ketones, their acid precursors and the secondary alcohols generated from reduction of short chain fatty acid derived ketones and these increases are more prevalent when *Y. lipolytica* is inoculated at $1x10^5$ and $1x10^8$ cells mL^{-1} than at $1x10^2$ cells mL^{-1} (Figure 2.3). Models co-inoculated with *D. hansenii* or *T. beigelli* tend towards the production of methyl alkanes and α-pinene and show reduced ketone production, separating along PC2, compared to solely *P. roqueforti* (Figure 2.3).

Table 2.2: Quantified amount[1] of aroma compounds and ketones[2] in resultant aroma profiles following incubation of each yeast species with and without *P. roqueforti*[3], in the blue cheese model at 25°C.

		Inoculum concentration							
Aroma compounds	Species	Yeast ($1x10^8$ cells mL^{-1})	Yeast ($1x10^8$ cells mL^{-1}) + spores	Yeast ($1x10^5$ cells mL^{-1})	Yeast ($1x10^5$ cells mL^{-1}) + spores	Yeast ($1x10^2$ cells mL^{-1})	Yeast ($1x10^2$ cells mL^{-1}) + spores	Milk	*P. roqueforti* spores ($1x10^5$ spores mL^{-1})
Overall	*K. lactis*	17.60^{bcde}	16.80^{bcde}	16.00^{bcde}	19.30^{bcd}	17.10^{bcde}	23.40^{abc}	0.62^{h}	4.64^{efgh}
	Y. lipolytica	10.00^{cdefgh}	27.90^{ab}	7.02^{defgh}	24.80^{ab}	10.20^{cdefgh}	14.70^{bcdefg}	0.81^{h}	15.70^{bcdef}
	D. hansenii	1.27^{gh}	34.20^{a}	1.14^{gh}	23.20^{abc}	1.13^{gh}	24.30^{ab}	1.25^{gh}	34.50^{a}
	T. beigelii	1.13^{gh}	1.39^{gh}	0.90^{gh}	4.43^{efgh}	1.88^{fgh}	18.90^{bcd}	1.25^{gh}	34.50^{a}
Ketones	*K. lactis*	0.11^{g}	0.13^{g}	0.12^{g}	1.37^{g}	0.19^{g}	6.10^{defg}	0.48^{g}	4.40^{efg}
	Y. lipolytica	1.57^{fg}	23.20^{abc}	1.37^{g}	19.90^{bcd}	1.7^{fg}	12.70^{cdefg}	0.48^{g}	15.30^{cdef}
	D. hansenii	0.86^{g}	33.60^{ab}	0.82^{g}	21.30^{abc}	0.75^{g}	23.30^{ab}	0.95^{g}	34.00^{a}
	T. beigelii	0.60^{g}	0.58^{g}	0.60^{g}	3.57^{fg}	0.59^{g}	18.00^{cde}	0.95^{g}	34.00^{a}

[1]SPME GC-MS signal intensities for compounds are expressed relative to the signal intensity observed from a 5µg/L 2-nonanone standard. Letters (a-h) show groupings from ANOVA ($p<0.05$) applied individually to the overall and ketone aroma compound data.

[2]Ketones totalled - 2-Butanone, 2-Pentanone, 3-Hydroxy-2-butanone, 3-Methyl-2-pentanone, 2-Hexanone, 2-Heptanone, 3-Octanone, 2-Octanone, 8-Nonen-2-one, 2-Nonanone, 2-Decanone and 2-Undecanone

[3] Incubated at for 10 days. Results averaged from three replicates of each model.

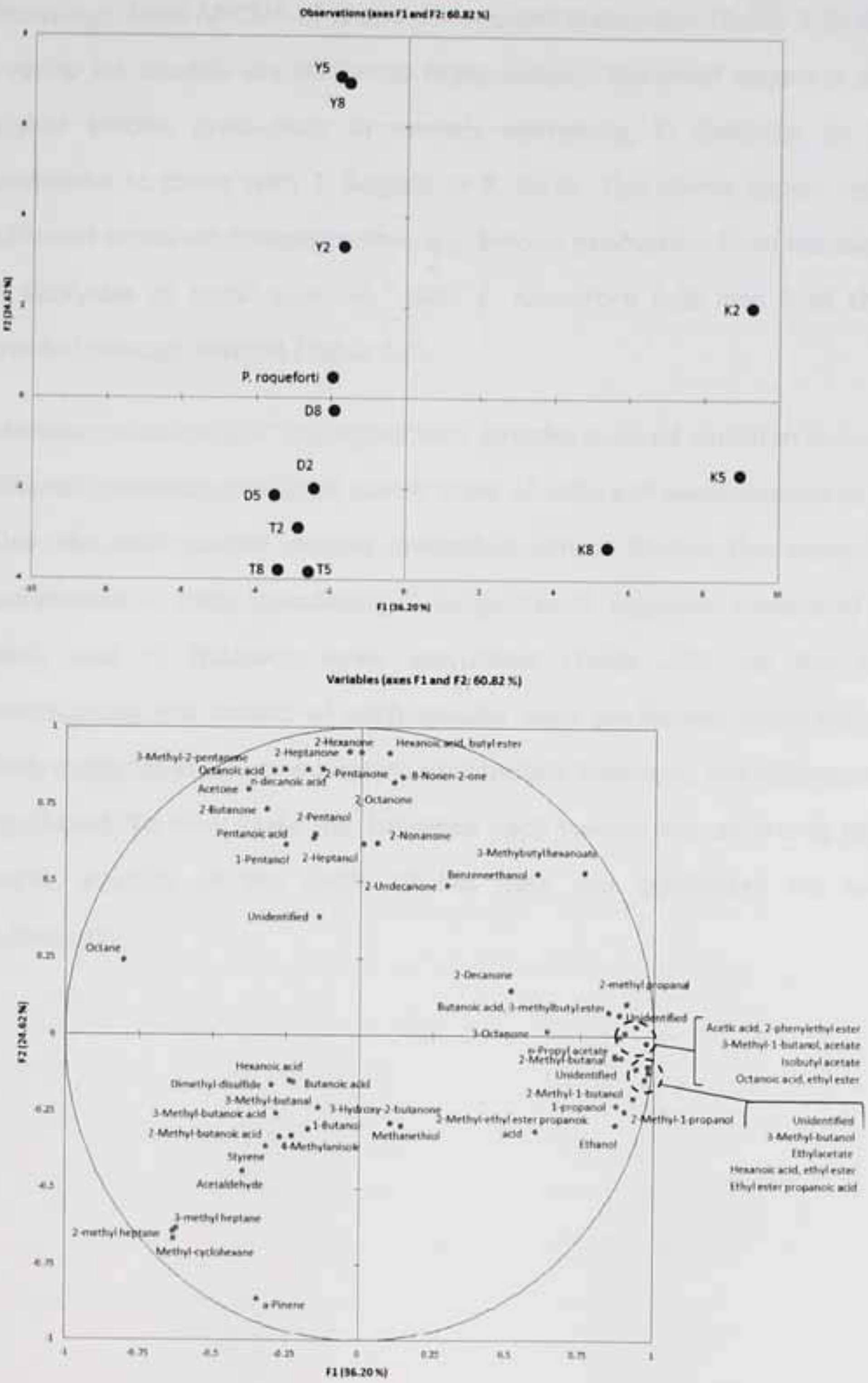


Figure 2.3 – PCA plots of models inoculated with yeasts at three concentrations and incubated at 25°C for 10 days with *P. roqueforti* at 1x10^5 spores/mL (a) bi-plot of samples[1;] (b) variables plot.

Y- *Y. lipolytica*; K- *K. lactis*; D- *D. hansenii*, T- *T. beigelli*.
8,5 and 2 - Inoculated at 1x10^8, 1x10^5 and 1x10^2 cells mL^{-1} respectively

[1]Samples prepared in triplicate. Replicates (3) averaged following SPME GC-MS analysis.

*Data was normalised against models containing *P. roqueforti* alone for each experiment to allow comparisons across yeast species.

Groupings from ANOVA of aroma compound production (Table 2.2) show a lot of overlap i.e. models are similar to many others. The most apparent separation is higher ketone production in models containing *Y. lipolytica* or *D. hansenii* compared to those with *T. beigelii* or *K. lactis*. This divide shows overlap across different inoculum concentrations e.g. ketone production from models containing *Y. lipolytica* at $1x10^2$ cells mL^{-1} with *P. roqueforti* falls into 5 of the 7 groups created through ANOVA (Table 2.2).

Aroma production of *P. roqueforti* only samples showed variation with significantly different amounts produced across trials of different yeast inoculums (Table 2.2). Also, the milk control models presented almost double the amount of aroma compounds in trials inoculating *T. beigelii* or *D. hansenii,* compared to when *K. lactis* and *Y. lipolytica* were inoculated (Table 2.2). As the experiments investigating the impact of each species were performed separately, this most likely indicates inaccurate creation of standard. However, the differences were not significant. To investigate the influence each species has on aroma production in depth, analysis of the SMPE GC-MS data was conducted for each species individually.

2.3.2.2.1 Analysis of aroma volatile generation from models inoculated with *Yarrowia lipolytica* at three concentrations

The aroma profiles generated from incubating *Y. lipolytica* in the dairy model show a clear divide between models inoculated with and without *P. roqueforti* (Figure 2.4). Ketones dominated the aroma profile of models containing *P. roqueforti* while models without *P. roquforti* showed a greater proportion of acids and aldehydes (PC1). The amount of the ketones 2-butanone, 2-pentantone, 2-hexanone, 2-heptanone, 8-nonen-2-one and 2-nonanone produced is significantly ($P<0.05$) greater in models containing *P. roqueforti* compared to those without *P. roqueforti* present (Appendix 8). On Principal Component 2 (PC2) models co-inoculated with *Y. lipolytica* and *P. roqueforti* diverged from those containing solely *P. roqueforti.* This divergence appeared to be concentration-dependent becoming larger when the inoculum concentration of *Y. lipolytica* was increased.

Models inoculated with *Y. lipolytica* at $1x10^5$ cells mL^{-1} and $1x10^8$ cells mL^{-1}; co-present with *P. roqueforti* showed greater ketone production than respective models containing *P. roqueforti* alone. The amount of ketones generated in these models was greater than the combined amount of ketones generated from models containing yeasts or *P. roqueforti* individually, suggesting a synergetic effect (Table 2.2). However, there was no significant increase in ketone production in these models compared to models inoculated solely with *P. roqueforti.* This means that the proposed synergetic increase in ketone production when *P. roqueforti* is incubated with *Y. lipolytica* at $1x10^5$ cells mL^{-1} and $1x10^8$ cells mL^{-1} is not statistically significant.

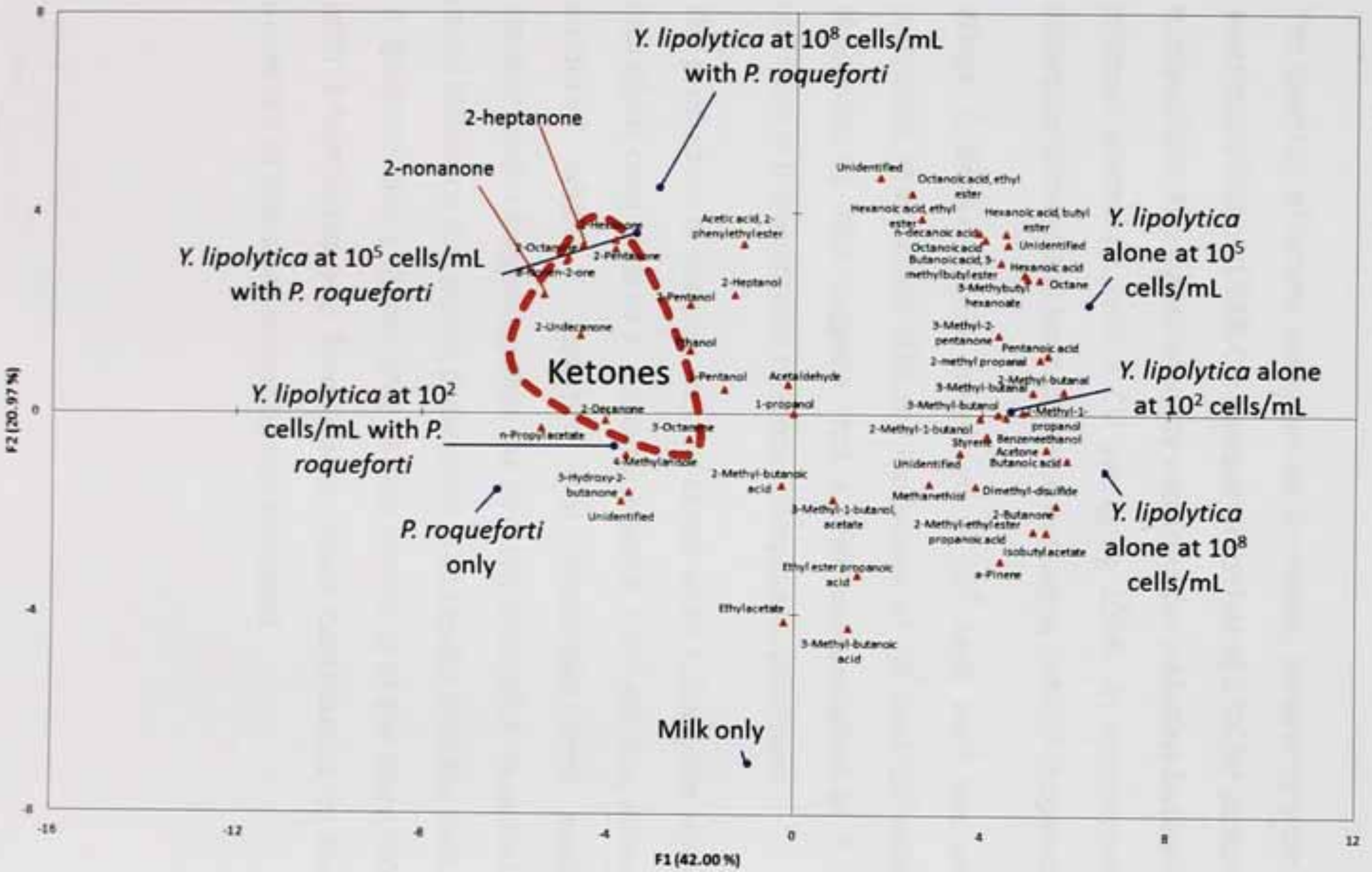


Figure 2.4: Bi-plot of SPME GC-MS analysis of model samples[1] inoculated with *Yarrowia lipolytica* at different concentrations, with and without *P. roqueforti* at $1x10^5$ spores mL^{-1}, following 10 days incubation at 25°C.

[1] Models were prepared in triplicate and replicates were averaged.

Models inoculated with *Y. lipolytica* and spores of *P. roqueforti* generated a greater overall abundance of aroma compounds than the yeast-only inoculums (Table 2.2). Following ANOVA the increase was found to be significant ($p<0.05$) for models inoculated to 10^8 and 10^5 cells mL^{-1} of *Y.lipolytica*. Ketone production was increased when *P. roqueforti* was co-inoculated with yeast and this increase was significant ($p<0.05$) when *Y. lipolytica* was inoculated into the model at $1x10^5$ cells mL^{-1} and $1x10^8$ cells mL^{-1}, further evidence for a synergy between *P. roqueforti* and *Y. lipolytica* and that ketone production increases with the inoculum concentration of *Y. lipolytica*.

The quantity of aroma compoundss in models containing only yeasts showed an average variation of 54% CV, compared to that of 57% for samples co-present with *P. roqueforti*. The signal intensity recorded for 2-Methyl-butanoic acid showed the greatest aberrancy, with a CV averaging 106%. By comparison quantities of 2-butanone showed the least variation averaging 16% CV (Appendix 9).

When *Y. lipolytica* was inoculated at 10^8 cells mL^{-1} the average CV is 41% compared to 65% and 60% for inoculums of 10^5 and 10^2 cells/ mL respectively (Appendix 9). This suggests that a high concentration of *Y. lipolytica* reduces variation in the quantities of aroma compounds produced.

The production of ketones was increased when *Y. lipolytica* was co-present with *P. roqueforti* compared to *P. roqueforti* alone. Furthermore, different ketones were produced when *Y. lipolytica* was inoculated into models at different concentrations suggesting that the concentration of *Y. lipolytica* present in Stilton could influence the aroma production. The results indicate that a high amount of *Y. lipolytica* may enhance blue cheese aroma as in the dairy model production of both 2-heptanone and 2-nonanone, major contributors to blue cheese aroma, increased as inoculum concentration increased.

2.3.2.2.2 Analysis of aroma volatile generation from models inoculated with *Kluyveromyces lactis* at three concentrations

PCA has shown that the aroma profiles from replicate models inoculated with *K. lactis* with *P. roqueforti* present, exhibited less variation as the inoculum concentration of *K.lactis* increased (Figure 2.5). Models inoculated to $1x10^8$ cells mL^{-1} of *K. lactis* co-present with *P. roqueforti* presented aroma profiles similar to that of models *containing K. lactis* alone. Models inoculated with *K. lactis* alone produced similar aroma profiles, irrespective of the inoculum concentration and tend towards 2-methy-ethyl ester propanoic acid on PC2 (Figure 2.5). In samples containing both *K. lactis* and *P. roqueforti*, ketones, acids and aldehydes were more dominant at lower yeast inoculum concentration.

Models containing *K. lactis* generated a larger amount of aroma compounds than models of *P. roqueforti* alone, though this increase was only significant ($p<0.05$) in models inoculated with *K. lactis* at 10^2 and 10^5 cells mL^{-1}, co-present with *P. roqueforti* (Table 2.2). Furthermore, models inoculated to 10^2 and 10^5 cells mL^{-1} of *K. lactis* did not show significantly greater aroma production than respective models containing *K. lactis* alone. This suggests that *K. lactis* directly contributes to aroma compound generation and has an additive effect on production of aroma compounds when co-inoculated with *P. roqueforti*.

As the concentration of *K. lactis* inoculated into the models increased, variation in the quantities of aroma compounds generated decreased. This is shown from the coefficient of variation for SPME signal intensities averaging 42%, 43% and 55% for inoculums of 10^8, 10^5 and 10^2 cells mL^{-1} of *K. lactis* respectively (Appendix 9). Models inoculated with or without *P. roqueforti* present showed a maximum 2% difference in the average coefficient of variation recorded.

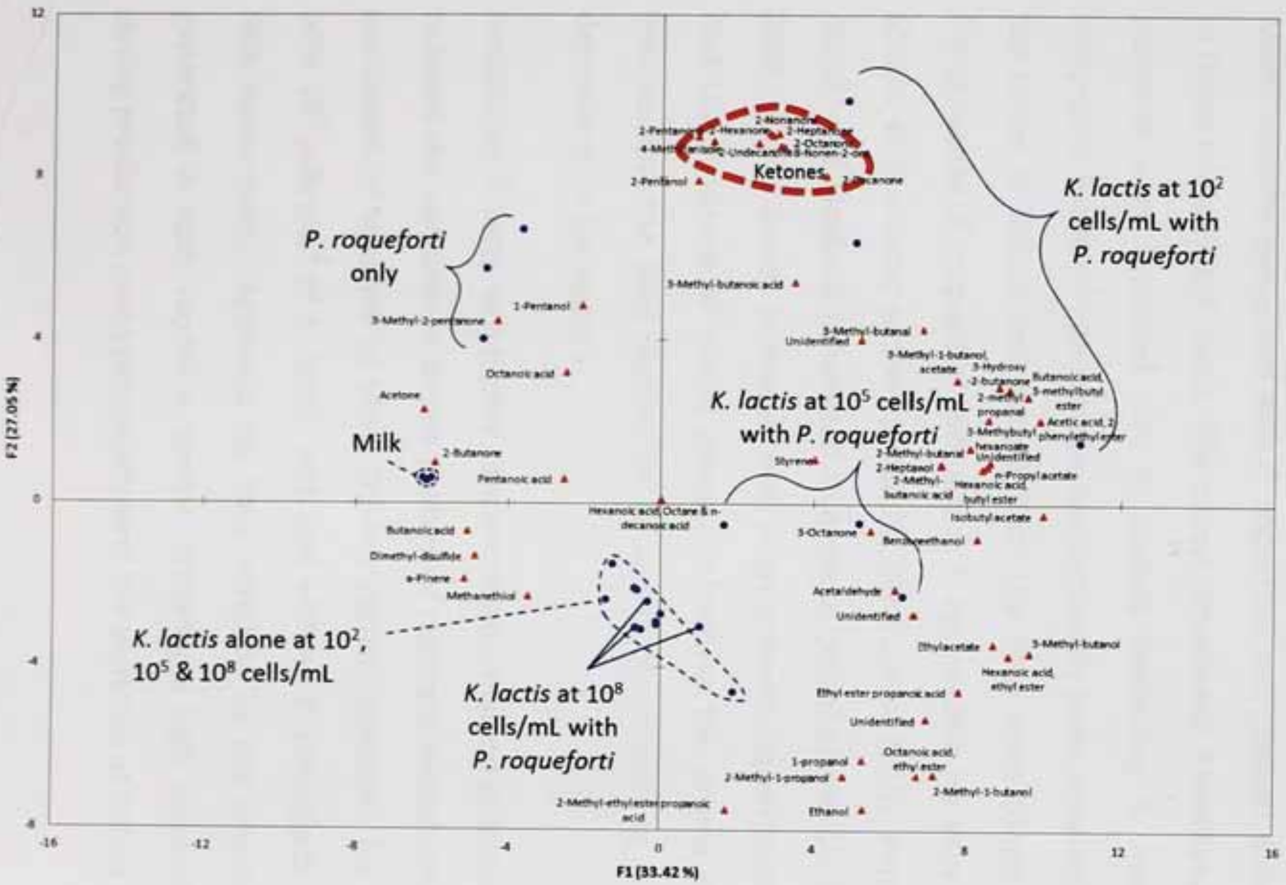


Figure 2.5: Bi-plot of SPME GC-MS analysis of model samples[1] inoculated with *Kluyveromyces lactis* at different concentrations, with and without *P. roqueforti* at $1x10^5$ spores mL^{-1}, following 10 days incubation at 25°C.

[1] Models were prepared in triplicate.

Production of the ketones 2-pentanone, 2-hexanone, 2-heptanone, 2-nonanone and 2-undecanone, along with 4-methylanisole, is significantly greater ($P<0.05$) in models containing *P. roqueforti* alone and those with *P. roqueforti* co-present with *K. lactis* at 10^2 cells mL^{-1}, compared to all other inoculum combinations (Appendix 10). All these compounds have been reported to contribute to blue cheese aroma (Berezińska *et al.*, 2007). Significantly more ($P<0.05$) 2-decanone is generated in models inoculated to 10^2 cells mL^{-1} of *K.lactis* and co-present with *P. roqueforti* (Appendix 10) with SPME signal intensities averaging 0.00866, compared to models containing *P. roqueforti* alone where an average of 0.00282 was measured (Appendix 9).

Model samples inoculated with *P. roqueforti* only present a distinct aroma profile to those containing *K. lactis.* The aroma compounds 3-methyl-2-pentanone and 1-pentanol were recorded only in models containing *P. roqueforti* alone. The compound 3-methyl-2pentanone has previously been reported to be abundant at the outer of Stilton and absent from the blue veins (Gkatzionis *et al.*, 2009). Paradoxically, *P. roqueforti* sporulation is responsible for vein generation yet it is absent at the outer section of Stilton (Gkatzionis, 2010). Pentan-1-ol presents a *'harsh'* and alcoholic fermented fruit odour (Hayaloglu *et al.*, 2008; Barron *et al.*, 2005). It was absent in models with yeast present. Lauverjat *et al.* (2009) showed that the structure of model cheeses influences the aroma release. The results indicate that the final distribution of aroma compounds in Stilton is likely to be dependent on the texture.

Inoculating *K. lactis* at a higher concentration, when co-present with *P. roqueforti,* reduced the variation in aroma profiles of replicate model samples. However the coefficient of variance of SPME GC-MS signals intensities for models inoculated with 10^2 cells mL^{-1} of *K. lactis,* with and without *P. roqueforti,* averaged 54% and 56% respectively (Appendix 9), thus variation in the amounts of compounds generated in each model is similar. Ensuring a high concentration of *K. lactis* during production could potentially limit the variation of Stilton aroma.

2.3.2.2.3 Analysis of aroma volatile generation from models inoculated with *Debaryomces hansenii* at three concentrations

Figure 2.6 shows the bi-plot of aroma compounds and model samples generated from PCA on the aroma compounds measured from models inoculated with *D. hansenii* (Appendix 7). Samples separate in PC1 on the basis of *P. roqueforti* presence or absence. All samples containing *D. hansenii* alone generated a similar aroma profile to that of milk alone, clustering on the bi-plot and also producing similar amounts of ketones and aroma compounds overall, as evidenced through ANOVA (Table 2.2). There is no significant difference ($p>0.05$) in the amounts of ketones and aroma compounds produced in all models containing *P. roqueforti.*

Models containing *P. roqueforti* presented significantly ($P<0.05$) greater amounts of the ketones 2, pentanone, 2-hexanone, 2-nonanone and 2-heptanone along with more 2-heptanol than those without (Appendix 11).

Significantly ($P<0.05$) less 2-butanone is generated in models containing *P. roqueforti*. Lawlor *et al.* (2001) showed that greater 2-butanone levels promoted perception of creamy odour following sensory analysis of ten cheese varieties. Models inoculated to different concentrations of *D. hansenii* and co-present with *P. roqueforti* are dispersed on PC2 (Figure 2.6).

Models inoculated to $1x10^8$ cells mL^{-1} of *D. hansenii* with *P. roqueforti* present a profile similar to *P. roqueforti* alone dominated by ketones and thus likely to embody a blue cheese like aroma. Samples inoculated at $1x10^5$ cells mL^{-1} exhibit a profile with a greater proportion of acids. Aldehydes and alcohols contribute more to the aroma profile of models inoculated to $1x10^2$ cells mL^{-1} of *D. hansenii* with *P. roqueforti* present.

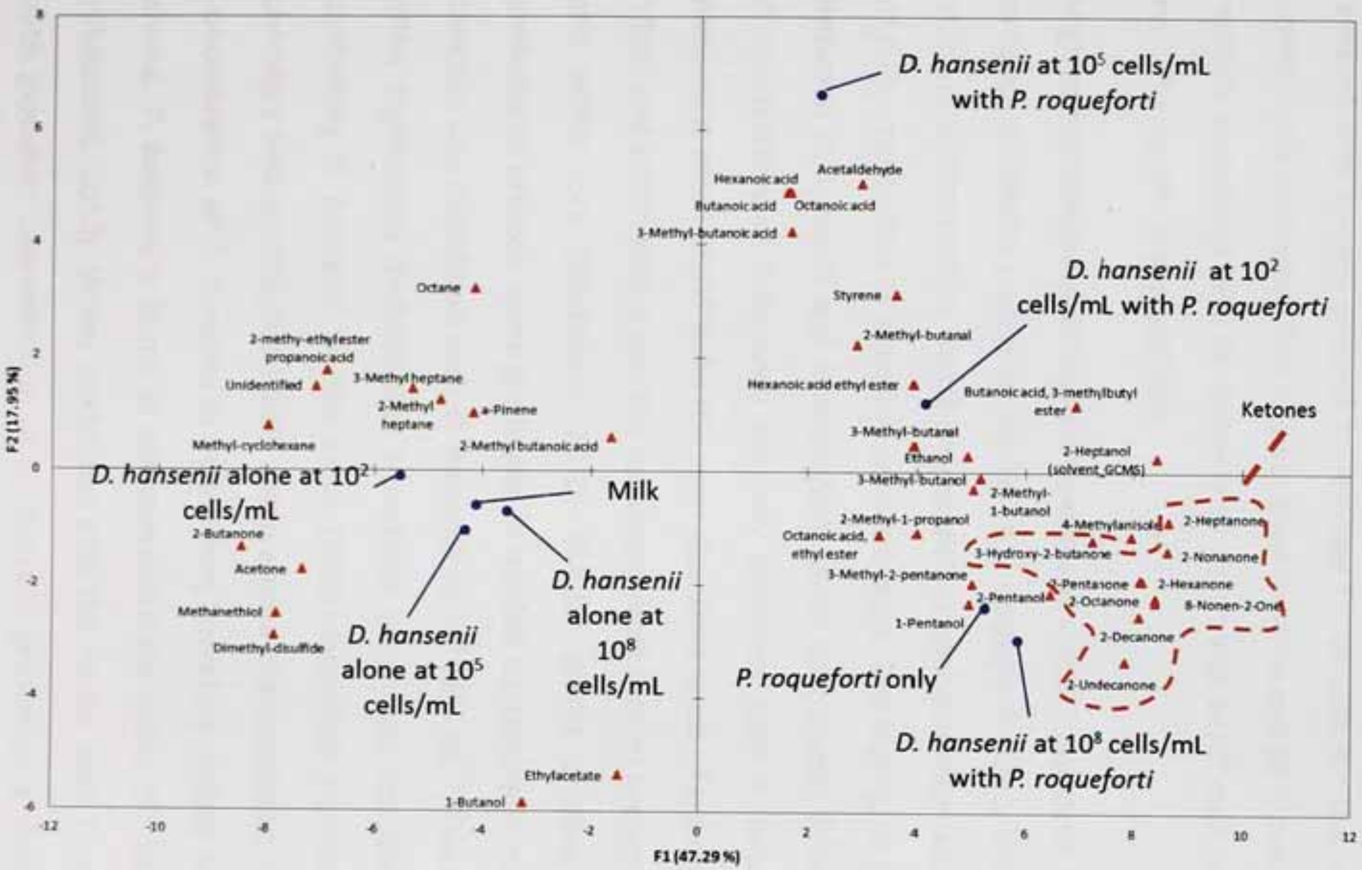


Figure 2.6: Bi-plot of SPME GC-MS analysis of blue cheese model samples[1] inoculated with *Debaryomyces hansenii* at different concentrations, with and without *P. roqueforti* at $1x10^5$ spores mL^{-1}, following 10 days incubation at 25°C.

[1] Models were prepared in triplicate and replicates have been averaged following analysis via SPME GC-MS.

Samples containing *P. roqueforti* showed greater variation in the amounts of volatiles between replicates than models without. An average CV of 59% and 38% respectively was calculated for the signal intensities recorded via SPME GC-MS (Appendix 9). Butanoic acid, pentanoic acid and octanoic acid were only found in samples containing *P. roqueforti*. Both butanoic acid and pentanoic acid have been described as contributing cheesy and rotten aroma notes to cheese (Frank *et al.*, 2004). The SPME signal intensities measured in replicate samples for these acids showed 141% CV, contributing to the higher variance observed models containing *P. roqueforti* (Appendix 9). Models inoculated to $1x10^8$ cells mL^{-1} of *D. hansenii* co-present with spores, present an average CV of 50% for the quantities of aroma compounds measured. This is lower than the 60% and 69% average CV observed in models inoculated with *D. hansenii* to $1x10^2$ and $1x10^5$ cells mL^{-1} and co-present with *P. roqueforti,* respectively.

High concentration of *D.hansenii* co-present with *P. roqueforti* has been shown to produce an aroma profile far similar to *P. roqueforti* alone, than when inoculated at lower concentration. Yeast only models produced similar aroma profiles to that of milk, irrespective of inoculum concentration. This highlights possible interaction between *D. hansenii* and *P. roqueforti,* given that aroma differences at differing concentrations of *D.hansenii* are only prevalent with *P. roqueforti* present. *D. hansenii* is often found to be the most abundant yeast of cheese microflora (Fleet, 1990) and within Stilton was the dominant yeast species present at the outer crust and white core (Gkatzionis, 2010). Similar aroma profiles, including similar amounts of ketones, were generated in models containing *P. roqueforti* alone and samples also inoculated with *D. hansenii* to 10^8 cells mL^{-1}. The only compound to differ significantly ($P<0.05$) was 1-pentanol which was less abundant in samples containing *D. hansenii*. Barron *et al.* (2005) identified 1-pentanol in farmhouse cheddars that contributed harsh, sharp aroma characteristics. Presence of a high concentration of *D. hansenii* in Stilton may therefore reduce negative aspects of aroma. *D. hansenii* is found in low concentration within the blue veins of Stilton (Gkatzionis, 2010). When inoculated into the model with *P. roqueforti* present, each inoculum concentration of *D. hansenii* presented a distinct aroma profile

(Figure 2.6) and thus different amounts in each section of Stilton is likely to be a key factor influencing the different aroma profiles observed for each section of the cheese (Gkatzionis *et al.*, 2009).

2.3.2.2.4 Analysis of aroma volatile generation from models inoculated with *Trichosporon beigelii* at three concentrations

Models inoculated with *T.beigelii* produced aroma profiles distinct from both milk and samples containing only *P. roqueforti* (Figure 2.7). Significantly ($P<0.05$) greater amounts of the ketones 2-decanone, 2-undecanone, 2-octanone, 8-nonen-2-one, 2-nonanone, 2-pentanone, 2-hexanone, 2-heptanone and also 1-pentanol was produced in models inoculated with *P. roqueforti* alone, compared to models containing *T. beigelii* (Appendix 12).

The amounts of ketones produced in samples containing both *T. beigelii* and *P. roqueforti* decreased as yeast inoculum concentration increased, ranging from an average SPME GC-MS signal peak area of 18.0 at 10^2 cells mL^{-1} to 0.57 at 10^8 cells mL^{-1} (Table 2.2), suggesting that *T. beigelii* inhibits *P. roqueforti* ketone production. The significantly ($P<0.05$) greater amount of ketones in models inoculated with *P. roqueforti* alone or when *T. beigelii* is co-inoculated at $1x10^2$ cells mL^{-1} (Table 2.2) separated these samples from other inoculum combinations on PC1 (Figure 2.7).

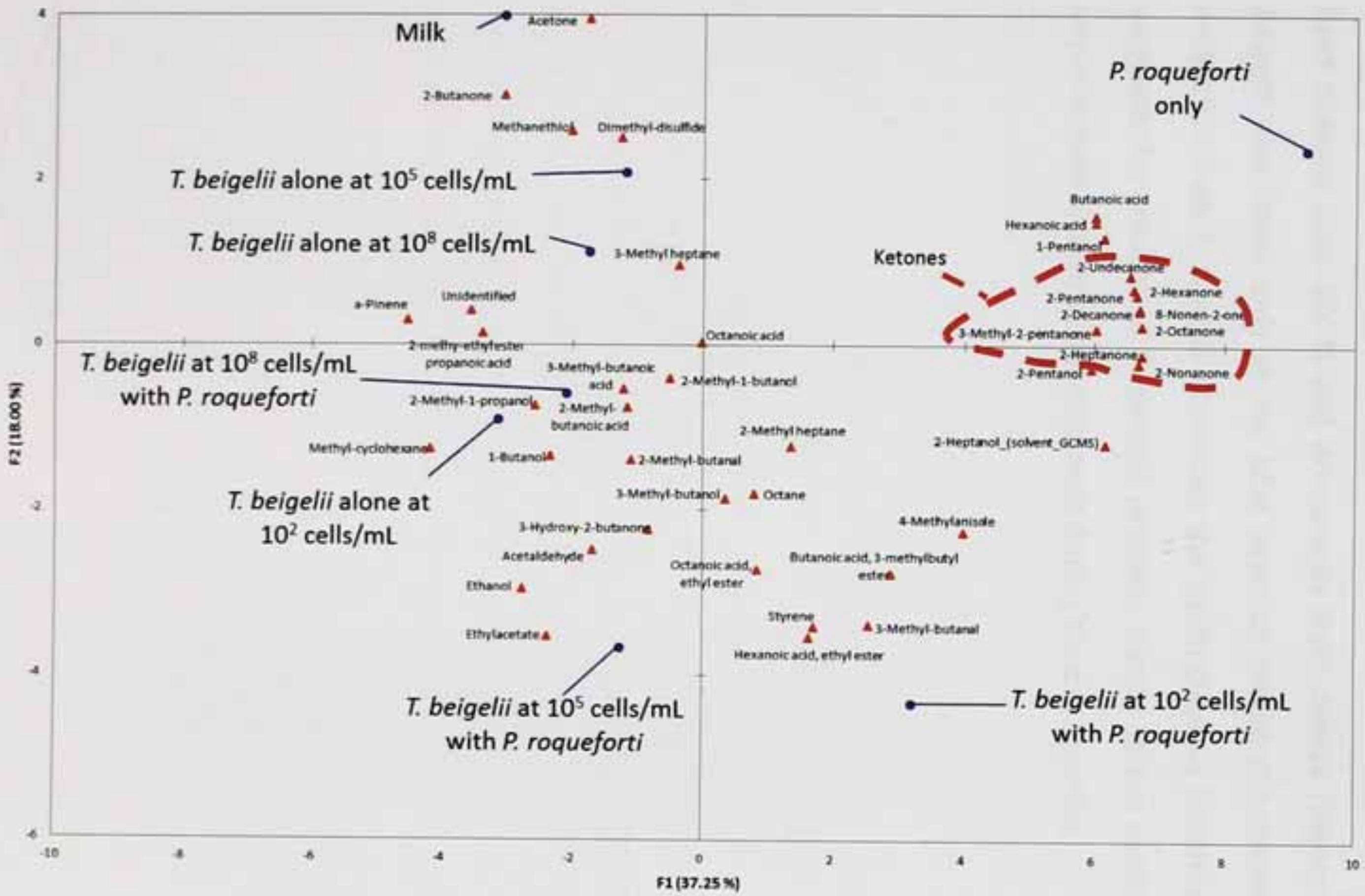


Figure 2.7: **Bi-plot of SPME GC-MS analysis of blue cheese model samples[1] inoculated with *Trichosporon beigelii* at different concentration, with and without *P. roqueforti* at 1x10^5 spores mL^{-1}, following 10 days incubation at 25°C.**

[1] Models were prepared in triplicate and replicates have been averaged following analysis via SPME GC-MS.

Variation in the SPME GC-MS signal intensities was greater for model replicates containing *P. roqueforti*, with an average CV of 58% compared to that of 49% in models containing *T. beigelli* alone (Appendix 9). Variation in the quantities of compounds recorded by SPME GC-MS is reduced at a *T. beigelii* inoculum concentration of $1x10^8$ cells mL^{-1} averaging 44% CV, compared to 60% and 56% for $1x10^5$ and $1x10^2$ cells mL^{-1} (Appendix 9) and this suggests that the variation is influenced by different amount of ketones produced by *P. roqueforti* in replicate models.

T. beigelii has been shown to be present in the secondary microflora of various hard cheeses (Das, 2004) and Gorgonzola style cheese (Viljoen *et al.*, 2003). *T. beigelii* was found only at the blue veins of Stilton (Gkatzionis, 2010) and the indication that *T. beigelii* supresses the production of ketones by *P. roqueforti* suggests the amount of *T. beigelli* present during Stilton production could be a key influence on aroma development during cheese ripening.

2.3.2.3 Temperature

Following study of the influence that yeast inoculum concentration in the model had upon aroma profiles generated an investigation into the effect the incubation temperature of the model system had upon aroma production was undertaken. *Y. lipolytica* and *K. lactis* (Table 2.1) were chosen to be studied because previous results (Section 2.4.2.2.1 and 2.4.2.2.2) showed that the inoculum concentration influenced the amount and variation of resultant aroma compounds produced and these effects were concentration-dependent.

Yeasts were inoculated at $1x10^2$ and $1x10^5$ cells mL^{-1} and models incubated at 5°C and 15°C. PCA bi-plots from SPME GC-MS measurements on aroma profiles models resulting from models incubated at 25°C showed clear distinction between samples inoculated to $1x10^2$ and $1x10^5$ cells mL^{-1} of yeast for *Y. lipolytica* (Figure 2.4) and *K. lactis* (Figure 2.5). Inoculating models at $1x10^5$ cells mL^{-1} meant yeast growth recorded in samples incubated at 5°C and 15°C could be compared to those measured in respective samples incubated at 25°C (Section 2.4.2.2)

Generation of aroma compounds in models incubated at 5°C and 15°C (Table 2.3) was far lower than that at 25°C (Table 2.2). This was most evident in models containing *P. roqueforti* alone where average SPME GC-MS signal intensities for models inoculated at 5°C, 15°C and 25°C were 0.06, 0.15 and 18.28. There was no significant difference in the amounts of aroma compound produced in repective models with and without *P. roqueforti* present. This is likely due to lack of *P. roqueforti* germination and growth as at low temperatures the germination time of *Penicillium* moulds is delayed and growth is slower (Lahlali *et al.*, 2005; Plaza *et al.*, 2003).

Table 2.3: Quantified amount of aroma compounds[1] and ketones[2] generated following incubation of each yeast species with and without *P. roqueforti*[3], in the blue cheese model at 5°C and 15°C.

		Incubation temp. (°C)	Yeast (1x10^5 cells mL^{-1})	Yeast (1x10^5 cells mL^{-1})+ spores	Yeast (1x10^2 cells mL^{-1})	Yeast (1x10^2 cells mL^{-1})+ spores	Milk	P. roqueforti spores (1x10^5 spores mL^{-1})
Overall	*K. lactis*	5	1.46^{ab}	1.47^{ab}	1.30^{abc}	0.10^{c}	0.09^{c}	0.06^{c}
	K. lactis	15	1.37^{abc}	1.58^{a}	0.31^{abc}	1.63^{a}	0.17^{c}	0.15^{c}
	Y. lipolytica	5	0.04^{c}	0.48^{abc}	0.05^{c}	1.05^{abc}	0.09^{c}	0.06^{c}
	Y. lipolytica	15	0.49^{abc}	1.46^{ab}	0.32^{abc}	0.87^{abc}	0.17^{c}	0.15^{c}
Ketones	*K. lactis*	5	4.35E-02^{a}	1.39E-01^{a}	2.66E-02^{a}	4.39E-02^{a}	6.94E-02^{a}	3.69E-02^{a}
	K. lactis	15	1.35E-02^{a}	1.09E-01^{a}	2.94E-01^{a}	1.31E-01^{a}	1.42E-01^{a}	1.17E-01^{a}
	Y. lipolytica	5	3.02E-02^{a}	3.94E-01^{a}	3.48E-02^{a}	9.38E-01^{a}	6.94E-02^{a}	3.69E-02^{a}
	Y. lipolytica	15	9.08E-02^{a}	1.26E+00^{a}	9.95E-02^{a}	6.28E-01^{a}	1.42E-01^{a}	1.17E-01^{a}

[1]SPME GC-MS signal intensities for compounds are expressed relative to the signal intensity observed from a 5μg/L 2-nonanone standard. Letters (a-h) show groupings from ANOVA ($p<0.05$) applied individually to the overall and ketone aroma compound data. Ketone production showed no significant difference for all models.

[2]Ketones totalled - 2-Butanone, 2-Pentanone, 3-Hydroxy-2-butanone, 3-Methyl-2-pentanone, 2-Hexanone, 2-Heptanone, 3-Octanone, 2-Octanone, 8-Nonen-2-one, 2-Nonanone, 2-Decanone and 2-Undecanone.

[3]Incubated for 20 days. Results averaged from three replicates of each model. Data for each replicate is shown in Appendix 13.

2.3.2.3.1 Temperature upon aroma profile of models inoculated with *K. lactis*

No significant difference ($p>0.05$) was observed in the amounts of ketones produced between models incubated at 5°C or 15°C, both with and without *P. roqueforti* co-present (Table 2.3) suggesting little germination and growth of *P. roqueforti.*

Results highlight that the aroma production resulting from models inoculated with *K. lactis* is dependent upon incubation temperature with regards to the compounds produced, but not the quantities of compounds observed in replicate samples. Models inoculated with *K. lactis* alone presented a lower proportion of ketones in the overall aroma profile, distinguished from models co-present with *P. roqueforti* along PC2 (Figure 2.8). However, two models incubated at 15°C containing *K. lactis* alone were exceptions and clustered with models inoculated with samples inoculated with solely *P. roqueforti* and those of controls. Also presenting a similar aroma to models containing *P. roqueforti* alone were models inoculated at $1x10^2$ cells mL^{-1} and incubated at 5°C. This cluster has a lower proportion of compounds produced during fermentation, shown upon PC1 (Figure 2.8).

The average coefficient of variation of peak areas recorded by SPME GC-MS analysis was lower in samples containing *P. roqueforti* at 32%, compared to 43% in samples containing *K. lactis* alone. This contrasts to the variation observed in aroma profiles of replicate samples, with samples containing *P. roqueforti* dispersing more when plotted following PCA analysis (Figure 2.8). Incubation temperature had little impact upon variation in amount of aroma compounds produced with models incubated at 5°C showing 36% CV and models incubated at 15°C presenting a CV of 38% (Appendix 14).

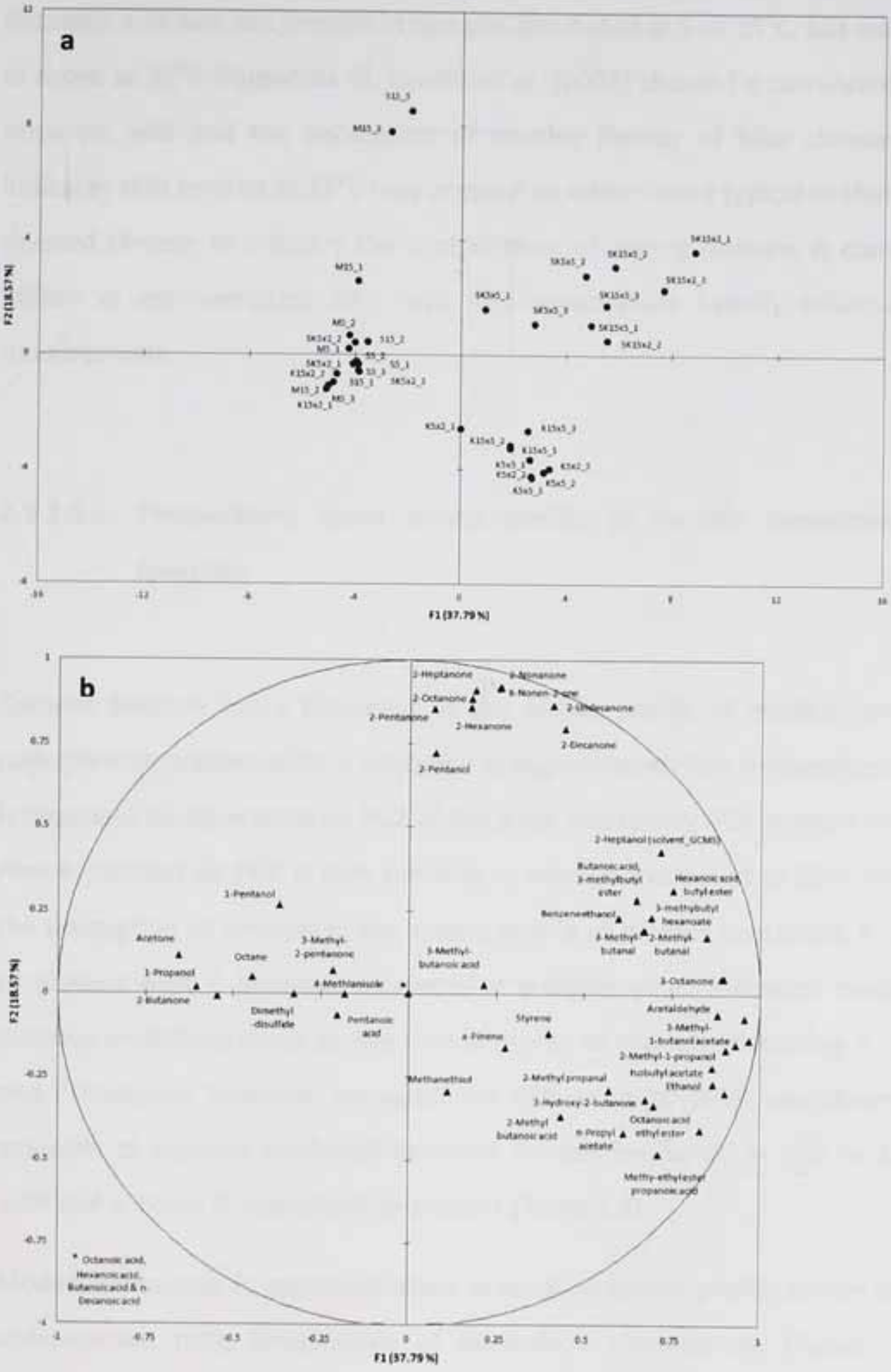


Figure 2.8: Bi- plots of SPME GC-MS analysis of models containing *K. lactis* inoculated at different concentrations with and without *P. roqueforti* at 1x10^5 cells mL^{-1}, and incubated at 5°C and 15°C (a) bi-plot of samples; (b) variables plot.

S: *P. roqueforti* spores, K: *K. lactis*, M: Milk only. 5/15 : 5°C/15°C incubation temp. x2/x5 : Yeast inoculation concentration of 1x10^2 or 1x10^5 cells mL^{-1}.

Butanoic acid was not present in samples incubated at 5 or 15°C, but was recorded in those at 25°C (Appendix 7). Lawlor *et al.* (2003) showed a correlation between butanoic acid and the perception of mouldy flavour of blue cheeses and this indicates that models at 25°C may present an odour more typical to that of mould-ripened cheese. In industry the temperature of during ripening is controlled, for Stilton at approximately 10°C and this temperature heavily influences aroma development.

2.3.2.3.2 Temperature upon aroma profile of models inoculated with *Y. lipolytica*

Ketones become more dominant in the aroma profile of models containing *P. roqueforti* co-present *with Y. lipolytica* at higher incubation temperatures and this is observed by separation on PC2 of the plots created by PCA analysis (Figure 2.9). Also evidenced on PC2 is that similarly to models incubated at 25°C (Figure 2.4), the proportion of ketones in the aroma profile of models containing *P. roqueforti* co-present with *Y. lipolytica* increases at a higher yeast inoculum concentration. Ketones contribute more to the aroma profile of models containing *P. roqueforti* and *Y. lipolytica*. However, no significant difference ($p > 0.05$) was observed in the amounts of ketones produced between models incubated at 5°C or 15°C, both with and without *P. roqueforti* co-present (Table 2.3).

Models containing *P. roqueforti* alone present an aroma profile similar to those of unfermented milk, irrespective of incubation temperature (Figure 2.9). This indicates that *Y. lipolytica* promotes *P. roqueforti* germination and thus enhances ketone production. A greater amount of ketones is present in all models with *Y. lipoltica* when incubated at 25°C (Table 2.2) suggesting that the influence temperature has on ketone production is greater than the role inoculum concentration plays. Models containing *P. roqueforti* showed greater variation compared to models without, with CV of 61% and 55% respectively.

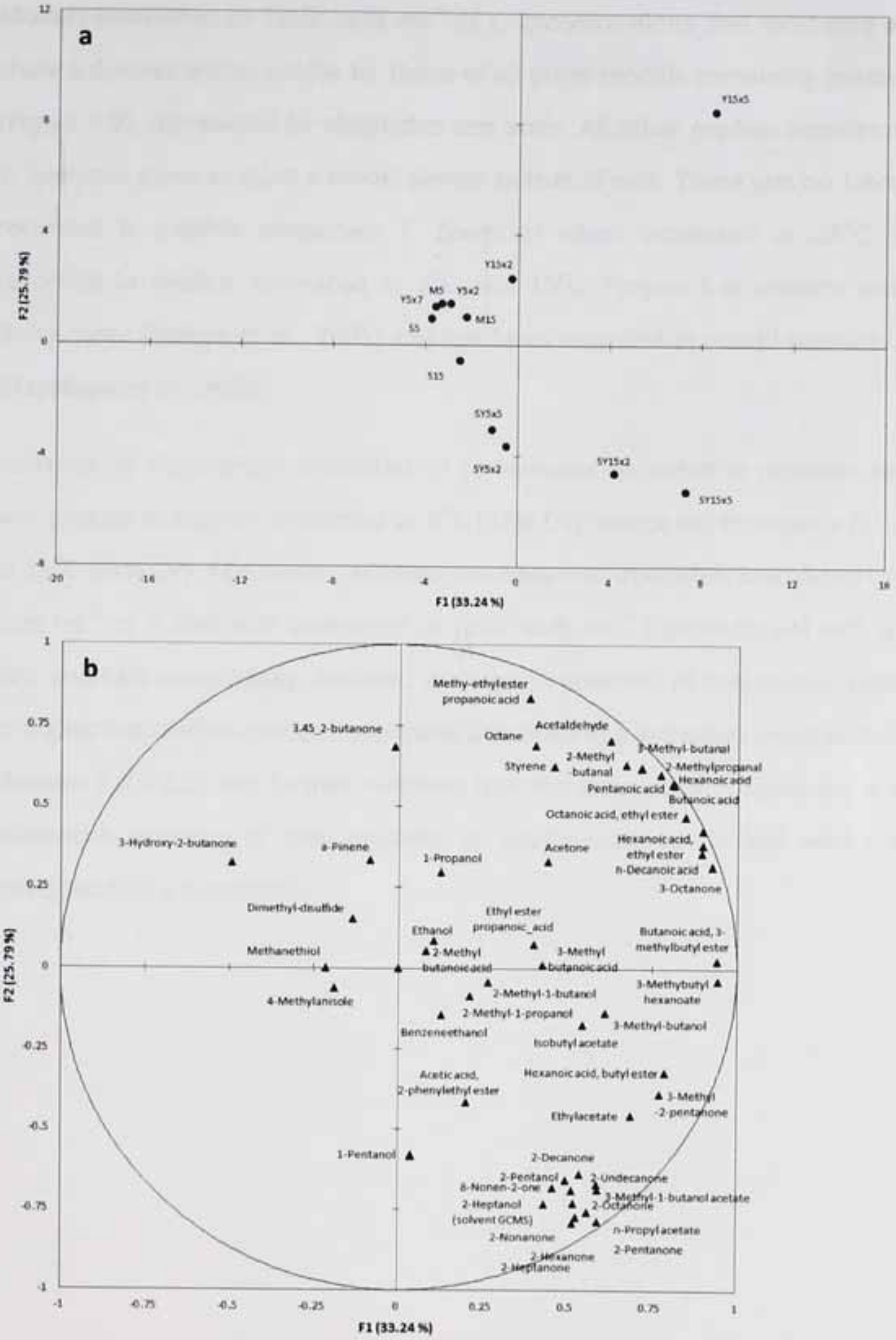


Figure 2.9: Bi- plots of SPME GC-MS analysis of models containing *Y. lipolytica* inoculated at different concentrations with and without *P. roqueforti* at 1x10^5 spores mL^{-1}, and incubated at 5°C and 15°C (a) bi-plot of samples[1]; (b) variables plot.

S: *P. roqueforti* spores, Y: *K. lactis*, M: Milk only. 5/15 : 5°C/15°C incubation temp. x2/x5 : Yeast inoculation concentration of 1x10^2 or 1x10^5 cells mL^{-1}.

[1] Replicates (3) averaged following analysis via SPME GC-MS.

Models inoculated to $1x10^5$ cells mL^{-1} of *Y. lipolytica* alone and incubated at 15°C show a distinct aroma profile to those of all other models containing yeasts alone (Figure 2.9), dominated by aldehydes and acids. All other models inoculated with *Y. lipolytica* alone present a model similar to that of milk. There was no 1-propanol recorded in models containing *Y. lipolytica* when incubated at 25°C. It was recorded in models incubated at 5°C and 15°C. Propan-1-ol imparts alcoholic, fruity notes (Barron *et al.*, 2005) and has been recorded in mould-ripened cheese (Hayaloglu *et al.*, 2008).

Variation in the average quantities of compounds recorded in replicate samples was greater in models incubated at 5°C (61% CV) compared to models incubated at 15°C (55% CV). Also lower variation was observed in models inoculated to $1x10^5$ cells mL^{-1} of *Y. lipolytica* compared to $1x10^2$ cells mL^{-1} (Appendix 14) with a CV of 52% and 64% respectively. Reduced variation in amounts of compounds measured at higher inoculation concentration was also observed in models incubated at 25°C (Section 2.4.2.2.2) and further indicates that the amount of *Y. lipolytica* in Stilton influences variation of the amounts of aroma compounds and which aroma compounds are generated.

2.4 CONCLUSIONS

Following incubation of each yeast species at three different concentrations in a blue cheese dairy model it has been shown that both the yeast inoculum concentration and incubation temperature influences resultant aroma profiles and variation (Section 2.4). Effects were species-specific.

Models incubated at 25°C showed distinct aroma profiles, not comparable to models incubated at 5°C and 15°C (data not shown). The amount of ketones generated in models incubated at 5°C and 15°C was significantly lower than those at 25°C. Also models incubated at 5°C and 15°C showed similar level of ketones to that produced in controls indicating that ketone production is heavily influenced by temperature. Yeasts achieved a similar concentration in models incubated at all three temperatures and this suggests that lack of *P. roqueforti* germination is the reason for lower ketone production in models incubated at 5°C and 15°C.

Accumulation of 2-heptanone and 2-nonanone has been shown to take approximately 60 days before a flavour typical of blue cheese is achieved (Dartey & Kinsella, 1971) and Stilton is ripened at approximately 10°C over a period of 10 weeks. The aroma profile from models incubated at 25°C is more similar to that of cheese on retail sale and it is suggested that in further work the incubation temperature of the model is standardised at this temperature.

The overall aroma profile of models inoculated to a high or low concentration of *Y. lipolytica* is similar however; 2-heptanone and 2-nonanone are proportionally greater in models inoculated to a higher concentration of *Y. lipolytica*. Production of 2-heptanone and 2-nonanone is enhanced when *Y. lipolytica* is co-present with *P. roqueforti* above amounts generated in models incubating *P. roqueforti* alone. Given that these two compounds are frequently cited as those most contributory to blue cheese aroma it could be theorised that a high concentration of *Y. lipolytica* enhances blue cheese aroma and suggest a synergistic interaction between *P. roqueforti* and *Y. lipolytica*. Models inoculated with *Y. lipolytica* present an aroma more similar to that of Stilton than for any other model combination (data not shown). *Y. lipolytica* is frequently isolated from blue cheese (Viljoen *et al.*, 2003) however the species is typically not identified as a dominant presence of Stilton flora (Gkaztionis, 2010). *Y. lipolytica* has been proposed to influence flavour development and quality of various blue cheeses (Addis *et al.*, 2001; Tempel & Jakobsen, 2000; Tempel, 1998) including Stilton (Gkatzionis, 2010).

The results of this work indicates that the amount of *Y. lipolytica* positively correlates with ketone production and so controlling the amount of *Y. lipolytica* present during Stilton production may allow the aroma intensity of each batch of Stilton to be manipulated towards consumers' preference.

Inoculating *K. lactis* at high concentration reduced variation in the aroma profiles observed for replicate samples when compared to models inoculated to a low concentration of *K. lactis.* Within industry ensuring a high level of *K. lactis* is present during cheese-making could potentially reduce product-to-product variation. However a high concentration of *K. lactis* may be detrimental to the sensory qualities of Stilton. Within the dairy model, inoculating *K. lactis* at high concentration reduced the proportion of ketones produced and the aroma profile was more similar to that observed in models without *P. roqueforti,* compared to models inoculated with a low concentration of *K. lactis*. If this decrease is perceivable it could mean that samples do not embody as great a blue cheese aroma.

Greater variation is noted in the amounts of aroma compounds produced between replicate samples when *P. roqueforti* is co-present in the model and this suggests that variable mould growth is a major contributory factor towards variable aroma profiles of Stilton. A high yeast concentration has been shown to reduce the variation in the quantities of aroma compounds measured in replicate samples via SPME GC-MS. Gkatzionis *et al.* (2009) recorded an average CV of 45% when analysing the aroma compounds from sections of real Stilton and analyses on models inoculated to a high concentration of *K. lactis* or *Y. lipolytica* shows similar values.

Whether the differences in aroma production, observed instrumentally, between models inoculated at high and low concentrations of *Y. lipolytica* or *K. lactis* are detectable by human perception is unknown. Therefore sensory investigation using models of *K. lactis* and *Y. lipolytica* will be conducted to understand the impact that aroma variation and ketone production have on aroma perception.

3. SENSORY INVESTIGATIONS

3.1 INTRODUCTION

3.1.1 Background

Sensory analysis involves humans evaluating the organoleptic properties of products. Sensory evaluation can provide insight into consumer preference and choice and is therefore important for product development. Aroma is a major aspect of consumer preference for cheese (Jaillais *et al.*, 1999) but perception of aroma is not well understood. Humans are unable to distinguish many individual compounds within mixtures (Qian *et al.*, 2002), smelling mixtures in a 'synthetic' manner (Cook *et al., 2005)*. Descriptive analysis of aromas collected through sensory testing may not equate to aroma perception. Aroma perception is an unclear concept and perception of a stimulus varies for each individual (Lawless, 1999). This leads to a lack of common vocabularly to describe aromas (Delarue & Sieffermann, 2004). Aroma release and perception is a temporal experience (Linforth *et al.*, 2000) adding further complexity to describing perception, as it changes over time. Whilst instrumental techniques can quantify each individual compound, how they interact in a mixture and are released during consumption is unknown.

From instrumental analysis of aroma profiles generated in models inoculated at different concentrations of *K. lactis* with *P. roqueforti* present and incubated at 25°C, results (Section 2.4.2.2.2) showed that at a high yeast inoculum concentration replicate model samples produced consistent aroma profiles whereas at low concentration replicates aroma profiles diverged (Figure 2.5). Furthermore models inoculated to 1×10^2 cells mL^{-1} produced significantly greater amounts of ketones than models which were inoculated to 1×10^8 cells mL^{-1}. When models were inoculated with *Y. lipolytica* co-present with *P. roqueforti* and incubated at 25°C, results (Section 2.4.2.2.1) showed that at higher yeast inoculum concentration the amount of 2-heptanone and 2-nonanone was greater than models inoculated to a low concentration (Table 2.2).

Conducting sensory analysis on the models would show whether these observations are perceivable by humans. This is necessary because instrumental results do not always relate to sensory perception (Cook *et al.*, 2005; Lawlor *et al.*, 2003). Comparisons of instrumental and sensory data have previously been applied for real cheese (Breuil & Meullenet, 2001; Lawlor *et al.*, 2001; Noël *et al.*, 1998), including blue varieties (Lawlor *et al.*, 2003) and cheese models (Martin *et al.*, 2002). These studies assosciated sensory attributes with the gross composition or volatile compounds of cheeses. All found that human perception of attributes cannot be fully explained or predicted from the instrumental data, indicating that further research is needed to fully understand the nature of sensory perception and the relationship to instrumental measures.

3.1.2 Descriptive tests

3.1.2.1 Flash profile

Different methods of collecting sensory data exist with test procedures developed on the basis of sample size, budget, data desired, time contraints, resources available and other factors; and using an appropriate method is vital (Issanchou *et al.*, 1997).

The Flash profile (FP) method, developed by Sieffermann (2000) is a variant of free choice profiling (FCP). With the option to use trained or untrained panellists, products are evaluated simultaneously and the method is simple, cheap and fast to conduct (Delarue & Sieffermann, 2004). Within FP panellists are free to generate descriptive attributes of their choice, avoiding hedonic terms; and then rank each product for each attribute. Individual responses are gathered and analysed using only the terms which discriminate between products. Generalised Procrustes Analysis (GPA) standardises the scale and terms used by individual panellists allowing uniform comparisons across data gathered for each product.

Information gathered from FP can be limited as only products in the same study can be compared since no nominal scale for intensity of each attribute is assigned (Delarue & Sieffermann, 2004). Also comparisons upon the samples are attribute specific and each attributes' weighting, or importance, is not reflected. However, when evaluating many products the FP method can prove to be more feasible than other techniques.

Gkatzionis (2010) carried out flash profile (FP) analysis comparing blue cheese model samples of *Y. lipolytica* with *P. roqueforti* to that of real cheeses, showing that the combination of yeast and mould present stronger 'blue cheese' notes than *P. roqueforti* models alone and greater than real Stilton.

3.1.2.2 Napping®

Napping® is rapid procedure which generates a relative spatial arrangement of the samples in a consensus configuration which represents panellists' perception. Napping® relies on panellists placing products within two dimensions based upon how similar they perceive them to be and using whatever criteria they individually wish. Multiple factor analysis (MFA) is used to generate a consensus map of products based upon all panellists' responses. MFA is a global analysis method which allows every panellist's differing evaluation of the same data set to be represented. Initially PCA upon each panellist's evaluation is performed and the data generated normalised and compiled into a global data set. PCA is then performed upon this global data set to generate the consensus map (Pagès, 2004).

Napping® has been shown to be advantageous compared to sorting procedures (King *et al.*, 1998) and similarity scaling (Risvik *et al.*, 1997) for evaluation of product sets where samples are similar. Nestrud & Lawless (2010) used the approach on an assortment of cheddar cheeses and Napping® creates interpretable product spaces from a limited number of expert panellists, providing they give some descriptors for each product during evaluation (Perrin & Pagès, 2009). Kennedy & Heymann (2009) used Napping® to evaluate chocolate and demonstrated that projective mapping can create equivalent maps to descriptive analysis using an untrained panel.

3.1.3 Discrimination testing

All the discrimination methods employ statistical analyses to reject a null hypothesis: that no difference is perceivable. They require a large number of panellists in order to have statistical confidence as the nature of the tests mean panellists can potentially guess their response (Kemp *et al.,* 2009). Using untrained panellists allows the assembly of a large panel quickly and is far easier, cost-effective and time-saving than training panellists.

3.1.3.1 Triangle tests

Triangle tests involve judging three unknown samples, where two of the samples are the same. The panel is asked to identify which sample is the odd-one-out in order to assess whether a difference is distinguishable. However, panellists have a one in three possibility ($p=1/3$) of guessing the correct answer.

Leuven *et al.* (2010) used triangle test with 15 panellists to determine if a difference in the aroma between semi-hard cheeses packaged under modified atmosphere and those without was perceivable and demonstrated that sensory results were in accordance with instrumental analysis of volatiles.

3.1.3.2 Paired comparison

Paired comparison tests ask the panel to directly compare each of the samples for certain properties or characteristics. Panellists only have a choice of two samples (p=0.5). Products are directly compared making the test suitable for determing if differences in the specific attributes of products are detectable (Kemp *et al.*, 2009).

The intensity of fruit flavour of milk-based samples have been analysed by paired comparison tests before and results were in agreement with the instrumental analysis (Shojaei *et al.*, 2006).

3.1.3.3 Constant reference

Constant reference tests are used to compare samples against that of a standard to assess how different from the standard samples are. Samples are ranked in relation to that of one provided as a reference. Constant reference analyses are commonly used in sensory tests (Kemp *et al.*, 2009) and cheese grading involves comparison to reference cheeses chosen as a standard (Fox *et al.*, 2000).

3.2 AIM OF SENSORY ANALYSIS

The aim of the sensory study was to identify whether the differences in the aroma profiles observed from SPME GC-MS analysis of models inoculated with *P. roqueforti* and different concentrations of *Y. lipolytica* (Section 2.4.2.2.1) *or K.lactis* (Section 2.4.2.2.2) and incubated at 25°C, are perceivable.

Flash Profile sensory analysis and Napping® were used to investigate whether humans can detect variation between the aromas generated in model replicates inoculated with *K. lactis* at high concentration compared to models inoculated at low concentration.

Triangle tests investigated whether differences in the aroma profiles of models inoculated with *Y. lipolytica* at different concentrations are detectable and paired comparison tests used to determine if there is a difference in the aroma intensities. Finally constant reference testing was peformed to investigate the similarilty of *Y. lipolytica* models at different concetrations to real blue cheese aroma.

3.3 METHODS

3.3.1 Model preparation

Models of *P. roqueforti* at $1x10^5$ spores mL^{-1} co-inoculated with *Y. lipolytica* or *K. lactis* at 10^8 or 10^2 cells ml^{-1} (400 mL in 1L bottles) were prepared in triplicate as described in Section 2.3.1. After incubation samples (15 mL) were aseptically transferred into 50 mL Falcon tubes (Fisherbrand) and frozen at -80°C. Samples were defrosted and then transferred into 30 mL opaque sealed glass bottles, to conceal their contents. Each sample was marked with a 3-digit random code.

3.3.2 Sensory facilities

All the sessions were conducted in standard individual sensory booths at the Sensory Science Centre, part of the Division of Food Sciences, University of Nottingham which conform to International Standards (ISO 8589: 1988).

3.3.3 Sensory panels

Sixty untrained panellists aged 18 to 72 participated in the discrimination tests. Untrained panellists were chosen as a large number of panellists are required for discrimination tests.

A panel comprising of 10 members (panellists), 8 women and 2 men, from 58 to 73 years old, trained in the evaluation of food products was employed for the Napping and Flash Profile analysis. These studies concerned variation in replicate samples. This decision to use a trained panel was based upon the fact a trained panel are more like to identify subtle differences between replicate samples in a reliable reproducible manner (Worch *et al*,, 2010).

3.3.4 Discrimination tests

For the discrimination tests the panel was split into three blocks of 20 panellists and each block analysed one set of replicate models i.e. one model containing $1x10^8$ cells mL^{-1} yeast was evaluated with the same respective $1x10^2$ cell mL^{-1} model. This was important as variation between replicate samples were being investigated as it allows comparison between individual replicates at each concentration.

Panellists were given a brief outline of the procedure prior to each session and were allowed breaks between each sensory test. Panellists were informed that the aroma of samples regarded blue cheese and informed to smell the samples without looking into the containers.

The ordering of samples for each block of panellists was generated via Fizz Sensory Analysis software (BioSystems, Couternon, France). Panel responses were collected on paper data recorded in Microsoft Excel 2010 (Microsoft, Washington, USA) and results analysed using XLSTAT-MX (Addinsoft). Results were analysed for each block of panellists i.e. between each individual replicate sample, and with responses of all sixty panellists totalled i.e. average for each model. A box for comments was included on the data collection paper of every test to allow further insight into panellist's perception.

3.3.4.1 Triangle test

The procedure followed the International Standard methods (BS ISO 4120:2004). Three model samples were simultaneously presented to each panellist, amongst which two were the same just with different codes. Panellists were asked to identify which of the three samples was the odd-one-out and to guess if they could not. Panellists were informed to sniff samples in the order presented (left to right) but could re-smell samples if desired (Appendix 15). The sessions lasted 5-10 mintues.

3.3.4.2 Paired comparison

The British Standard method (BS ISO 5495:2007) was followed. Panellists were provided with two samples simultaneously, one at each inoculum concentration. Panellists were asked to identify which sample had the 'most intense aroma' (Appendix 16). Panellists were asked to smell samples left-to-right as presented and were allowed to re-smell samples. Each session lasted approximately 5 minutes.

3.3.4.3 Constant reference

Reference samples composed of 2.5g Danish Blue cheese left to equilibrate at 22°C as for models. The chosen amount of cheese gave comparable aroma intensity to that of the model samples. Reference samples were labelled as 'REF' and panellists were informed that each model sample would be compared to this reference. Further samples of Danish Blue cheese were prepared and were given random three digit codes to act as an internal blind control. All sample bottles in this test were covered with foil to conceal the contents and the panellists were asked to smell the samples without looking in the containers.

Each panellist was provided with the identified reference sample and 3 coded test samples: a model at each of the inoculum concentrations and a blind control. Panellists were asked to acquaint themselves with the aroma of the reference sample. Following this they were then asked to smell each test sample in turn (left-to-right as presented) and determine if the aroma differs from the reference sample (Appendix 17). Panellists could re-smell samples if desired but were asked to reacquaint with the reference sample before doing so. Panellists were asked to indicate the magnitude of difference on the scale provided. Ranking procedure followed the British Standards methodology (BS ISO 8587:2006).

3.3.5 Napping® procedure

3.3.5.1 Napping® data collection

The procedure performed was based on Perrin & Pagès (2009). Panellists were given a brief outline of the procedure prior to each session. They were provided with 60 x 40 cm blank paper and simply informed to smell all the samples and place them physically on the paper with similar samples being closer together and those differing further part. Panellists were informed that the distance between samples represented the degree of similarity and that how they perceived similarities was their choice.

Samples were presented simultaneously and panellists could smell samples in any order and as many times as they wished, re-arranging their map with no time constraints. After concluding their configuration they wrote the corresponding product codes where they positioned each sample along with a few descriptors of the overall aroma and the differences from samples at differing positions. Napping® was conducted twice with a one day gap in between sessions. Sample codes were independent for each Napping® session.

The co-ordinates of samples on each panellist's map were recorded. MFA analysis was conducted in XLSTAT-MX 2012 (Addinsoft) to give a consensus spatial arrangement. The attributes that each panellist chose to describe samples were prospectively added onto the global map.

3.3.6 Flash profile procedure

3.3.6.1 Flash profile data collection

The procedure performed was based on Delarue & Loescher (2004). The flash profile analysis consisted of three sessions. To introduce the Flash Profile technique, the panellists were given a brief outline of the procedures prior to each session. During all sessions the panel was informed that the samples were related to cheese aroma but there was no information on the individual characteristics of each sample. During the first session each panellist had to smell the samples and individually generate their own provisional list of attributes that best described the differences between the aromas of the samples. All six samples were presented simultaneously. There was no limitation regarding the number of sensory attributes that they could generate but they were instructed to avoid hedonic terms. The panellists were asked to focus on attributes that discriminate/characterise the overall set of the samples and not on those which concerned individual or a few samples. This session lasted about 30 min.

Between the first and the second session the attributes generated by the whole panel were pooled and presented in a single list. At the beginning of the second session, each panellist had to choose their definitive list of attributes from the pooled list. They were asked to read the panel's list and, if desired, to review and update their personal list by adding, excluding or replacing attributes. Then the panellists proceeded to the evaluation of the samples on a ranking mode, using their own definitive list of terms. All six samples were presented simultaneously in a randomised order.

A 170 mm scale was used for each attribute, marked at the left end with '-' for the attribute not perceived and at the right end '+' for the attribute strongly perceived. Ties were allowed. The panellists could smell the samples as many times as they liked. Pauses were allowed during the evaluation and the panellists could take as much time as they needed to evaluate them. The third session was a repeat of the second session. The time length of the evaluation sessions (2 and 3) varied for each panellist. The panellists did not necessarily participate in the sensory sessions at the same time but they all had to wait for the whole panel to complete the first session before proceeding to the following sessions in order to ensure that attributes from the whole panel were communicated to each member.

During all sessions panellists could smell the samples as many times as they wanted but were not allowed to taste the samples or look inside the container. Within the flash profile sessions, codes for attribute generation were independent and during attribute ranking sample codes changed after the evaluation of two attributes. Different codes were also used for repeated rankings. Samples were also presented in randomised placements. To prevent carry over effect during the two attributes being ranked simultaneously, for the second ranking panellists were asked to rank attributes in a different combination and also each panellist ranked attributes in a different order.

3.3.6.2 Flash Profile data treatment

The discrimination efficiency of the attributes for each panellist was tested by a one-way analysis of variance (ANOVA) on the rank data. Attributes that were found not to discriminate the samples were excluded from the concerned panellist's list. Panellists' repeatability between the two sessions was tested by Spearman correlation test. Only the attributes with reproducible ranking between the sessions were considered. Panellists with poor overall performance were excluded from the data set. Generalised Procrustes Analysis (GPA) was applied for the consensus configuration between panellists' sensory maps. The GPA calculates a consensus from data matrices of a sensory profiling experiment. In the case of Flash profile a data matrix corresponds to each panellist. The GPA plot demonstrates how similar or different the samples were to each other according to their schematic interpretation. The data were collected on Microsoft Excel spreadsheets. ANOVAs and Spearman correlation tests were performed with

XLSTAT PRO (Addinsoft); and GPAs were performed with XLSTAT-MX (Addinsoft). Pearson correlations were calculated to relate the volatiles recorded from SPME GC-MS to the sensosry attributes of the Flash Profile.

3.4 RESULTS

3.4.1 Sensory evaluation of models inoculated with *P.roqueforti* and *Y. lipolytica* at different concentrations

3.4.1.1 Triangle test

Triangle tests gave very strong evidence (alpha<0.001) that the aroma profiles generated in models of *P. roqueforti* and different concentrations of *Y. lipolytica* are distinguishable (Table 3.1). For two blocks of replicate samples, 13 of the 20 panellists correctly identified which sample was the odd-one-out and (α-level of 0.01) data from the third set of replicates shows even greater discernibility (alpha < 0.001). When results from the three replicate sets are totalled, 42 panellists out of 60 correctly identified which sample was different within the set. Instrumental analysis (Section 2.4.2.2.1) showed that these models deviate in the amount of ketones produced (Table 2.2) and also the proportion of 2-heptanone and 2-nonanone within the whole aroma profile (Figure 2.4).

The vocabulary generated showed that the majority of panellists easily distinguished between the aromas of models inoculated at high or low concentration of *Y. lipolytica*, with *P. roqueforti* co-present. Comments (Table 3.2) showed mixed responses and highlighted the variation in aroma perception of each panellist. Samples at a low concentration of *Y. lipolytica* were described as '*creamy*', '*fruity*', and '*sweet*' and ocassionally as '*Stilton*' itself. Samples at a high concentration were described as '*mouldy*', '*mushroom*', '*nutty*' and '*ammonia*'.

Sensory tests indicate that changes in the aroma of models inoculated with *Y. lipolytica* to different concentrations are perceivable, suggesting that the composition of ketones may be a key factor determining aroma and flavour aspects of Stilton.

In industry the level of *Y. lipolytica* in dairies is not controlled. Results suggest that differences in the concentration of *Y. lipolytica* in Stilton may be perceivable.

Table 3.1: Results of triangle test on models inoculated with *P.roqueforti* and *Y. lipolytica* to a high and low concentration[1].

Triangle test	Correct response	α-level
Rep 1vs 1	13	0.01
Rep 2 vs 2	13	0.01
Rep 3 vs 3	16	<0.001
Total[2]	42	<0.001

[1] *Y. lipolytica* inoculated to $1x10^2$ and $1x10^8$ cells mL^{-1} with *P. roqueforti* at $1x10^5$ spores mL^{-1} co-present. Models incubated at 25°C for 10 days.

[2] Sixty panellists participated overall. Twenty panellists evaluated each set of replicate samples.

Table 3.2 –Comments about aroma of samples recorded during triangle discrimination test on models inoculated with *P. roqueforti* and *Y. lipolytica* to a high and low concentration[1].

Y. lipolytica at $1x10^5$ cells mL^{-1}	*Y. lipolytica* at $1x10^2$ cells mL^{-1}
Lactic acid	Weaker (3)
Cheddar	Blue cheese (9)
Intense (2)	Less sour
Smelly socks	Ripe
Less pungent (4)	Intense
Blue cheese (7)	Stronger (4)
Cheesy (3)	Chemical (3)
Nutty	Stilton (3)
More pungent	Fruity
Processed	Sweeter
Cheese puffs	Sharper
Mouldy	Acidy
Mushroom	Savoury
Mini cheddars	Goats cheese
Alcoholic	Creamy
Stronger	Alcoholic
Acrid	
Ammonia	

For attibutes reported multiple times, the number of times is indicated in brackets.

[1] *P. roqueforti* at $1x10^5$ spores mL^{-1} co-present. Models incubated at 25°C for 10 days.

3.4.1.2 Paired comparison

A two-sided paired test was performed in order to investigate whether there are perceivable differences in the intensity of aroma between models inoculated with *P. roqueforti* and different concentations of *Y. lipolytica*. Responses showed that overall more panellists' perceived models inoculated at $1x10^2$ cells mL^{-1} as presenting a more intense aroma than those at $1x10^8$ cells mL^{-1} (Table 3.3). However, the differences were not statistically significant.

Replicate set 2 (Table 3.3) showed that 14 of 20 panellists perceived models inoculated at $1x10^2$ cells mL^{-1} of *Y. lipolytica* to have a more intense aroma than those at $1x10^8$ cells mL^{-1}, giving a significance level of α=0.2. Models of replicate sets 3 showed less distinguishability (α>0.2) with 13 panellists perceiving models at $1x10^2$ cell mL^{-1} of *Y. lipolytica* to be ore intense. In contrast, 12 of the 20 panellists which evaluated replicate set 1 perceived the models inoculated to $1x10^8$ cells mL^{-1} of *Y. lipolytica* to have a more intense aroma than models at $1x10^2$ cells mL^{-1}. This could be the result of individual panellists having different perception of aroma intensity and the sensory characteristics that define it. Alternatively, as the test was a forced choiced method and the response did not support a statistically significant difference being perceivable, it could mean that judges were simple guessing.

By relating comments from triangle tests (Table 3.1) to results of the paired comparison it would appear that creamy, fruity odours are more often percieved as intense (describing models at low concentration of *Y. lipolytica*) than mushroomy and nutty character (describing models at a high concentration of *Y. lipolytica*). However, as responses from the paried comparison tests did not show a statistically significant difference is perceivable, interpretation of written comments with regards to aroma intensity is only speculative.

Overall, models at both concentrations of *Y. lipolytica* present aromas of similar intentity. This suggests that differences in the amount of *Y. lipolytica* in Stilton may not affect the intensity of the aroma of the cheese.

Table 3.3: Results from paired comparison tests investigating whether a difference in aroma intensity is perceivable[1] between models inoculated with *P. roqueforti* and *Y. lipolytica* at high or low concentration[2].

Paired Comparison-More intense?	*Y. lipolytica* inoculum concentration (cells mL^{-1})		Statistically significant? (α=0.05)[4]
	$1x10^8$	$1x10^2$	
Rep 1vs 1	12	8	No
Rep 2 vs 2	6	14	No
Rep 3 vs 3	7	13	No
Total[3]	25	35	No

[1] Panellists were asked to identify which sample had the 'more intense' aroma.

[2] *Y. lipolytica* inoculated to $1x10^2$ and $1x10^8$ cells mL^{-1} with *P. roqueforti* at $1x10^5$ spores mL^{-1} co-present. Models incubated at 25°C for 10 days.

[3] Sixty panellists participated overall. Twenty panellists evaluated each set of replicate samples.

[4] Two tailed test, responses compared to stastical table in BS ISO 5495:2007.

3.4.1.3 Constant reference

Model samples of *P. roqueforti* and *Y. lipolytica* at high or low concentration were compared to real Danish Blue using a provided scale (Appendix 17). The frequency of response for each rank was recorded (Table 3.4). Data recorded for both model samples did not follow normal distribution (Appendix 18). Panellist's responses comparing model samples to the reference may not show normal distribution due to panellists finding the samples difficult to evaluate or from the comparison scale being open to individual interpretation and not a standardised rating measurement. Responses for comparisons of the internal blind reference also did not present a normal distribution. Due to the data not being normally distributed, each response was assigned a numerical value for degree of difference from blue cheese reference aroma and analysed via ranking methods.

Friedman's test upon the data showed that, when replicate sets were totalled, models were deemed not to come from the same population (p-value <0.0001) (Appendix 19). Individual analysis upon each block of replicates showed that samples of replicate set 1 could have been from one population, with a possible error of 12% to assume that samples were distinguishable. This means that panellists of this sample block could not easily distinguish whether the samples were different from one another and the internal reference; or that panellists perceived that the aroma of all samples in replicate set 1 were similar to the reference. Friedman's test upon model replicate sets 2 and 3 (Appendix 19) showed that for both sets of models, samples were deemed to be from significantly different populations (p-values of 0.002 and 0.010 respectively) showing that panellists perceived that the aroma of model samples differed from the reference (Danish Blue aroma).

Table 3.4: Response frequencies[1] from constant reference tests comparing the aroma generated from models containing *P. roqueforti* and *Y. lipolytica* at high and low concentration[2] to that of a typical blue cheese aroma[3].

Constant Reference – Comparison to typical blue cheese aroma	**Response Frequency**		
	***Y. lipolytica* at $1x10^8$ cells mL^{-1}**	***Y. lipolytica* at $1x10^2$ cells mL^{-1}**	**Blind Ref.**
No difference	3	3	17
Very slight difference	10	5	19
Slight / moderate difference	9	22	13
Moderate difference	8	10	4
Moderate / large difference	13	6	3
Large difference	11	8	3
Very large difference	6	6	1

[1] Sixty panellists evaluated the models. Three replicate sample sets were evaluated by 20 panellists each.

[2] *Y. lipolytica* inoculated to $1x10^2$ and $1x10^8$ cells mL^{-1} with *P. roqueforti* at $1x10^5$ spores mL^{-1} co-present. Models incubated at 25°C for 10 days.

[3] Danish Blue cheese was used as the blue cheese aroma reference

ANOVA showed that aroma perception of models inoculated to $1x10^8$ and $1x10^2$ cells mL^{-1} of *Y. lipolytica* both deviated from the blind reference and thus are thought to present an aroma less like that of blue cheese (Table 3.5). Models inoculated to $1x10^8$ cells mL^{-1} deviate more than those at $1x10^2$ cells mL^{-1}, but the difference between the two is not significant and therefore neither is perceived as being more or less like blue cheese aroma. ANOVA of all individual responses between the replicate sets showed that each session was not significantly different ($p<0.05$) and thus results are comparable for all three set of replicate models (Appendix 20). Results suggest that different levels of *Y. lipolytica* in Stilton may not affect the like-ness to a blue cheese aroma.

Table 3.5: ANOVA from constant reference test on aroma of models[1] inoculated with *P. roqueforti* and *Y.lipolytica* at high and low concentration[2] compared models to a real blue cheese[3].

Q1 / Fisher (LSD) / Analysis of the differences between the categories with a confidence interval of 95%:

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
High vs Ref	35.000	7.526	2.448	0.000	Yes
High vs Low	5.333	1.147	2.448	0.295	No
Low vs Ref	29.667	6.379	2.448	0.001	Yes

Category	LS means	Groups	
High	65.000	A	
Low	59.667	A	
Ref	30.000		B

Q1 / Dunnett (two sided) / Analysis of the differences between categories and the control category Q1-Ref with a confidence interval of 95%:

Category	Difference	Standardized difference	Critical value	Critical difference	Pr > Diff	Significant
Ref vs High	-35.000	-7.526	2.863	13.314	0.001	Yes
Ref vs Low	-29.667	-6.379	2.863	13.314	0.001	Yes

[1] Sixty panellists evaluated the models. Three replicate sample sets were evaluated by 20 panellists each.

[2] *Y. lipolytica* inoculated to $1x10^2$ (Low) and $1x10^8$ cells mL^{-1} (High) with *P. roqueforti* at $1x10^5$ spores mL^{-1} co-present. Models incubated at 25°C for 10 days.

[3] Danish blue cheese was used as the reference sample (Ref).

3.4.1.4 Conclusions of sensory analysis of *Y. lipolytica models*

Discrimination testing demonstrated that the difference between the aroma profiles of models inoculated at high and low concentrations of *Y. lipolytica* co-present with *P. roqueforti* and incubated at 25°C is detectable by most panellists (Section 3.4.1.1). This suggests that the concentration of *Y. lipolytica* in Stilton could influence the aroma perception.

From instrumental analysis, the levels of ketones and especially 2-heptanone and 2-nonanone were significantly greater in models inoculated at high concentration of *Y. lipoltyica* (Table 2.2). However, following paired comparison testing the difference between models inoculated at high or low concentration of *Y. lipolytica* was not found to regard the aroma intensity (Section 3.4.1.2). This suggests that differences in the amounts of some aroma compounds are difficult to detect. Laska & Hubener (2001) demonstrated that humans cannot distinguish between 2-heptanone and 2-octanone, or 2-nonanone and 2-decanone. Instrumental data showed that between samples of high and low *Y. lipolytica* concentration the proportion of these ketones were altered (Figure 2.4) and 2-heptanone and 2-nonanone are considered most important to blue cheese aroma (Frank *et al.*, 2004; Urbach, 1997).

In addition, the aroma of each model samples was compared to that of Danish Blue cheese. Danish Blue was chosen as it presented a 'typical' blue cheese aroma in sensory studies (Chambers *et al.*, 2005; Lawlor *et al.*, 2003). Neither sample was perceived to embody a more similar blue cheese aroma than the other.

The level of *Y. lipolytica* in Stilton is not controlled and results suggest that the aroma of Silton cheese with different concentrations *of Y. lipolytica* may be distinguishable however; the potential nature of this difference is unknown.

3.4.2 Sensory evaluation of models containing *P. roqueforti* and *K. lactis* at different concentrations

3.4.2.1 Napping®

Panellists evaluated the aroma profiles generated from blue cheese models inoculated with *K. lactis* at $1x10^8$ and $1x10^2$ cells mL^{-1+} co-present with *P. roqueforti* by the Napping® method on two occasions. Consensus projective maps (Figure 3.1) show both evaluations are in agreement presenting a clear divide between samples with different concentrations of *K. lactis*. Variation between each set of replicates alters only slightly between the two sessions. Most notable is that in session 1, replicates 'K^2a' and 'K^2c' were similar to one another than replicate 'K^2b'; yet in session 2 replicates 'K2^b' and 'K^2c' are perceived to be more alike. No difference is observable between the degrees of variation of replicates of the same yeast concentration.

Samples at $1x10^8$ cells mL^{-1} were described as *'fruity'*, *'grassy'*, *'ester'*, *'mild'*, *'acidic'*, *'floral'*, *'beer'*, *'milky'* and *'cleaning fluid'*, while samples at $1x10^2$ cells mL^{-1} were characterised as *'mouldy'*, *'sharp'*, *'blue cheese'*, *'malty'*, *'mushrooms'*, *'sweaty socks'* and *'ammonia'*. Instrumental findings showed that the aroma profile of samples inoculated to $1x10^2$ cell mL^{-1} of *K. lactis* was dominated by ketones (Figure 2.5) and sensory panel members assigned terms to these samples which relate to description of blue cheese aromas (Chambers *et al.*, 2005).

Also, instrumental data showed that replicate samples of models inoculated at $1x10^8$ cells mL^{-1} had highly similar aroma profiles whereas the aroma profiles of replicates of models inoculated at $1x10^2$ cells mL^{-1} presented variation (Figure 2.5). This was not perceivable by humans (Figure 3.1) and suggests that enforcing a high concentration of *K. lactis* may not reduce variation in the aroma profiles of Stilton cheeses. However, differences in the aroma between models at high and low concentration of *K. lactis* are perceivable and results suggest that a low concentration of *K. lactis* in Stilton may be beneficial to production of blue cheese aroma.

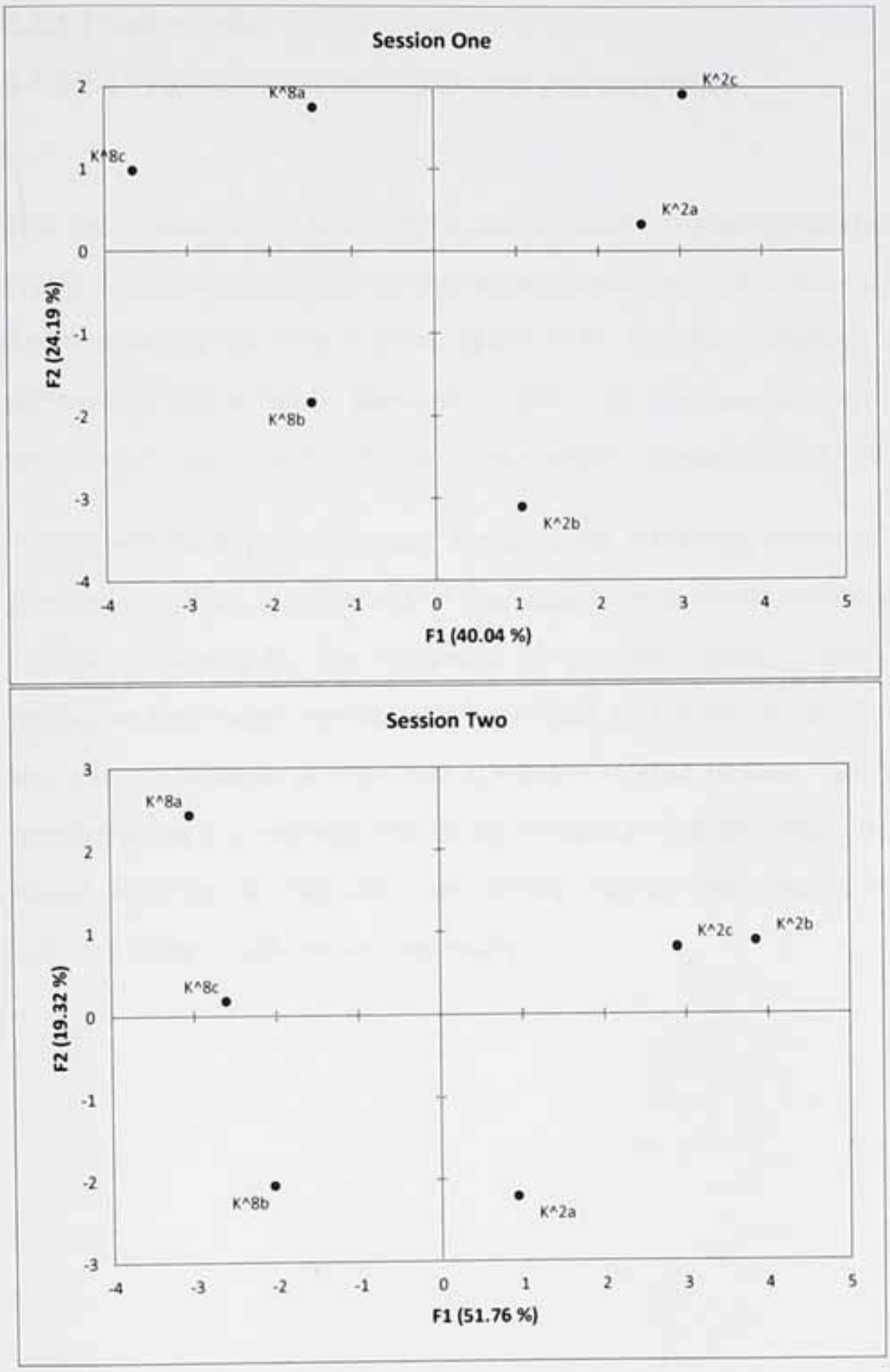


Figure 3.1: Plots showing consensus maps generated from Napping® analysis on aroma generated in models inoculated with *K. lactis at* different concentrations with *P. roqueforti* co-present at $1x10^5$ spores mL^{-1} and incubated at 25°C for 10 days.

K^8: K. lactis inoculated at $1x10^8$ cells mL^{-1}. K^2: K. lactis inoculated at $1x10^2$ cell mL^{-1}

a,b,c: Replicate samples

3.4.2.2 Flash profile

3.4.2.2.1 Panellists' discrimination and reproducibility

The first session of the Flash profile analysis of the models generated 65 attributes (Table 3.6). Following this 38 terms were chosen for ranking the models with each panellist opting for 7 or 8 terms (Table 3.7). The discrimination ability of each attribute varied between panellists (Table 3.8). The panellists generated 5 to 7 terms which significantly differentiated samples, as assessed via ANOVA ($p<0.05$).

The reproducibility of panellists' rankings for attributes was variable. Following Spearman analysis the rankings of four panellists were not reproducible and were excluded (Table 3.8). The remaining six panellists gave a total of 22 ranking responses that were reproducible ($p \leq 0.103$) and retained for GPA. This p-value was chosen because at this level attributes related to blue cheese aroma were discriminatory and reproducible while unrelated attributes showed much higher p-values. Also the samples were very similar making their discrimination a difficult task and using a high p-value necessary.

Table 3.6 – List of terms generated during session 1 of Flash Profile analysis on models samples inoculated with *P. roqueforti* and *K. lactis*.

Sugary	Floral	Blue Stilton
Sour	Flowery	Mouldy cheese
Ammonia	Warm Hay	Mouldy
Rancid butter	Grassy	Stale beer
Buttery	Herby	Beer
Pungent	Sage	Fermenting beer
Acid	Malt vinegar	Fermented apples
Plastic	Malt	Fruit
Emulsion paint	Vinegar	Pear drops
Paint	Cardboard	Bread
Ester	Wet cardboard	Sour bread dough
Ether-ial	Wallpaper paste	Bread dough
Cleaning fluid	Musty	Stale mouldy bread
Natural Yoghurt	Dirty washing	Digestive Biscuits
Yeasty	Sweaty socks	Compost Heap
Off milk	Edam – sweaty smell	Vegetables
Sour Milk	Strong cheddar	Asparagus
Milky	Cheddar cheese	Cooked vegetables e.g. cabbage
Creamy	Cheese	Mushroom
Reisty	Processed cheese	Mushroom – not fresh
Strong nasal vapour affecting mouth	Ripe Cheese	Dusty
Hops	Blue cheese	

Table 3.7: List of terms used by more than one panel member to rank samples during flash profile of models inoculated with *P. roqueforti* and *K. lactis* at high and low concentration[1].

Rank Attribute	No. of panellists
Blue cheese	6
Sweaty socks	5
Sour milk	4
Yeasty	4
Floral	3
Mushrooms	3
Musty	3
Stilton	3
Ammonia	2
Beer	2
Creamy	2
Emulsion paint	2
Fermenting Apple	2
Malt vinegar	2
Mouldy	2
Pear drops	2
Processed Cheese	2
Rancid butter	2
Sour bread dough	2
Vinegar	2

[1] Models were inoculated with $1x10^8$ or $1x10^2$ cells mL^{-1} of *K. lactis* co-present with *P. roqueforti* at for $1x10^5$ spores mL^{-1}, and incubated at 25°C for 10 days.

Table 3.8: F-values of ANOVA, Spearman coefficients and p-values for panellists attribute evaluations[1] by Flash Profile on models inoculated with *P. roqueforti* and a high or low concentration of *K. lactis*[2].

Panellist 1	F (95%)	Spearman coeffeicient	P
Blue cheese/sweaty socks	8.541	0.568	0.103*
Beer/yeast	0.900	0.021	0.714
Cheddar cheese	36.000	0.875	0.017*
Emulsion paint	36.000	0.875	0.017*
Creamy/milky		1.000	< 0.0003*
Grassy/herby		1.000	< 0.0004*
Flowery	4.114	0.301	0.297

Panellist 2	F (95%)	Spearman coeffeicient	P
Blue cheese	7.200	0.510	0.136
Sour Milk	1.425	0.007	0.919
Mushroom-not fresh	8.541	0.568	0.103*
Sour bread dough	1.425	0.007	0.919
Sweaty socks	0.800	0.040	0.714
Fermented apples	19.800	0.784	0.033*
Cleaning fluid	1.800	0.040	0.714

Panellist 3	F (95%)	Spearman coeffeicient	P
Rancid Butter	31.920	0.861	0.017*
Blue Stilton	2.323	0.102	0.564
Sour bread dough	2.300	0.099	0.564
Mouldy	0.550	0.138	0.497
Cooked vegetables (cabbage)	0.800	0.040	0.714
Fermenting beer	19.800	0.784	0.033*
Blue cheese	9.300	0.595	0.103*

Panellist 4	F (95%)	Spearman coeffeicient	P
Natural Yoghurt	19.800	0.784	0.033*
Vinegar	19.800	0.784	0.033*
Yeasty	1.800	0.040	0.714
Blue cheese	12.800	0.687	0.058*
Musty	2.618	0.138	0.497
Mushrooms	2.031	0.066	0.658
Sour milk	4.050	0.295	0.297

Panellist 5	F (95%)	Spearman coeffeicient	P
Sugary	0.133	0.641	0.058*
Creamy	9.086	0.605	0.103*
Floral	8.700	0.576	0.103*
Mouldy	21.771	0.802	0.033*
Fatty	1.636	0.024	0.803
Stilton	5.600	0.419	0.175
Pear drops	4.114	0.301	0.297
Rancid butter	9.000	0.585	0.103*

Panellist 6	F (95%)	Spearman coefficient	P
Blue cheese	12.982	0.692	0.058*
Off milk	9.300	0.595	0.103*
Ammonia	5.896	0.438	0.175
Ester	37.200	0.880	0.017*
Processed Cheese	0.698	0.070	0.564
Sweaty socks	14.160	0.713	0.058*
Mushroom	0.525	0.174	0.419

* Attribute used within GPA analysis.

[1]Only panellists having discriminatory, reproducible ranking descriptors are shown.

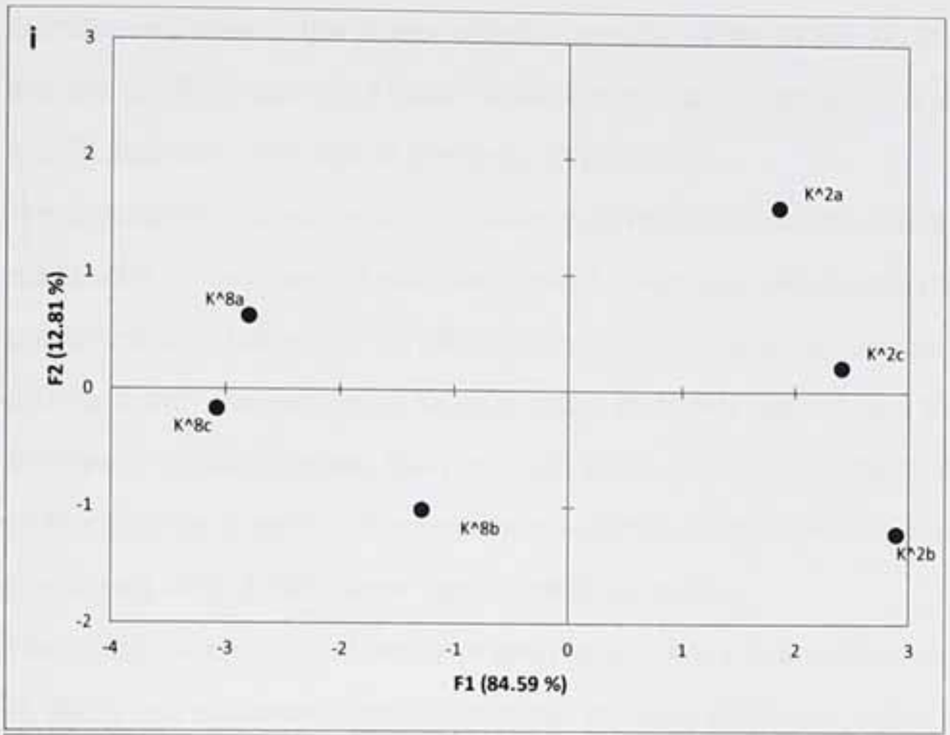
[2] Models were inoculated with $1x10^8$ or $1x10^2$ cells mL^{-1} of *K. lactis* co-present with *P. roqueforti* at for $1x10^5$ spores mL^{-1}, and incubated at 25°C for 10 days.

3.4.2.2.2 GPA

GPA plots produced from Flash profile evidence that the different inoculum concentrations of *K. lactis* in the model are recognisable (Figure 3.2). Models inoculated to $1x10^2$ cells mL^{-1} of *K. lactis* tend to the right on F1, whilst models inoculated to $1x10^8$ cells mL^{-1} sepearate to the left (Figure 3.2i). By comparing the sample plots (Figure3.2i) with the attribute plots (Figure3.2ii), *K. lactis* inoculated at $1x10^2$ cells mL^{-1} exhibited 'blue cheese' and 'rancid butter' attributes (right on Figure 3.2ii). In comparison, samples at $1x10^8$ cells mL^{-1} of *K.lactis* presented 'floral', 'grassy' 'emulsion paint' notes (right on Figure 3.2ii).

Replicate samples separate upon the F2 axes (Figure3.2i). Replicate K^8b (model inoculated to $1x10^8$ cells mL^{-1} of *K. lactis*) tends tends towards 'fermented beer' and 'vinegar' characteristics on the attribute plot (bottom left on Figure 3.2ii). Replicate K^2a (model inoculated to $1x10^2$ cells mL^{-1} of *K. lactis*) tends more towards 'creamy' attributes when compared with the attribute plot (top right, Figure 3.2ii). Interestingly these two samples were also shown to differ from their respective replicates in Napping® sessions one and two (Figure 3.1). The F2 axis represents ~13% of data.

It appears that variation between replicates is less than between the two sets of models which show a clear divide on F1 between both samples (Figure 3.2i) and majority of attributes used to describe the aroma (Figure 3.2ii). Furthermore, there is no noticeable difference in the degree of variation between replicates at each concentration, suggesting that the differences observed from SPME analysis (Figure 2.5) are not reflected in the sensory characteristics of models.



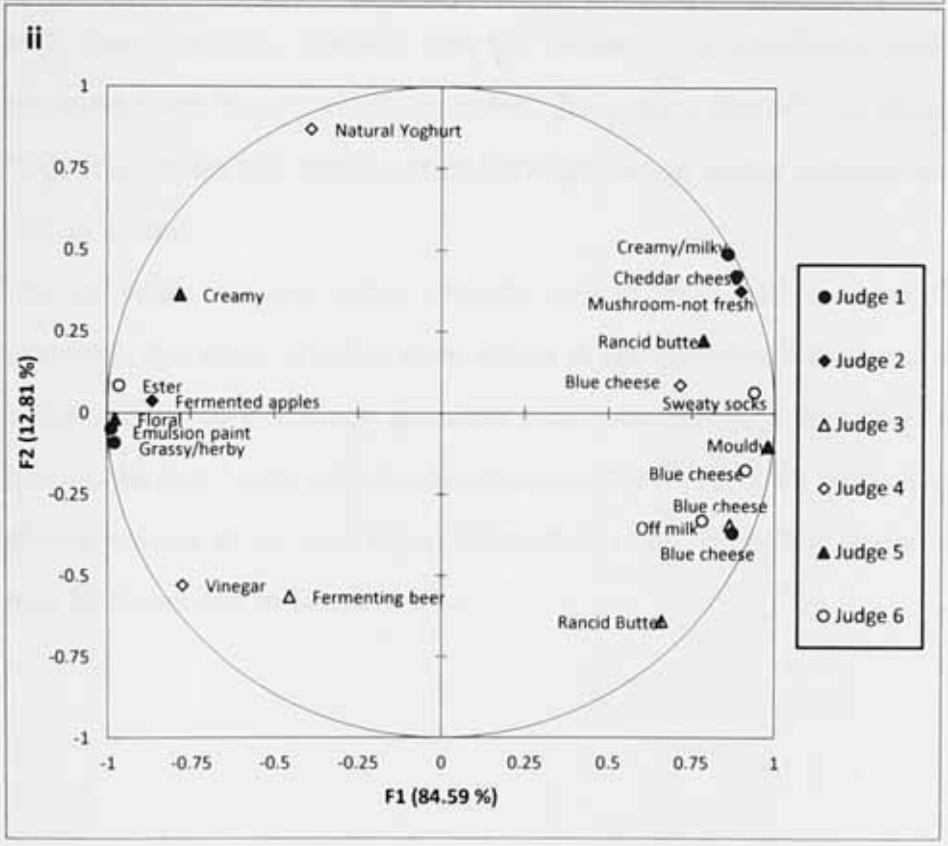


Figure 3.2: Consensus plots of Flash Profile analysis on aroma models inoculated with *K. lactis at* different concentrations with *P. roqueforti* co-present at 1x10^5 spores mL^{-1} and incubated at 25°C for 10 days.

i. consensus configuration of samples. ii. variables plot.

K^8: *K. lactis* inoculated at 1x10^8 cells mL^{-1}. K^2: *K. lactis* inoculated at 1x10^8 cells mL^{-1}.

a,b,c : Replicate samples

Correlation between the aroma volatiles recorded from SPME GC-MS (Appendix 7) and the attribute ratings of Flash Profile shows that 20 compounds significantly ($r<0.9$) associate with aroma attributes (Table 3.9).

The description 'blue cheese' is positively correlated with the ketones 2-pentanone, 2-hexanone, 2-nonanone and 2-decanone and 4-methylanisole and n-propyl acetate (Table 3.9). All these compounds, along with 2-heptanone, associate with the descriptor 'sweaty socks' and have been shown to contribute to the flavour of blue cheeses (Barron *et al.*, 2005; Lawlor *et al.*, 2001; Alonso, 1999). Of the ketones, 2-pentanone associates with the most attributes, also negatively correlating with *'floral'*, *'ester'* and *'fermented apples'*.

The volatile 2-methyl ethyl ester propanoic acid has a fruity odour (Sympoura *et al.* 2009) and associates with 8 attributes, showing significant negative correlation with 'sweaty socks' , *'cheddar cheese'*, *'mouldy'* and *'mushroom-not fresh'* and positively with *'ester'*, *'emulsion paint'*, *'fermented apples'* and *'floral'* (Table 3.9). Thus production of 2-methyl ethyl ester propanoic acid is possibly detrimental to Stilton aroma.

The attributes *'creamy/milky'* *'cheddar cheese'* and *'mushroom-not fresh'* all positively correlate with the same group of compounds: 2-Pentanol; 3-Hydroxy-2-butanone; Isobutyl acetate; Butanoic acid, 3-methylbutyl ester; 3-Methybutyl hexanoate and Acetic acid, 2-phenylethyl ester (Table 3.9). Blue cheeses are often shown to have mushroom notes (Chambers *et al.*, 2005) and these compounds may be beneficial to Silton aroma.

Table 3.9
Correlation (pearson, significant r=<0.9) of aroma volatiles recorded via SPME GC-MS to aroma attributes generated during Flash profiling of models inoculated with *K. lactis* at different concentration, with and without *P. roqueforti*

	Volatile correlation	
Aroma Attribute	Positive	Negative
Blue cheese	2-Pentanone; n-Propyl acetate; 2-Hexanone; 4-Methylanisole; 2-Nonanone; 2-Decanone	
Cheddar cheese	2-Pentanol; 3-Hydroxy-2-butanone; Isobutyl acetate; Butanoic acid, 3-methylbutyl ester; 3-Methylbutyl hexanoate; Acetic acid, 2-phenylethyl ester	2-Methyl-ethyl ester propanoic acid
Creamy/milky	2-Pentanol; 3-Hydroxy-2-butanone; Isobutyl acetate; 2-Heptanol; Butanoic acid, 3-methylbutyl ester; 3-Methybutyl hexanoate; Acetic acid, 2-phenylethyl ester	
Emulsion paint	2-Methyl-ethyl ester propanoic acid	2-Pentanol
Ester	2-Methyl-ethyl ester propanoic acid	2-Pentanone
Fermented apples	Ethanol; 1-propanol; 2-Methyl-ethyl ester propanoic acid	Acetone; 2-Pentanone; n-Propyl acetate; 2-Hexanone; 2-Heptanone; 4-Methylanisole; 2-Nonanone
Floral	2-Methyl-ethyl ester propanoic acid	2-Pentanone; 2-Pentanol; Isobutyl acetate
Grassy/herby		2-Pentanol; Isobutyl acetate
Mouldy	2-Pentanol	2-Methyl-ethyl ester propanoic acid
Mushroom-not fresh	2-Pentanol; 3-Hydroxy-2-butanone; Isobutyl acetate; Butanoic acid, 3-methylbutyl ester; 3-Methybutyl hexanoate; Acetic acid, 2-phenylethyl ester	2-Methyl-ethyl ester propanoic acid
Natural Yoghurt	Unidentified	
Sweaty socks	Acetone; 2-Pentanone; 2-Pentanol; n-Propyl acetate; Isobutyl acetate; 2-Hexanone; 2-Heptanone; 4-Methylanisole; 2-Nonanone; 2-Decanone	Ethanol; 2-Methyl-ethyl ester propanoic acid
Vinegar		Acetone; 2-methyl propanal; 3-Hydroxy-2-butanone

3.4.2.3 Conclusions of sensory analysis of *K. lactis models*

Sensory analysis demonstrated that the inoculum concentration of *K. lactis* within the blue cheese model impacts the aroma perceived. Models inoculated at low concentration presented a blue cheese related aroma correlated with the production of ketones (2-pentanone, 2-hexanone, 2-nonanone and 2-decanone), 3-methylanisole and n-propyl acetate. Contrary to this, models at a high concentration of *K. lactis* produce fruity, milky and floral aromas which are likely to be derived from esters and acids (especially 2-methyl ethyl ester propanoic acid) which were more abundant in their aroma profiles.

Following sensory analysis variation is observed between replicate models whereas, instrumental data showed the aroma profiles of models at a high concentration of *K. lactis* clustered, being more alike than replicate models inoculated at a low *K. lactis* concentration (Figure 2.4). Sensory analysis indicates that variation in the aroma profiles of replicate models is too small to detect. Controlling *K. lactis* concentration in industrial production could decrease aroma variation, but this may not be perceivable by the consumer.

The results of Napping® and GPA were comparable supporting the consistency of the sensory analysis. The second Napping® session generated bi-plots very similar to that of the GPA plots created from Flash Profile demonstrating that Napping® using a small panel of experts can produce projective maps comparable to more extensive analysis (Perrin & Pagès, 2009).

4. DISCUSSION

The yeast secondary flora of blue cheese is believed to influence aroma development during ripening (Beresford *et al.*, 2001; Viljoen, 2001; Jakobsen & Narvhus, 1996). Studies have suggested that controlling the yeast secondary flora offers potential to manipulate flavour development of cheese (Law & Tamine, 2010; Das, 2004; Jakobsen & Narvhus, 1996).

Investigating growth parameters of the model has highlighted that yeast inoculum concentration (Section 2.4.2.2) and incubation temperature (Section 2.4.2.3) are important factors influencing aroma profiles generated in the model and indicates that the species and amounts of yeasts present in Stilton could affect the aroma production in Stilton (Objective 1, Section 1.3). Aroma development is a key aspect of consumer preference for cheese (Jaillais *et al.*, 1999) and this work indicated that controlling *Yarrowia lipolytica* in Stilton offers potential to manipulate the composition of aroma compounds including ketones, and controlling *Kluyveromyces lactis* provides potential for influencing variation in the aroma.

In previous work it was observed that *Y. lipolytica* co-present with *P. roqueforti* enhanced the amounts of ketones produced in models (Gkatzionis, 2010). The current study demonstrated that this effect depends on the concentration of the yeast. The proportions of key aroma compounds such as 2-pentanone, 2-hexanone, 2-heptanone and 2-nonanone increased at a higher concentration of *Y. lipolytica* (Figure 2.4). The aroma profiles observed following incubation *K. lactis* with *P. roqueforti* in the model evidenced that the variation between replicate samples reduced as the yeast inoculum concentration increased (Figure 2.5) and thus identifying potential to limit variation in real cheese production by applying a high concentration of *K. lactis* (Objective 2, Section 1.3). The impact of the concentration of *Trichospon beigelli* on aroma generation has been investigated (Objective 1, Section 1.3). *Trichosporon beigelli* was indicated to suppress the production of ketones in the model and this was more prevalent at higher yeast inoculum concentrations (Figure 2.7). *T. beigelii* is infrequently identified in the blue veins of Stilton (Gkatzionis, 2010). The presence of *T. beigelli* at high concentrations may have undesirable effects upon quality of the final product due to reducing the amount of ketones. The concentration of *Debaryomyces hanensii* inoculated into the model was evidenced to affect the aroma profile generated. The aroma profile generated from incubating high concentrations of *D. hansenii* co-present with *P. roqueforti* showed ketone production similar to models containing *P. roqueforti* alone (Figure 2.6). *D. hansenii* is reported to be the most abundant yeast species in the microflora of Stilton (Gkatzionis, 2010). The results of this study suggest that this species is important for flavour development.

The observations of the effect that different inoculum concentrations of *K. lactis* and *Y. lipolytica* had on the aroma profiles generated in models prompted the study of the effect of incubation temperature (Objective 2, Section 1.3).

Results showed that the amount of aroma compounds produced in models incubated at 5°C and 15°C was similar to the controls (Table 2.3) and lower than in models incubated at 25°C (Table 2.2). At low incubation temperature the presence of yeasts was found to be vital for the production of ketones. Various yeasts have been reported to impact *P. roqueforti* sporulation (Gkatzionis, 2009; Tempel & Jakobsen, 2000) yet the basis of this is largely unknown. Results indicate that yeast influence cheese ripening (Jakobsen & Narvhus, 1996). Interestingly the aroma profiles of models incubated at 25°C are more similar to the aroma profiles of real Stilton (Gkatzionis e*t al.*, 2009).

Sensory studies using models inoculated at high and low concentrations of *Y. lipolytica* and *K.lactis*, co-present with *P. roqueforti* and incubated at 25°C were thus conducted to investigate if the respective differences in aroma profile and variation were perceivable by humans (Objective 3, Section 1.3).

Discrimination testing (Section 3.4.1) showed that the differences between models inoculated with *Y. lipolytica* at high and low concentration, with *P. roqueforti,* were perceivable (Section 3.4.1.1) but did not affect the aroma intensity (Section 3.4.1.2) or degree of similarity to a typical blue cheese aroma (Section 3.4.1.3).

Comments from panellists (Table 3.2) highlighted the differences in individual's aroma perception. Samples at both concentrations were described as '*stronger*' and '*intense*' when the difference in aroma was described. This shows the difficulties relating sensory data collected to the true aroma perceived (Lawless, 1999). Further investigation will need to be undertaken to understand the nature of the difference in aroma between models inoculated to a high or low concentration of *Y. lipolytica*.

Flash profiling (Section 3.4.2.2) and Napping® (Section 3.4.2.1) on models containing *K. lactis* with *P. roqueforti* showed that a difference in aroma is detectable between samples inoculated to a low or high concentration of *K. lactis*. No perceivable difference in the degree of aroma variation for replicate samples was observed between models inoculated to high and low concentration of *K. lactis*. The results of Flash profile and Napping® results were comparable demonstrating that ultra-fast profiling techniques can produce interpretable and reproducible data (Delarue & Sieffermann, 2004; Dairou & Sieffermann, 2002). Sensory analysis (Section 3.4) showed that humans detected the major trends in aroma profiles of models, as were observed by SPME GC-MS analysis (Section 2.4.2.2) (Objective 3, Section 1.3). However, instrumental data and human perception did not directly relate with regards to aroma variation between replicate models containing *K. lactis*.

SPME GC-MS analysis for quantification of volatiles is often reported to lack reproducibility and precision (Stashenko & Martínez, 2007) yet within this study the average variation in the quantities of aroma compounds generated in model samples (Appendix 9, Appendix 14) is similar to that recorded for real Stilton (Gkatzionis *et al.*, 2009).

Within this study yeasts were studied at species level. Yeasts show strain-dependent properties which impact on the organoleptic properties of cheese (Lanciotti *et al.*, 2005). This work could be used as basis for screening of strains to identify those with desired attributes.

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6. APPENDICES

Appendix 1. Information about salt substitutes.

Seaweed (www.seagreens.co.uk)

Seagreens® food granules, nutritional information (100g):

Protein	5g	
Carbohydrate	55g	
Sugars	3g	
Fat	4g	
of which:		
	Saturates	0.45g
	Mono-unsaturates (cis)	1.23g
	Mono-unsaturates (trans)	< 0.01g
	Polyunsaturates	0.39g
	Polyunsaturates (trans)	<0.01g
Dietary Fibre	50g	
of which:		
	Insoluble fibre	40g
	Soluble fibre	7g
Sodium	3.5g	
Moisture	10%	
Energy	167 kcalories (683 kJoules)	

sub4salt® (www.jungbunzlauer.com)

sub4salt® components:

Sodium Gluconate

Potassium Chloride

Sodium Chloride

1g sub4salt® contains 0.26g Na

Appendix 2. Collection of provided[1] enzymatically active yeast isolates of Stilton cheese.

Code	Species	Code	Species	Code	Species
SW01	*D. hansenii*	**DW01**	*K. lactis*	**Y31**	*Y. lipolytica*
SW02	*K. lactis*	**DW02**	*K. lactis*	**Y32**	*K. lactis*
SW03	*D. hansenii*	**DW03**	*K. lactis*	**Y33**	*D. hansenii (A)*
SW04	*K. lactis*	**DW04**	*K. lactis*	**Y34**	*D. hansenii (B)*
SW05	*K. lactis*	**DW05**	Unknown species	**Y35**	*D. hansenii (A)*
SW06	*K. lactis*	**DW06**	*K. lactis*	**Y36**	*K. lactis*
SW07	*K. lactis*	**DW07**	*Y. lipolytica*	**Y37**	*K. lactis*
SW08	*P. roqueforti*			**Y38**	*D. hansenii (A)*
SW09	*K. lactis*	**DW09**	*K. lactis*	**Y39**	*K. lactis*
SW10	*K. lactis*	**DW10**	*K. lactis*	**Y40**	*D. hansenii (B)*
SW11	*K. lactis*	**DW11**	*K. lactis*	**Y41**	*K. lactis*
SW12	Unknown species	**DW12**	*K. lactis*	**Y42**	*D. hansenii (A)*
SW13	*K. lactis*	**DW13**	*K. lactis*	**Y43**	*K. lactis*
SW14	*K. lactis*	**DW14**	*K. lactis*	**Y44**	*K. lactis*
SW15	*K. lactis*	**DW15**	*K. lactis*	**Y45**	*D. hansenii (B)*
SW16	*P. roqueforti*	**DW16**	*P. roqueforti*		
SO01	K. lactis	**DO01**	*Y. lipolytica*	**Y1**	*Y. lipolytica*
SO02	Y. lipolytica	**DO02**	*Y. lipolytica*	**Y2**	*Y. lipolytica*
SO03	K. lactis	**DO03**	Unknown species	**Y3**	*Y. lipolytica*
SO04	K. lactis	**DO04**	*D. hansenii*	**Y4**	*D. hansenii (A)*
SO05	Unknown mould	**DO05**	*Y. lipolytica*	**Y5**	*D. hansenii (A)*
SO06	Unknown mould	**DO06**	*D. hansenii*	**Y6**	*D. hansenii (A)*
SO07	*K. lactis*	**DO07**	*K. lactis*	**Y7**	*D. hansenii (B)*
SO08	Unknown mould	**DO08**	*D. hansenii*		
SO09	Unknown mould	**DO09**	Unknown species	**Y9**	*D. hansenii (B)*
SO10	*Y. lipolytica*	**DO10**	*Y. lipolytica*		
SO11	*Y. lipolytica*	**DO11**	*Y. lipolytica*	**Y11**	*D. hansenii (B)*
SO12	*Y. lipolytica*	**DO12**	*Y. lipolytica*	**Y12**	*D. hansenii (B)*
SO13	*K. lactis*	**DO13**	*Y. lipolytica*	**Y13**	*D. hansenii (B)*
SO14	*K. lactis*	**DO14**	*Y. lipolytica*	**Y14**	*D. hansenii (B)*
SO15	*K. lactis*	**DO15**	*P. roqueforti*	**Y15**	*D. hansenii (B)*
SO16	*K. lactis*				
SO17	*P. roqueforti*				
SB01	*Y. lipolytica*	**DB01**	*Y. lipolytica*	**Y16**	*Trichosporon beigelii*
SB02	*K. lactis*	**DB02**	*Y. lipolytica*	**Y17**	*Trichosporon beigelii*
SB03	*Y. lipolytica*	**DB03**	*K. lactis*	**Y18**	*Trichosporon beigelii*
SB04	*Y. lipolytica*	**DB04**	*K. lactis*	**Y19**	*Trichosporon beigelii*
SB05	Unknown species	**DB05**	*K. lactis*	**Y20**	*Kluyveromyces lactis*
SB06	Unknown species	**DB06**	Unknown species	**Y21**	*D. hansenii (B)*
SB07	*Y. lipolytica*	**DB07**	*Y. lipolytica*	**Y22**	*K. lactis*
SB08	Unknown species	**DB08**	*K. lactis*	**Y23**	*K. lactis*
SB09	Unknown species	**DB09**	*K. lactis*	**Y24**	*K. lactis*
SB10	*Y. lipolytica*	**DB10**	*K. lactis*	**Y25**	*D. hansenii (B)*
SB11	*Y. lipolytica*	**DB11**	*K. lactis*		
SB12	*Y. lipolytica*	**DB12**	*K. lactis*	**Y27**	*K. lactis*
SB13	Unknown species	**DB13**	Unknown species	**Y28**	*K. lactis*
SB14	*P. roqueforti*	**DB14**	*Y. lipolytica*		
SB15	*K. lactis*	**DB15**	*P. roqueforti*		
SB16	*K. lactis*				
SB17	*P. roqueforti*				

(A) and (B) represent different morphologies of *D. hansenii*.

[1]Collection provided by Food and Drink iNET project, 2011

Appendix 3. Counts of yeasts with and without *P. roqueforti*.

Inoculated into the dairy model at 1x10^5 cells mL^{-1} and incubated for 10 days at 25°C.

Model inoculum (1x10^5 cells / spores mL^{-1})	Yeast count (CFU mL^{-1}) Incubation length			
	Day 0	Day 3	Day 6	Day 10
K. lactis (DB09)	1.67E+05	4.17E+07	3.67E+09	2.33E+09
K. lactis (DB09)	3.17E+05	1.33E+07	2.83E+09	1.83E+09
T. beigelii (Y19)	2.50E+04	3.50E+06	1.00E+08	2.17E+08
T. beigelii (Y19)	6.17E+04	1.67E+06	5.00E+07	5.00E+07
D. hansenii (DO04)	3.33E+05	5.00E+06	1.67E+07	1.33E+09
D. hansenii (DO04)	3.83E+05	2.67E+06	1.67E+08	1.83E+09
Y. lipolytica (SB04)	1.50E+05	2.00E+07	7.00E+08	2.33E+09
Y. lipolytica (SB04)	1.83E+05	1.50E+07	5.50E+09	3.50E+09
K. lactis (DB09) with *P. roqueforti*	1.00E+05	8.17E+07	4.67E+09	1.67E+10
K. lactis (DB09) with *P. roqueforti*	1.67E+05	6.17E+07	1.17E+09	1.00E+10
T. beigelii (Y19) with *P. roqueforti*	1.33E+05	1.00E+06	1.67E+08	4.67E+08
T. beigelii (Y19) with *P. roqueforti*	3.50E+05	2.83E+06	1.17E+08	3.33E+08
D. hansenii (DO04) with *P. roqueforti*	2.67E+05	1.33E+07	1.67E+07	5.00E+07
D. hansenii (DO04) with *P. roqueforti*	6.17E+04	1.67E+06	3.33E+08	1.50E+08
Y. lipolytica (SB04) with *P. roqueforti*	1.83E+05	2.00E+07	5.50E+09	2.17E+09
Y. lipolytica (SB04) with *P. roqueforti*	2.83E+05	3.50E+07	1.07E+09	2.00E+09
P. roqueforti	6.83E+04	8.11E+04	9.87E+04	1.17E+05
P. roqueforti	4.33E+04	1.68E+05	2.86E+05	5.67E+05

Appendix 4. ANOVA of yeast counts at Day 10 (Appendix 3) from models inoculated with each yeast species, with and without *P. roqueforti* co-present.

Category	LS means	Groups	
K. lactis (DB09) with *P. roqueforti*	13333333333.333	A	
Y. lipolytica (SB04)	2916666666.667		B
K. lactis (DB09)	2083333333.333		B
Y. lipolytica (SB04) with *P. roqueforti*	2083333333.333		B
D. hansenii (DO04)	1583333333.333		B
T. beigelii (Y19) with *P. roqueforti*	400000000.000		B
T. beigelii (Y19)	133333333.333		B
D. hansenii (DO04) with *P. roqueforti*	100000000.000		B

Appendix 5. Counts of yeasts growing in models with salt substitutes in co-presence with *P. roqueforti*.

All species inoculated at 1x10^5 cells/spores mL^{-1} and incubated at 25°C.

Yeast Inoculum	Salt supplement	Incubation time			
		Day 0	**Day 3**	**Day 7**	**Day 10**
K. lactis (Y44)	Seaweed	2.00E+04	2.67E+07	1.50E+10	4.33E+08
K. lactis (Y44)	Seaweed	1.33E+04	4.17E+06	1.33E+08	5.00E+07
Y. lipolytica (SO10)	Seaweed	3.00E+05	1.00E+07	5.00E+07	5.00E+07
Y. lipolytica (SO10)	Seaweed	4.00E+05	7.83E+06	6.67E+07	5.00E+07
K. lactis (Y44)	NaCl	1.33E+04	5.67E+06	2.50E+08	6.17E+08
K. lactis (Y44)	NaCl	1.83E+04	2.50E+07	1.17E+08	3.50E+08
Y. lipolytica (SO10)	NaCl	1.50E+05	1.00E+07	1.00E+09	3.83E+09
Y. lipolytica (SO10)	NaCl	2.00E+05	1.83E+07	6.00E+08	3.33E+07
K. lactis (Y44)	sub4salt	1.33E+05	1.33E+08	2.50E+08	1.28E+09
K. lactis (Y44)	sub4salt	1.83E+05	4.00E+07	2.00E+08	2.17E+09
Y. lipolytica (SO10)	sub4salt	1.33E+04	4.33E+06	5.00E+07	4.83E+08
Y. lipolytica (SO10)	sub4salt	1.17E+04	2.67E+06	5.00E+07	1.50E+09
K. lactis (Y44)	None –milk	1.83E+05	5.00E+04	2.67E+08	2.50E+09
K. lactis (Y44)	None –milk	2.50E+05	5.00E+04	1.83E+08	1.33E+10
Y. lipolytica (SO10)	None –milk	1.17E+04	2.33E+06	2.67E+09	2.83E+10
Y. lipolytica (SO10)	None –milk	1.17E+04	4.67E+06	3.00E+09	1.50E+09
None	None –milk	0.00E+00	0.00E+00	0.00E+00	0.00E+00
None	None –milk	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Appendix 6. ANOVA of yeast counts following ten days incubation at 25°C in models containing salt supplements (Appendix 5) in co-presence of *P. roqueforti.*

Category	LS means	Groups
Y. lipolytica, milk	14916666666.667	A
K. lactis, milk	7916666666.667	A
Y. lipolytica, NaCl	1933333333.333	A
K. lactis, sub4salt	1725000000.000	A
Y. lipolytica, sub4salt	991666666.667	A
K. lactis, NaCl	616666666.667	A
K. lactis, NaC	350000000.000	A
K. lactis, seaweed	241666666.667	A
Y. lipolytica, seaweed	50000000.000	A

Appendix 7. Aroma compounds generated in blue cheese models following incubation at 25°C for 10days.

SPME GC-MS signal intensities for compounds are expressed relative to the signal intensity observed from a 5µg/L 2-nonanone standard.

	Yeast inoculum (CFU mL^{-1}) *Y. lipolytica*																	
LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Acetaldehyde	1.98E-02	0.00E+00	6.51E-03	0.00E+00	1.39E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.60E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Methanethiol	7.41E-03	6.04E-03	6.90E-04	4.98E-04	3.39E-04	2.12E-04	4.32E-04	2.76E-03	2.45E-04	5.12E-04	0.00E+00	9.60E-04	1.92E-03	0.00E+00	2.99E-04	3.09E-04	2.39E-04	2.04E-04
Ethanol	1.51E-01	1.03E-01	8.50E-02	7.66E-02	7.75E-02	5.24E-02	5.86E-02	1.52E-02	1.26E-01	5.05E-02	3.13E-02	2.27E-01	5.30E-02	1.41E-01	8.48E-02	1.81E-01	6.11E-02	5.14E-02
Acetone	2.21E-01	1.64E-01	1.43E-01	1.29E-01	1.43E-01	1.15E-01	2.22E-01	4.30E-01	4.03E-01	8.42E-02	6.86E-02	9.72E-02	1.53E-01	2.76E-01	2.38E-01	1.76E-01	1.00E-01	5.68E-02
1-propanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl propanal	1.95E-02	1.49E-02	1.44E-02	2.12E-03	3.46E-03	4.78E-04	3.44E-03	1.59E-03	2.24E-02	1.14E-03	4.19E-04	0.00E+00	1.37E-03	6.76E-03	6.42E-03	0.00E+00	7.00E-04	2.28E-04
Unidentified	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.68E-03	6.58E-04	0.00E+00	0.00E+00	0.00E+00	9.70E-04	0.00E+00	3.84E-02	1.86E-03	9.00E-04
2-Butanone	1.58E-01	1.07E-01	1.03E-01	5.18E-02	4.43E-02	2.79E-02	1.33E-01	1.35E-01	1.78E-01	2.40E-02	1.55E-02	2.57E-02	9.88E-02	2.04E-01	1.58E-01	2.23E-02	2.34E-02	2.13E-02
Ethylacetate	9.62E-03	6.84E-03	6.49E-03	5.90E-03	4.06E-03	2.13E-03	7.81E-03	0.00E+00	9.36E-03	4.35E-03	3.01E-03	7.82E-03	2.66E-03	2.94E-02	4.22E-03	1.15E-02	4.45E-03	7.81E-03
2-Methyl-1-propanol	1.19E-02	9.24E-03	8.28E-03	3.17E-03	3.21E-03	1.62E-03	7.99E-03	2.08E-02	2.92E-02	3.47E-03	1.73E-03	4.28E-03	6.83E-03	1.43E-02	1.29E-02	2.41E-03	6.26E-03	6.01E-03
3-Methyl-butanal	3.52E-02	2.32E-02	2.44E-02	5.26E-03	6.12E-03	8.59E-04	5.14E-03	5.34E-03	8.45E-02	2.34E-03	1.91E-04	6.32E-04	2.89E-03	1.64E-02	1.55E-02	3.08E-04	5.93E-03	2.49E-03
1-Butanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Methyl-butanal	3.96E-02	2.30E-02	2.85E-02	4.49E-03	7.40E-03	5.78E-04	5.58E-03	3.87E-03	6.00E-02	2.89E-03	4.78E-04	1.42E-03	6.02E-03	1.82E-02	1.94E-02	5.00E-04	2.53E-03	1.67E-03
2-Pentanone	9.72E-02	6.78E-02	6.02E-02	1.98E+00	2.33E+00	2.48E+00	6.48E-02	8.93E-02	9.79E-02	1.06E+00	1.31E+00	9.32E-01	4.25E-02	6.36E-02	7.19E-02	1.09E+00	2.32E-01	4.38E-01
2-Pentanol	3.62E-03	1.80E-03	2.20E-03	2.46E-03	4.04E-03	1.26E-03	9.05E-04	2.83E-03	2.60E-03	3.77E-02	1.67E-02	5.37E-02	5.89E-04	0.00E+00	1.29E-03	1.77E-02	6.60E-03	4.35E-03
3-Hydroxy-2-butanone	4.93E-03	2.47E-03	1.34E-03	0.00E+00	7.83E-04	6.99E-04	3.56E-03	3.63E-03	4.98E-03	0.00E+00	0.00E+00	5.65E-04	2.53E-03	6.08E-03	4.35E-03	5.35E-02	2.20E-03	1.07E-02
Ethyl ester propanoic acid	7.35E-04	6.36E-04	1.22E-03	0.00E+00	0.00E+00	0.00E+00	4.97E-04	0.00E+00	0.00E+00	3.10E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.51E-04	0.00E+00	0.00E+00
Methyl-cyclohexane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
n-Propyl acetate	0.00E+00	0.00E+00	0.00E+00	2.97E-04	8.68E-05	0.00E+00	1.57E-04	0.00E+00	0.00E+00	4.37E-04	0.00E+00	7.55E-04	5.21E-05	0.00E+00	8.02E-05	0.00E+00	1.15E-03	3.09E-04
3-Methyl-butanol	1.12E-01	7.50E-02	7.67E-02	2.56E-02	2.64E-02	8.32E-03	6.89E-02	3.32E-01	3.87E-01	3.47E-02	1.19E-02	5.07E-02	5.63E-02	9.26E-02	8.23E-02	1.03E-01	2.77E-02	2.62E-02
2-Methyl-1-butanol	1.07E-02	7.71E-03	8.89E-03	3.47E-03	2.82E-03	1.27E-03	9.11E-03	2.34E-02	2.94E-02	4.84E-03	2.04E-03	4.92E-03	7.27E-03	1.15E-02	1.12E-02	1.87E-02	2.34E-03	4.83E-03

	Yeast inoculum (CFU mL^{-1})																	
	Y. lipolytica																	
LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Dimethyl-disulfide	1.16E-02	1.78E-02	2.38E-03	2.38E-04	3.59E-04	1.74E-04	1.65E-03	8.22E-03	1.57E-04	1.17E-03	3.74E-04	1.31E-03	7.72E-03	1.27E-03	4.31E-04	9.58E-04	1.25E-03	2.95E-04
3-Methyl-2-pentanone	7.24E-04	5.00E-04	2.99E-04	2.42E-04	2.27E-04	2.52E-04	4.56E-04	1.62E-03	9.17E-04	7.51E-04	1.90E-04	3.20E-04	0.00E+00	2.82E-04	5.49E-04	4.43E-04	0.00E+00	1.81E-04
2-Methyl-ethyl ester propanoic acid	1.48E-02	1.36E-02	1.19E-02	8.99E-03	6.02E-03	0.00E+00	1.54E-02	1.62E-02	2.70E-02	8.74E-03	3.72E-03	5.93E-03	1.11E-02	1.90E-02	2.38E-02	3.61E-03	1.03E-02	9.69E-03
2-Methyl-heptane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-Pentanol	7.29E-03	3.40E-03	3.16E-03	4.29E-03	3.08E-03	2.00E-03	5.53E-03	1.43E-02	1.25E-02	1.56E-02	8.53E-03	8.37E-03	3.57E-03	3.71E-03	6.81E-03	1.66E-02	2.07E-02	9.11E-03
Isobutyl acetate	9.94E-03	1.56E-02	1.70E-02	1.01E-02	8.30E-03	9.95E-04	7.15E-03	2.89E-02	3.09E-02	1.01E-02	1.32E-02	4.44E-03	1.19E-02	2.17E-02	2.45E-02	0.00E+00	1.04E-02	9.98E-03
3-Methyl-heptane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Hexanone	1.64E-02	1.26E-02	1.27E-02	4.27E-01	5.02E-01	5.02E-01	1.32E-02	6.00E-03	2.13E-02	3.01E-01	3.40E-01	2.43E-01	8.75E-03	1.54E-02	1.50E-02	2.21E-01	5.59E-02	1.07E-01
Octane	4.84E+00	2.31E+00	2.30E+00	1.81E+00	2.19E+00	1.27E+00	2.26E+00	2.45E-01	3.71E+00	1.03E+00	1.08E+00	1.74E+00	1.81E+00	4.60E+00	3.54E+00	0.00E+00	0.00E+00	1.73E+00
Butanoic acid	2.88E-02	2.12E-02	1.96E-02	1.61E-02	1.60E-02	5.70E-03	1.90E-02	2.24E-02	4.46E-02	1.85E-02	8.15E-03	1.35E-02	1.84E-02	3.11E-02	3.86E-02	8.74E-03	1.64E-02	1.75E-02
3-Methyl-butanoic acid	7.23E-03	4.76E-03	3.17E-03	2.68E-03	2.34E-03	2.02E-03	4.91E-03	7.01E-02	4.35E-02	8.83E-04	1.81E-03	1.23E-02	6.56E-03	8.60E-03	6.69E-03	1.85E-03	6.86E-03	4.33E-03
2-Methyl-butanoic acid	0.00E+00	0.00E+00	1.09E-04	0.00E+00	1.99E-04	1.93E-04	0.00E+00	0.00E+00	0.00E+00	1.03E-04	0.00E+00	0.00E+00	0.00E+00	2.51E-04	2.12E-04	0.00E+00	0.00E+00	9.67E-05
Pentanoic acid	7.99E-02	3.43E-02	3.59E-02	0.00E+00	0.00E+00	0.00E+00	3.85E-02	8.68E-03	5.60E-02	1.71E-02	0.00E+00	3.20E-02	2.85E-02	7.44E-02	5.52E-02	0.00E+00	0.00E+00	2.31E-02
3-Methyl-1-butanol, acetate	0.00E+00	6.36E-04	4.46E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.18E-04	1.59E-03	5.85E-04	6.75E-04	7.42E-04	0.00E+00	0.00E+00	0.00E+00	9.42E-04	3.59E-04	4.40E-04
2-Heptanone	1.21E+00	8.49E-01	8.13E-01	1.14E+01	1.28E+01	1.78E+01	8.90E-01	1.58E-01	7.13E-01	1.04E+01	1.37E+01	9.46E+00	7.24E-01	9.88E-01	1.24E+00	1.14E+01	4.55E+00	5.90E+00
Styrene	1.20E-02	1.63E-03	1.30E-03	1.32E-03	5.11E-04	3.67E-03	5.85E-02	5.47E-02	1.23E-02	2.72E-03	2.33E-03	1.06E-03	1.48E-01	3.83E-03	4.74E-02	1.57E-03	3.44E-03	3.83E-04
2-Heptanol	2.07E-01	1.51E-01	1.32E-01	8.00E-02	7.39E-02	2.34E-02	1.09E-01	2.02E-01	2.49E-01	1.38E+00	6.69E-01	1.76E+00	1.04E-01	1.52E-01	2.06E-01	1.89E-01	2.27E-01	4.02E-01
a-Pinene	1.06E-03	7.32E-04	6.94E-04	2.36E-04	2.75E-04	0.00E+00	7.59E-04	7.48E-04	7.05E-04	4.02E-04	1.81E-04	4.44E-04	4.46E-04	1.11E-03	9.62E-04	4.18E-04	5.19E-04	5.37E-04
Unidentified	4.30E-04	0.00E+00	3.76E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.71E-03	0.00E+00	1.90E-04	0.00E+00	1.25E-04	0.00E+00	0.00E+00	0.00E+00	8.84E-04	0.00E+00
Unidentified	4.86E-03	2.84E-03	3.34E-03	2.25E-03	3.19E-03	6.09E-04	1.97E-03	0.00E+00	6.09E-03	3.08E-03	1.37E-03	2.99E-03	1.63E-03	3.13E-03	4.71E-03	7.97E-04	4.74E-04	1.29E-03
3-Octanone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.72E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.81E-03
Hexanoic acid	5.44E+00	2.79E+00	2.56E+00	1.97E+00	2.32E+00	1.39E+00	2.45E+00	0.00E+00	3.95E+00	1.30E+00	9.91E-01	2.08E+00	2.29E+00	4.56E+00	3.77E+00	0.00E+00	0.00E+00	1.88E+00
2-Octanone	9.04E-03	6.63E-03	6.08E-03	3.46E-01	4.09E-01	1.01E+00	8.53E-03	1.04E-03	6.71E-03	5.25E-01	6.56E-01	4.09E-01	7.30E-03	7.53E-03	8.32E-03	6.13E-01	1.36E-01	1.67E-01

Yeast inoculum (CFU mL^{-1})

Y. lipolytica

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Hexanoic acid, ethyl ester	8.27E-02	5.39E-02	5.23E-02	4.33E-02	4.49E-02	2.25E-02	8.35E-03	7.73E-04	2.84E-02	2.59E-02	1.05E-02	6.70E-02	1.09E-02	2.99E-02	3.61E-02	7.42E-03	3.02E-03	1.08E-02
4-Methylanisole	1.18E-04	0.00E+00	9.29E-06	0.00E+00	0.00E+00	2.42E-04	0.00E+00	0.00E+00	3.40E-05	4.01E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.10E-04	0.00E+00	1.09E-03
Butanoic acid, 3-methylbutyl ester	1.12E-02	6.74E-03	5.88E-03	3.46E-03	4.78E-03	3.27E-03	1.95E-03	0.00E+00	1.53E-02	3.04E-03	2.10E-03	5.19E-03	3.33E-03	4.86E-03	5.36E-03	1.06E-02	5.08E-04	1.60E-03
8-Nonen-2-one	0.00E+00	9.23E-04	4.01E-03	1.10E+00	1.30E+00	2.95E+00	2.29E-02	1.42E-03	1.97E-03	1.71E+00	2.03E+00	1.40E+00	1.56E-02	0.00E+00	2.78E-03	1.99E+00	3.69E-01	5.21E-01
2-Nonanone	2.41E-01	1.58E-01	1.66E-01	2.78E+00	3.09E+00	5.86E+00	2.10E-01	1.97E-02	2.14E-01	4.43E+00	5.27E+00	4.26E+00	2.31E-01	1.98E-01	2.34E-01	5.44E+00	1.97E+00	2.18E+00
Benzeneethanol	3.00E-02	1.37E-02	1.16E-02	1.21E-02	1.15E-02	6.84E-03	8.93E-03	1.52E-01	9.83E-02	3.43E-03	2.61E-03	2.20E-03	1.36E-02	4.05E-02	2.23E-02	4.53E-04	1.31E-03	4.31E-03
Hexanoic acid, butyl ester	2.44E-03	1.34E-03	9.04E-04	8.57E-04	1.76E-03	5.64E-04	7.60E-04	0.00E+00	2.82E-03	1.01E-03	7.37E-04	9.94E-04	9.07E-04	1.10E-03	1.20E-03	1.64E-04	0.00E+00	9.59E-04
Octanoic acid	1.26E+00	6.72E-01	6.99E-01	6.13E-01	7.17E-01	4.74E-01	5.27E-01	0.00E+00	8.00E-01	6.53E-01	3.51E-01	5.41E-01	5.72E-01	1.10E+00	1.03E+00	1.11E-01	0.00E+00	5.50E-01
2-Decanone	0.00E+00	3.49E-04	5.23E-04	3.79E-03	0.00E+00	0.00E+00	1.03E-03	1.23E-04	0.00E+00	1.44E-02	0.00E+00	0.00E+00	8.24E-04	8.60E-04	0.00E+00	0.00E+00	3.57E-03	2.99E-03
Octanoic acid, ethyl ester	3.34E-02	2.34E-02	2.09E-02	2.04E-02	2.20E-02	1.58E-02	9.01E-03	6.31E-04	2.23E-02	8.32E-03	8.76E-03	3.81E-02	1.12E-02	7.45E-03	1.83E-02	7.86E-03	4.73E-03	1.24E-02
3-Methybutyl hexanoate	5.03E-03	2.84E-03	2.50E-03	1.38E-03	1.78E-03	1.71E-03	1.13E-03	0.00E+00	7.69E-03	1.53E-03	9.44E-04	2.25E-03	1.62E-03	2.44E-03	2.01E-03	1.01E-03	0.00E+00	1.03E-03
Acetic acid, 2-phenylethyl ester	9.15E-03	1.50E-02	1.47E-02	6.08E-02	2.69E-02	9.35E-03	2.97E-03	5.60E-03	1.82E-02	4.84E-03	3.53E-03	1.35E-02	2.80E-03	9.54E-03	4.79E-03	6.52E-03	1.35E-02	1.64E-02
2-Undecanone	2.90E-02	1.70E-02	1.83E-02	4.83E-02	5.63E-02	1.08E-01	1.79E-02	3.04E-03	2.80E-02	2.56E-01	2.30E-01	2.58E-01	2.10E-02	2.70E-02	2.66E-02	1.76E-01	5.74E-02	5.96E-02
n-decanoic acid	1.03E-01	4.67E-02	4.36E-02	5.30E-02	8.41E-02	4.23E-02	4.35E-02	3.57E-03	8.41E-02	7.29E-02	2.90E-02	3.12E-02	3.33E-02	1.04E-01	8.80E-02	6.85E-03	0.00E+00	3.44E-02
Unidentified	6.85E-03	4.45E-03	3.90E-03	4.50E-03	4.67E-03	3.88E-03	1.66E-03	4.18E-04	4.48E-03	2.62E-03	2.48E-03	7.08E-03	2.18E-03	3.23E-03	3.46E-03	4.60E-03	7.94E-04	2.51E-03

Yeast inoculum (CFU mL^{-1})

K. lactis

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Acetaldehyde	4.96E-02	0.00E+00	9.19E-02	6.65E-01	6.56E-02	4.15E-01	4.85E-01	8.44E-02	6.87E-02	1.50E-01	4.34E-01	4.55E-01	1.30E-01	3.70E-01	3.11E-01	5.03E-01	2.07E-01	1.62E-01
Methanethiol	2.23E-03	0.00E+00	0.00E+00	1.82E-04	2.79E-03	0.00E+00	0.00E+00	8.71E-04	2.14E-03	1.90E-03	0.00E+00	0.00E+00	8.63E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethanol	5.30E+00	6.94E+00	5.35E+00	5.09E+00	5.27E+00	4.77E+00	5.24E+00	5.07E+00	4.75E+00	5.47E+00	4.41E+00	4.40E+00	6.75E+00	4.54E+00	4.68E+00	4.07E+00	1.22E+00	1.96E+00

Yeast inoculum (CFU mL^{-1})

K. lactis

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Acetone	1.75E-03	0.00E+00	2.61E-03	8.06E-03	2.61E-03	6.35E-03	6.77E-03	4.57E-03	3.45E-03	1.21E-02	1.06E-02	1.09E-02	8.41E-03	6.02E-03	4.45E-03	1.59E-02	1.91E-02	1.60E-02
1-propanol	2.03E-02	0.00E+00	2.56E-02	2.87E-02	2.29E-02	2.12E-02	2.15E-02	2.01E-02	2.12E-02	2.76E-02	1.29E-02	1.50E-02	4.45E-02	1.76E-02	1.56E-02	1.97E-02	4.01E-03	1.13E-02
2-methyl propanal	3.17E-03	1.28E-03	5.31E-03	6.98E-03	4.25E-03	4.33E-03	5.29E-03	4.12E-03	3.33E-03	1.18E-02	1.39E-02	1.77E-02	1.49E-02	5.47E-03	4.82E-03	3.49E-02	2.84E-02	1.49E-02
Unidentified	1.08E-02	0.00E+00	1.93E-02	5.88E-03	3.44E-02	4.19E-03	1.05E-02	3.78E-02	1.17E-02	6.09E-02	3.58E-03	2.69E-02	7.34E-02	1.08E-02	1.14E-02	4.61E-02	2.32E-02	1.11E-02
2-Butanone	2.19E-03	2.87E-03	3.38E-03	1.06E-02	3.29E-03	7.88E-03	1.17E-02	7.99E-03	5.83E-03	1.30E-02	8.83E-03	8.58E-03	1.66E-02	1.02E-02	9.00E-03	1.27E-02	9.67E-03	9.58E-03
Ethylacetate	7.29E+00	7.96E+00	6.20E+00	7.66E+00	6.71E+00	6.93E+00	7.09E+00	6.05E+00	7.48E+00	8.79E+00	6.50E+00	7.18E+00	7.93E+00	6.74E+00	6.70E+00	7.98E+00	8.38E+00	9.21E+00
2-Methyl-1-propanol	2.75E-01	5.45E-01	2.94E-01	2.48E-01	2.61E-01	1.91E-01	2.57E-01	2.41E-01	2.27E-01	3.70E-01	1.61E-01	1.61E-01	6.42E-01	1.80E-01	2.01E-01	2.94E-01	2.82E-02	7.65E-02
3-Methyl-butanal	1.49E-03	0.00E+00	1.26E-03	1.90E-03	1.36E-03	1.32E-03	1.07E-03	6.92E-04	1.11E-03	6.64E-03	1.19E-02	2.04E-02	2.97E-03	2.04E-03	6.86E-04	2.94E-02	1.97E-02	5.06E-03
1-Butanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Methyl-butanal	4.43E-03	7.43E-03	6.66E-03	1.02E-02	4.66E-03	7.43E-03	4.81E-03	3.66E-03	3.00E-03	3.33E-02	6.80E-02	1.06E-01	1.15E-02	9.85E-03	4.54E-03	9.65E-02	4.73E-02	1.41E-02
2-Pentanone	9.80E-04	1.07E-03	1.73E-03	1.71E-03	1.33E-03	1.06E-03	2.50E-03	2.15E-03	2.27E-03	2.94E-02	1.51E-02	1.33E-02	5.06E-03	1.77E-03	1.98E-03	4.87E-02	1.10E-01	9.35E-02
2-Pentanol	5.76E-04	9.19E-04	0.00E+00	4.16E-04	6.31E-04	0.00E+00	3.88E-04	0.00E+00	6.97E-04	3.52E-03	2.09E-03	1.85E-03	0.00E+00	3.17E-04	2.46E-04	3.76E-03	3.54E-03	3.40E-03
3-Hydroxy-2-butanone	1.50E-03	0.00E+00	0.00E+00	3.14E-02	3.44E-03	0.00E+00	1.23E-02	9.64E-03	3.18E-03	2.64E-02	3.62E-02	5.92E-02	1.39E-02	1.83E-02	3.83E-02	1.08E-01	4.82E-02	7.31E-02
Ethyl ester propanoic acid	3.59E-01	3.83E-01	3.74E-01	3.95E-01	3.40E-01	3.29E-01	3.59E-01	3.02E-01	3.20E-01	4.43E-01	2.73E-01	2.91E-01	6.04E-01	3.45E-01	0.00E+00	4.26E-01	2.64E-01	3.94E-01
Methyl-cyclohexane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
n-Propyl acetate	5.53E-02	4.14E-02	5.52E-02	5.89E-02	4.98E-02	4.72E-02	4.46E-02	4.03E-02	4.02E-02	4.78E-02	2.51E-02	2.88E-02	6.79E-02	4.10E-02	3.22E-02	8.69E-02	1.17E-01	1.12E-01
3-Methyl-butanol	1.90E+00	1.87E+00	1.87E+00	1.82E+00	1.66E+00	1.56E+00	1.82E+00	1.64E+00	1.77E+00	2.33E+00	1.73E+00	1.97E+00	2.48E+00	1.64E+00	1.51E+00	3.32E+00	1.76E+00	2.17E+00
2-Methyl-1-butanol	7.73E-01	5.90E-01	8.39E-01	8.16E-01	7.70E-01	6.85E-01	6.88E-01	6.25E-01	6.25E-01	8.28E-01	6.41E-01	7.56E-01	1.09E+00	5.96E-01	5.87E-01	8.67E-01	2.47E-01	3.98E-01
Dimethyl-disulfide	1.53E-03	4.50E-04	2.97E-04	1.43E-04	1.81E-03	0.00E+00	0.00E+00	9.55E-04	1.83E-03	6.07E-04	0.00E+00	1.11E-04	8.04E-04	0.00E+00	0.00E+00	0.00E+00	1.14E-04	0.00E+00
3-Methyl-2-pentanone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.58E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Methyl-ethyl ester propanoic acid	1.41E-01	1.54E-01	1.51E-01	1.37E-01	1.36E-01	1.21E-01	8.76E-02	6.94E-02	7.11E-02	8.14E-02	4.82E-02	4.00E-02	1.41E-01	7.14E-02	6.39E-02	4.18E-02	1.83E-02	1.61E-02
2-Methyl-heptane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-Pentanol	3.06E-03	7.03E-03	3.82E-03	4.80E-03	2.25E-03	5.45E-03	3.73E-03	3.38E-03	1.65E-03	8.05E-03	1.88E-03	2.53E-03	4.57E-03	4.77E-03	4.31E-03	1.43E-02	3.20E-03	3.53E-03

Yeast inoculum (CFU mL^{-1})

K. lactis

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Isobutyl acetate	1.82E-01	1.64E-01	1.91E-01	1.94E-01	1.62E-01	1.54E-01	1.71E-01	1.31E-01	1.40E-01	3.51E-01	1.43E-01	1.81E-01	2.15E-01	1.23E-01	9.42E-02	3.31E-01	3.26E-01	3.50E-01
3-Methyl-heptane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Hexanone	6.68E-04	6.74E-04	8.70E-04	7.87E-04	8.08E-04	5.10E-04	1.13E-03	8.12E-04	7.46E-04	1.06E-02	4.70E-03	5.02E-03	1.76E-03	7.79E-04	7.57E-04	1.82E-02	4.78E-02	3.73E-02
Octane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Butanoic acid	1.01E-02	9.63E-03	1.16E-02	1.07E-02	8.21E-03	9.20E-03	1.34E-02	1.01E-02	8.64E-03	1.34E-02	7.17E-03	7.96E-03	2.30E-02	1.07E-02	8.41E-03	1.20E-02	7.21E-03	5.89E-03
3-Methyl-butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.76E-03	0.00E+00	0.00E+00	0.00E+00	9.90E-04	0.00E+00	0.00E+00	1.46E-04	0.00E+00	6.21E-03	2.04E-03
2-Methyl-butanoic acid	2.29E-04	3.26E-04	2.03E-04	0.00E+00	1.90E-04	1.41E-04	1.40E-04	1.54E-04	0.00E+00	1.34E-04	1.09E-04	2.80E-04	0.00E+00	0.00E+00	9.11E-05	2.15E-03	2.46E-04	3.36E-04
Pentanoic acid	1.75E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.03E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-1-butanol, acetate	2.96E-01	2.14E-01	2.52E-01	2.90E-01	2.26E-01	2.44E-01	2.27E-01	1.60E-01	1.71E-01	3.27E-01	1.88E-01	2.72E-01	2.68E-01	1.93E-01	1.27E-01	3.28E-01	9.42E-01	7.35E-01
2-Heptanone	6.13E-02	6.39E-02	4.89E-02	7.18E-02	4.42E-02	6.60E-02	6.14E-02	4.61E-02	5.87E-02	1.14E+00	6.24E-01	6.09E-01	7.64E-02	8.10E-02	6.33E-02	1.41E+00	4.47E+00	3.37E+00
Styrene	7.97E-04	1.44E-03	8.47E-04	1.62E-03	8.59E-04	6.96E-04	1.02E-03	1.17E-03	1.30E-03	2.27E-03	8.34E-04	1.09E-03	2.86E-03	7.26E-04	9.72E-04	6.23E-03	1.17E-03	6.89E-04
2-Heptanol	3.45E-02	3.09E-02	2.62E-02	3.44E-02	2.34E-02	2.53E-02	3.39E-02	2.56E-02	2.75E-02	6.12E-01	2.59E-01	3.04E-01	3.84E-02	2.70E-02	2.14E-02	3.20E-01	1.08E-01	1.28E-01
a-Pinene	1.30E-03	1.64E-03	1.49E-03	7.42E-04	8.88E-04	8.62E-04	1.38E-03	1.16E-03	9.47E-04	1.32E-03	6.50E-04	6.88E-04	1.76E-03	1.14E-03	6.17E-04	8.91E-04	6.69E-04	4.48E-04
Unidentified	0.00E+00	0.00E+00	2.24E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.16E-04	0.00E+00	0.00E+00	2.07E-04	5.87E-04	0.00E+00	0.00E+00	0.00E+00	3.86E-04	8.40E-04	0.00E+00
Unidentified	1.33E-03	1.24E-03	1.38E-03	1.24E-03	1.15E-03	1.10E-03	1.36E-03	4.16E-04	6.72E-04	2.45E-02	9.44E-03	1.68E-02	1.32E-03	1.13E-03	9.01E-04	5.39E-02	4.08E-03	1.29E-02
3-Octanone	0.00E+00	0.00E+00	0.00E+00	7.84E-05	0.00E+00	0.00E+00	5.84E-05	0.00E+00	0.00E+00	5.93E-03	5.47E-04	1.44E-03	0.00E+00	0.00E+00	0.00E+00	1.33E-03	0.00E+00	4.24E-04
Hexanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Octanone	6.63E-04	6.97E-04	3.17E-04	8.53E-04	5.10E-04	0.00E+00	8.49E-04	3.78E-04	6.85E-04	2.51E-02	1.33E-02	1.50E-02	4.43E-04	0.00E+00	0.00E+00	3.79E-02	2.22E-01	1.30E-01
Hexanoic acid, ethyl ester	6.01E-02	5.15E-02	5.14E-02	6.37E-02	4.99E-02	4.80E-02	5.32E-02	3.47E-02	3.60E-02	1.53E-01	7.69E-02	1.20E-01	6.10E-02	5.31E-02	3.08E-02	1.55E-01	1.25E-02	3.86E-02
4-Methylanisole	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.31E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.47E-03	6.00E-03	4.93E-03
Butanoic acid, 3-methylbutyl ester	9.92E-04	8.25E-04	4.24E-04	9.76E-04	5.25E-04	7.84E-04	1.53E-03	1.05E-03	9.52E-04	3.22E-02	1.29E-02	2.49E-02	1.50E-03	1.05E-03	8.60E-04	6.67E-02	1.74E-02	4.16E-02
8-Nonen-2-one	4.98E-03	8.53E-03	2.00E-03	7.62E-03	7.30E-04	6.32E-03	2.83E-03	0.00E+00	7.11E-03	8.23E-02	3.49E-02	4.12E-02	0.00E+00	1.11E-02	8.89E-03	9.81E-02	5.49E-01	3.39E-01
2-Nonanone	3.84E-02	5.22E-02	1.22E-02	4.10E-02	1.28E-02	5.74E-02	1.92E-02	1.44E-02	5.44E-02	5.55E-01	3.18E-01	3.63E-01	1.70E-02	7.82E-02	8.23E-02	8.46E-01	3.16E+00	2.68E+00

Yeast inoculum (CFU mL^{-1})

K. lactis

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Benzeneethanol	1.04E-03	2.17E-03	1.10E-03	3.04E-03	1.50E-03	8.13E-04	1.19E-03	8.23E-04	2.93E-04	6.38E-03	3.08E-03	1.00E-02	2.51E-03	1.75E-03	4.90E-04	9.48E-03	1.09E-03	1.05E-03
Hexanoic acid, butyl ester	7.24E-05	2.14E-04	0.00E+00	0.00E+00	7.73E-05	1.23E-04	1.32E-04	1.11E-04	0.00E+00	7.80E-04	2.88E-04	4.88E-04	1.00E-04	1.98E-04	0.00E+00	1.45E-03	0.00E+00	5.94E-04
Octanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Decanone	6.29E-04	0.00E+00	1.87E-04	5.71E-04	5.41E-05	0.00E+00	3.01E-04	4.14E-04	0.00E+00	1.13E-03	7.41E-04	1.54E-03	0.00E+00	0.00E+00	9.60E-04	2.93E-03	1.23E-02	1.07E-02
Octanoic acid, ethyl ester	5.15E-02	4.68E-02	3.34E-02	4.91E-02	3.69E-02	3.24E-02	4.95E-02	3.70E-02	4.49E-02	8.82E-02	2.96E-02	5.27E-02	5.76E-02	4.61E-02	2.59E-02	5.28E-02	4.27E-03	1.09E-02
3-Methybutyl hexanoate	1.65E-04	3.31E-04	0.00E+00	0.00E+00	1.83E-04	3.21E-04	0.00E+00	2.02E-04	0.00E+00	1.64E-03	2.51E-04	6.30E-04	0.00E+00	0.00E+00	0.00E+00	2.08E-03	3.25E-04	1.79E-03
Acetic acid, 2-phenylethyl ester	2.96E-01	2.93E-01	2.62E-01	3.49E-01	2.35E-01	2.48E-01	2.43E-01	1.80E-01	2.32E-01	5.02E-01	4.26E-01	8.82E-01	3.17E-01	2.02E-01	1.35E-01	1.03E+00	7.21E-01	1.12E+00
2-Undecanone	3.41E-03	4.53E-03	1.80E-03	2.98E-03	1.73E-03	4.72E-03	2.03E-03	1.85E-03	3.59E-03	1.04E-02	6.01E-03	1.03E-02	2.72E-03	6.05E-03	6.33E-03	2.41E-02	1.62E-01	9.81E-02
n-decanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	8.73E-03	1.05E-02	5.82E-03	9.23E-03	5.24E-03	5.88E-03	7.86E-03	5.91E-03	7.87E-03	2.32E-02	4.68E-03	1.35E-02	9.31E-03	5.68E-03	4.01E-03	1.06E-02	1.18E-03	1.51E-03

Yeast inoculum (CFU mL^{-1})

D. hansenii

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Acetaldehyde	1.03E-03	1.09E-03	9.32E-04	7.27E-04	3.60E-03	1.98E-03	1.67E-03	7.14E-04	1.02E-03	2.01E-03	5.65E-02	2.23E-03	5.60E-04	1.92E-03	6.99E-04	1.60E-02	2.73E-03	1.46E-03
Methanethiol	2.22E-03	3.21E-03	4.45E-03	2.53E-04	0.00E+00	0.00E+00	1.88E-03	2.29E-03	4.44E-03	0.00E+00	0.00E+00	0.00E+00	2.42E-03	2.80E-03	1.68E-03	0.00E+00	3.35E-04	2.78E-04
Ethanol	1.08E-01	1.67E-02	2.02E-02	8.33E-03	2.10E-01	1.12E-01	2.12E-02	2.13E-02	1.79E-02	2.11E-02	3.69E-02	1.44E-01	1.67E-02	4.79E-02	1.46E-02	5.33E-01	6.38E-02	2.79E-02
Acetone	2.63E-01	3.32E-01	3.54E-01	2.51E-01	9.94E-02	1.08E-01	3.43E-01	3.08E-01	3.67E-01	4.77E-01	1.20E-01	1.15E-01	3.16E-01	3.94E-01	2.91E-01	2.61E-01	1.48E-01	1.02E-01
1-propanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl propanal	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	6.86E-03	1.05E-02	1.45E-02	3.96E-03	3.49E-03	4.88E-03	9.86E-03	9.68E-03	1.36E-02	2.32E-02	8.35E-03	1.03E-02	7.14E-03	2.67E-02	2.65E-02	1.01E-02	1.09E-02	1.26E-03
2-Butanone	1.74E-01	2.40E-01	2.56E-01	9.72E-02	3.87E-02	3.85E-02	2.43E-01	2.15E-01	2.70E-01	2.64E-01	4.21E-02	4.28E-02	2.25E-01	2.63E-01	1.96E-01	8.01E-02	5.85E-02	4.66E-02
Ethylacetate	2.18E-03	3.76E-03	1.64E-03	1.10E-03	8.62E-03	1.46E-03	1.94E-03	1.76E-03	4.38E-03	7.03E-04	1.03E-03	3.44E-03	2.08E-03	3.09E-03	3.11E-03	2.21E-03	2.88E-03	5.05E-04

	Yeast inoculum (CFU mL^{-1})																	
	D. hansenii																	
LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
2-Methyl-1-propanol	1.48E-02	4.91E-03	1.04E-02	5.32E-03	2.12E-03	1.47E-02	2.70E-03	9.77E-04	3.23E-03	1.78E-03	1.27E-03	6.81E-03	5.61E-03	3.95E-03	2.18E-03	4.23E-02	7.68E-03	8.05E-03
3-Methyl-butanal	5.49E-04	2.50E-04	6.96E-04	2.70E-04	8.02E-04	1.50E-02	2.65E-04	6.93E-04	9.37E-04	1.10E-02	6.41E-04	6.08E-03	2.46E-04	9.75E-04	7.61E-04	1.20E-01	1.36E-02	1.66E-03
1-Butanol	0.00E+00	0.00E+00	2.50E-03	4.61E-04	0.00E+00	1.42E-03	1.26E-03	0.00E+00	5.82E-04	0.00E+00	1.65E-04	0.00E+00	1.05E-03	1.24E-03	5.36E-04	1.52E-03	0.00E+00	7.29E-04
2-Methyl-butanal	4.06E-03	1.38E-03	2.14E-03	5.07E-04	7.93E-04	3.62E-03	1.78E-03	1.90E-03	1.52E-03	1.22E-02	3.86E-04	2.50E-03	1.49E-03	3.01E-03	6.08E-04	2.58E-02	5.20E-03	6.04E-04
2-Pentanone	2.09E-02	2.79E-02	3.13E-02	1.25E+00	1.52E+00	6.99E-01	2.19E-02	1.84E-02	2.57E-02	7.28E-01	5.40E-01	8.13E-01	2.00E-02	2.48E-02	1.83E-02	5.02E-01	2.90E-01	1.27E+00
2-Pentanol	5.24E-03	5.62E-03	9.88E-03	1.04E-02	1.27E-02	8.55E-03	5.39E-03	4.48E-03	6.45E-03	1.39E-02	7.52E-03	8.61E-03	7.86E-03	6.46E-03	3.94E-03	1.61E-02	1.56E-02	9.61E-03
3-Hydroxy-2-butanone	1.62E-03	0.00E+00	0.00E+00	1.58E-03	1.94E-03	2.23E-03	9.51E-04	0.00E+00	1.04E-03	3.53E-03	1.55E-03	1.37E-03	0.00E+00	0.00E+00	0.00E+00	3.19E-03	1.61E-03	1.47E-03
Ethyl ester propanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Methyl-cyclohexane	4.31E-02	7.63E-02	7.36E-02	2.90E-02	2.05E-02	2.56E-02	5.55E-02	5.90E-02	7.46E-02	7.82E-02	3.63E-02	3.59E-02	6.38E-02	7.67E-02	5.44E-02	5.03E-02	4.61E-02	3.28E-02
n-Propyl acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-butanol	2.11E-02	3.13E-02	4.89E-02	6.80E-02	5.28E-02	1.46E-01	5.65E-03	2.53E-03	1.11E-02	3.30E-02	1.80E-02	1.02E-01	4.06E-03	7.75E-03	4.81E-03	7.48E-01	1.05E-01	7.26E-02
2-Methyl-1-butanol	6.97E-03	8.16E-03	1.05E-02	8.46E-03	6.64E-03	2.18E-02	3.94E-03	2.71E-03	2.74E-03	5.97E-03	6.31E-03	1.09E-02	3.10E-03	2.30E-03	4.33E-03	8.15E-02	2.71E-02	2.03E-02
Dimethyl-disulfide	7.65E-03	2.90E-02	2.37E-02	4.25E-03	5.04E-03	7.98E-03	8.57E-03	1.72E-02	1.48E-02	4.49E-03	1.68E-04	1.94E-03	1.54E-02	1.40E-02	2.38E-02	1.08E-03	6.02E-03	2.28E-03
3-Methyl-2-pentanone	8.30E-04	7.74E-04	5.14E-04	7.55E-04	6.14E-04	3.01E-04	3.43E-04	1.56E-04	1.57E-04	1.42E-03	1.31E-04	0.00E+00	7.84E-05	1.19E-04	1.98E-04	2.26E-04	4.37E-04	4.77E-04
2-Methyl-ethyl ester propanoic acid	1.00E-02	2.14E-02	2.48E-02	9.10E-03	7.96E-03	6.26E-03	1.57E-02	2.14E-02	1.93E-02	2.65E-02	1.52E-02	1.54E-02	2.27E-02	3.15E-02	2.17E-02	2.52E-02	1.81E-02	1.12E-02
2-Methyl-heptane	6.46E-02	9.95E-02	1.04E-01	5.03E-02	4.25E-02	4.23E-02	8.43E-02	1.01E-01	1.04E-01	1.28E-01	8.08E-02	6.78E-02	1.05E-01	1.30E-01	1.04E-01	1.21E-01	9.38E-02	6.17E-02
1-Pentanol	3.70E-03	4.67E-03	8.49E-03	2.83E-03	8.23E-03	7.50E-03	6.90E-03	6.20E-03	8.97E-03	5.83E-03	9.19E-03	1.26E-02	6.34E-03	4.88E-03	7.75E-03	2.16E-02	1.86E-02	1.63E-02
Isobutyl acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-heptane	0.00E+00	3.04E-03	1.96E-03	1.41E-03	1.72E-03	9.06E-04	2.55E-03	2.66E-03	3.22E-03	4.09E-03	1.55E-03	2.83E-03	3.61E-03	2.94E-03	2.33E-03	1.10E-03	1.77E-03	1.42E-03
2-Hexanone	1.26E-03	1.01E-03	2.67E-03	1.59E-01	2.06E-01	1.17E-01	1.59E-03	7.38E-04	1.44E-03	6.50E-02	8.26E-02	1.47E-01	1.58E-03	2.67E-03	1.61E-03	8.21E-02	4.70E-02	2.64E-01
Octane	4.53E-02	6.43E-02	6.42E-02	3.76E-02	2.95E-02	3.55E-02	5.61E-02	5.74E-02	6.02E-02	9.13E-02	5.03E-02	4.83E-02	5.99E-02	7.39E-02	5.36E-02	6.21E-02	5.70E-02	4.97E-02
Butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.64E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.72E+00	0.00E+00	4.11E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.64E-03
3-Methyl-butanoic acid	2.04E-03	3.63E-04	1.00E-03	1.98E-04	1.90E-04	3.43E-04	1.26E-04	1.03E-04	1.45E-04	5.56E-03	2.75E-04	1.61E-03	4.61E-04	1.66E-03	1.72E-04	4.73E-03	5.40E-04	5.03E-05

Yeast inoculum (CFU mL^{-1})

D. hansenii

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
2-Methyl-butanoic acid	5.67E-04	2.26E-04	3.10E-04	0.00E+00	0.00E+00	3.13E-04	1.82E-04	0.00E+00	1.71E-04	5.56E-04	0.00E+00	0.00E+00	0.00E+00	1.24E-03	0.00E+00	5.15E-04	5.89E-04	4.00E-04
Pentanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-1-butanol, acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Heptanone	2.24E-01	2.35E-01	2.81E-01	1.48E+01	1.87E+01	1.72E+01	1.86E-01	1.22E-01	2.16E-01	9.46E+00	1.12E+01	1.56E+01	1.33E-01	1.96E-01	1.21E-01	1.11E+01	7.44E+00	1.97E+01
Styrene	9.71E-04	5.78E-03	6.94E-03	5.65E-03	9.34E-02	5.50E-03	3.69E-03	1.62E-03	1.86E-03	1.02E-02	1.21E-01	4.34E-02	4.30E-03	3.26E-03	3.69E-03	6.88E-03	3.41E-03	2.21E-03
2-Heptanol	4.03E-03	4.17E-03	6.02E-03	1.75E-01	7.94E-02	6.88E-02	2.45E-03	2.08E-03	2.64E-03	1.60E-01	1.31E-01	4.65E-02	2.20E-03	7.49E-03	1.61E-03	1.39E-01	8.92E-02	5.79E-02
a-Pinene	2.16E-03	2.69E-03	3.96E-03	1.32E-03	2.41E-03	1.63E-03	1.77E-03	1.65E-03	1.28E-03	3.50E-03	2.65E-03	2.26E-03	2.31E-03	3.78E-03	2.32E-03	3.22E-03	2.99E-03	1.32E-03
Unidentified	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Octanone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Hexanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.44E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Octanone	1.46E-03	2.23E-03	2.58E-03	8.12E-01	7.56E-01	1.00E+00	3.03E-03	2.52E-03	2.75E-03	1.23E-01	3.46E-01	5.86E-01	2.28E-03	1.18E-03	1.47E-03	2.77E-01	2.30E-01	8.25E-01
Hexanoic acid, ethyl ester	9.79E-03	1.29E-03	1.56E-03	1.48E-03	1.70E-02	3.78E-03	1.08E-04	0.00E+00	1.15E-04	1.25E-02	8.30E-04	1.01E-02	2.54E-04	7.03E-04	2.48E-04	2.04E-03	6.28E-04	7.55E-04
4-Methylanisole	0.00E+00	3.83E-04	3.61E-04	1.65E-03	1.97E-03	3.91E-03	0.00E+00	3.02E-04	0.00E+00	1.25E-04	1.78E-03	2.61E-03	2.65E-04	1.66E-03	1.81E-04	1.19E-03	4.22E-03	2.67E-03
Butanoic acid, 3-methylbutyl ester	1.62E-03	4.39E-04	9.93E-04	1.70E-03	1.59E-02	9.51E-03	3.50E-04	3.49E-04	1.10E-03	9.26E-03	1.90E-03	1.14E-02	6.31E-04	0.00E+00	3.82E-04	2.14E-02	3.72E-03	2.49E-03
8-Nonen-2-one	1.89E-03	1.72E-03	9.68E-04	2.23E+00	1.83E+00	2.54E+00	1.20E-03	2.66E-03	1.32E-03	2.85E-01	8.86E-01	1.55E+00	1.70E-03	2.59E-03	1.26E-03	7.44E-01	5.57E-01	2.25E+00
2-Nonanone	4.61E-02	3.80E-02	3.86E-02	1.21E+01	1.04E+01	1.25E+01	3.73E-02	6.89E-03	4.52E-02	3.17E+00	6.49E+00	1.05E+01	7.99E-03	1.13E-02	7.31E-03	5.58E+00	5.10E+00	1.24E+01
Benzeneethanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Hexanoic acid, butyl ester	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Octanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.01E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Decanone	0.00E+00	1.05E-03	1.45E-03	7.80E-02	4.19E-02	7.73E-02	1.27E-03	6.89E-04	7.50E-04	9.83E-03	1.09E-02	5.65E-02	0.00E+00	1.82E-03	3.95E-04	1.27E-02	6.63E-03	5.70E-02
Octanoic acid, ethyl ester	1.10E-03	8.19E-05	2.85E-04	2.36E-04	4.96E-04	4.88E-04	5.55E-04	0.00E+00	6.87E-04	7.73E-04	6.89E-05	5.53E-04	1.56E-04	4.18E-04	1.62E-04	4.69E-04	1.31E-04	5.46E-04
3-Methybutyl hexanoate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Yeast inoculum (CFU mL^{-1})

D. hansenii

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Acetic acid, 2-phenylethyl ester	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Undecanone	1.96E-03	2.02E-03	1.30E-03	6.65E-01	3.29E-01	4.10E-01	1.24E-03	8.60E-04	1.83E-03	5.81E-02	4.67E-02	2.34E-01	1.28E-03	3.35E-03	1.35E-03	4.06E-02	3.99E-02	4.39E-01
n-decanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Yeast inoculum (CFU mL^{-1})

T. beigelii

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
Acetaldehyde	4.97E-03	1.38E-04	3.05E-03	1.96E-03	4.65E-03	5.78E-03	6.58E-04	5.73E-03	1.92E-03	1.38E-03	3.67E-02	2.45E-03	1.22E-02	3.11E-03	1.69E-03	1.20E-03	2.55E-03	2.38E-03
Methanethiol	1.49E-04	0.00E+00	1.53E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.56E-04	0.00E+00	1.51E-04	0.00E+00	0.00E+00	2.86E-04	0.00E+00	1.74E-04	9.95E-05	0.00E+00	0.00E+00
Ethanol	2.86E-01	3.09E-01	1.52E-01	2.91E-01	6.10E-02	3.91E-02	5.25E-02	5.92E-02	5.63E-02	3.23E-02	8.62E-01	7.07E-03	1.08E+00	4.65E-02	4.88E-02	1.79E-01	6.47E-02	3.43E-01
Acetone	2.79E-01	2.72E-01	2.65E-01	3.40E-01	1.85E-01	3.10E-01	3.05E-01	2.35E-01	1.99E-01	1.37E-01	2.15E-01	1.76E-01	7.55E-02	4.36E-01	3.07E-01	1.24E-01	7.89E-02	2.23E-01
1-propanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl propanal	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	1.00E-02	1.29E-02	1.20E-03	1.24E-02	5.31E-03	9.07E-03	5.63E-03	2.47E-03	2.03E-03	6.74E-03	9.77E-03	1.14E-02	1.33E-02	2.52E-02	2.80E-02	6.54E-03	3.23E-03	9.35E-03
2-Butanone	1.42E-01	1.33E-01	1.09E-01	1.60E-01	2.25E-02	5.05E-02	1.38E-01	4.37E-02	3.32E-02	2.91E-02	6.33E-02	3.39E-02	1.16E-02	2.16E-01	1.95E-01	3.41E-02	3.70E-02	3.34E-02
Ethylacetate	4.24E-03	3.33E-03	1.80E-03	4.77E-03	6.59E-03	2.96E-03	1.36E-03	1.51E-03	2.08E-03	2.50E-03	1.76E-02	1.36E-03	1.13E-02	3.14E-03	3.03E-03	6.42E-03	2.45E-03	5.01E-03
2-Methyl-1-propanol	2.47E-03	3.17E-03	1.25E-03	2.57E-03	1.11E-01	7.98E-02	2.79E-03	2.19E-02	4.23E-02	1.59E-03	2.88E-02	3.88E-03	4.82E-01	2.19E-03	2.30E-03	2.44E-03	3.23E-03	1.58E-02
3-Methyl-butanal	2.14E-03	1.83E-03	4.39E-04	4.16E-04	1.35E-03	7.52E-04	4.27E-04	7.55E-04	0.00E+00	5.84E-04	1.69E-02	2.33E-04	6.89E-04	1.28E-03	8.99E-04	1.22E-02	4.29E-04	4.33E-03
1-Butanol	9.46E-04	5.20E-04	7.85E-04	8.63E-04	4.21E-04	2.14E-04	4.70E-04	9.01E-04	1.29E-03	6.08E-04	4.04E-01	7.74E-04	1.10E+00	2.61E-03	0.00E+00	1.15E-03	7.24E-04	1.22E-03
2-Methyl-butanal	2.34E-03	2.95E-03	2.84E-04	1.53E-03	1.41E-03	3.07E-03	1.03E-03	2.19E-04	6.39E-04	4.26E-04	1.42E-02	1.01E-03	0.00E+00	2.11E-03	1.90E-03	2.35E-03	3.35E-04	2.96E-03
2-Pentanone	2.74E-02	3.34E-02	1.07E-01	4.33E-02	7.95E-02	1.34E-01	1.80E-01	1.14E-01	1.15E-01	1.47E-01	2.46E-01	1.15E-01	4.76E-02	4.37E-02	3.11E-02	6.53E-01	5.40E-01	2.03E-01
2-Pentanol	7.28E-03	6.39E-03	5.67E-03	1.09E-02	1.84E-02	2.21E-02	9.84E-03	1.06E-02	1.24E-02	9.41E-03	1.66E-02	7.50E-03	3.77E-03	8.91E-03	5.04E-03	1.42E-02	1.14E-02	2.03E-02

Yeast inoculum (CFU mL^{-1})

T. beigelii

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
3-Hydroxy-2-butanone	2.51E-03	1.43E-03	1.68E-03	1.32E-03	3.66E-03	4.36E-03	1.86E-03	4.77E-03	1.79E-03	1.70E-03	2.77E+00	1.18E-03	0.00E+00	1.34E-03	1.21E-03	2.27E-03	1.08E-03	1.33E-03
Ethyl ester propanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Methyl-cyclohexane	6.10E-02	6.33E-02	1.91E-02	7.34E-02	4.89E-02	6.05E-02	5.00E-02	3.01E-02	2.73E-02	4.19E-02	4.58E-02	3.83E-02	3.24E-02	7.17E-02	5.66E-02	5.01E-02	3.69E-02	6.37E-02
n-Propyl acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-butanol	1.61E-02	1.72E-02	1.72E-02	2.62E-02	2.10E-01	1.75E-01	8.49E-03	3.87E-02	4.33E-02	1.72E-02	1.00E-01	1.58E-02	2.13E-01	9.89E-03	5.15E-03	4.03E-02	2.62E-02	1.23E-01
2-Methyl-1-butanol	1.71E-03	5.38E-03	2.49E-03	3.11E-03	7.69E-02	6.20E-02	4.46E-03	1.87E-02	3.30E-02	6.41E-03	1.56E-02	2.77E-03	1.96E-02	1.53E-03	2.05E-03	6.01E-03	3.56E-03	1.65E-02
Dimethyl-disulfide	7.10E-04	9.53E-04	1.37E-04	2.89E-04	2.67E-04	5.58E-04	1.32E-04	2.17E-04	3.09E-05	4.01E-04	5.06E-03	4.08E-05	2.32E-04	3.78E-03	2.50E-03	7.38E-04	2.48E-05	9.25E-04
3-Methyl-2-pentanone	2.50E-04	2.48E-04	1.77E-04	2.73E-04	3.43E-04	4.68E-04	9.81E-05	8.60E-05	1.90E-04	4.63E-04	2.09E-04	1.34E-04	0.00E+00	4.37E-04	1.34E-04	3.31E-04	3.49E-04	1.03E-03
2-Methyl-ethyl ester propanoic acid	1.55E-02	1.83E-02	1.04E-02	2.72E-02	1.49E-02	1.98E-02	1.32E-02	1.71E-02	1.07E-02	1.41E-02	1.55E-02	1.48E-02	8.44E-03	2.96E-02	1.55E-02	1.50E-02	1.26E-02	2.24E-02
2-Methyl-heptane	8.24E-02	1.09E-01	3.25E-02	1.48E-01	7.98E-02	1.30E-01	6.58E-02	4.71E-02	4.09E-02	7.13E-02	7.92E-02	6.92E-02	4.94E-02	1.44E-01	7.58E-02	9.41E-02	7.59E-02	1.30E-01
1-Pentanol	6.19E-03	1.22E-02	2.39E-03	1.29E-02	4.42E-03	7.75E-03	5.23E-03	2.14E-03	2.75E-03	3.18E-03	6.07E-03	4.73E-03	1.87E-03	4.59E-03	4.97E-03	8.88E-03	7.37E-03	7.33E-03
Isobutyl acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-heptane	2.23E-03	2.90E-03	1.21E-03	2.27E-03	2.49E-03	3.71E-03	2.17E-03	0.00E+00	1.68E-03	1.78E-03	1.42E-03	1.69E-03	1.86E-03	2.81E-03	1.65E-03	1.74E-03	1.28E-03	3.17E-03
2-Hexanone	1.29E-03	9.78E-04	1.24E-03	1.72E-03	9.11E-04	3.45E-03	2.11E-03	1.40E-03	8.03E-04	8.91E-03	2.32E-02	2.57E-03	1.85E-03	3.62E-03	1.46E-03	7.58E-02	1.10E-01	2.36E-02
Octane	5.93E-02	5.94E-02	2.18E-02	8.39E-02	5.39E-02	6.49E-02	4.19E-02	2.84E-02	2.62E-02	4.44E-02	4.36E-02	4.10E-02	3.56E-02	7.18E-02	5.04E-02	5.87E-02	5.08E-02	7.48E-02
Butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.59E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-butanoic acid	5.62E-04	4.19E-04	8.30E-04	1.19E-03	3.10E-03	2.12E-01	1.94E-04	1.74E-03	1.16E-03	0.00E+00	2.23E-03	2.99E-04	1.27E-03	1.24E-03	3.72E-04	4.76E-03	0.00E+00	1.57E-02
2-Methyl-butanoic acid	1.52E-04	0.00E+00	0.00E+00	5.66E-04	0.00E+00	4.15E-02	3.08E-04	8.29E-04	1.78E-04	9.31E-05	0.00E+00	2.92E-04	9.36E-04	5.11E-04	0.00E+00	2.15E-04	2.58E-04	6.28E-03
Pentanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-1-butanol, acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Heptanone	1.36E-01	1.15E-01	1.10E-01	1.51E-01	8.09E-02	9.27E-02	1.88E-01	5.49E-02	4.18E-02	2.20E+00	3.06E+00	1.26E-01	7.02E-02	1.27E-01	1.20E-01	1.17E+01	1.26E+01	3.59E+00
Styrene	2.49E-03	2.84E-03	1.61E-03	3.59E-03	1.88E-02	1.51E-02	5.19E-03	3.93E-03	1.78E-03	7.30E-02	3.06E-02	1.63E-01	2.57E-03	2.32E-03	1.01E-03	2.07E-01	2.02E-01	3.29E-01

Yeast inoculum (CFU mL^{-1})

T. beigelii

LRI Suggested Compound	10^8	10^8	10^8	10^8 + spores	10^8 + spores	10^8 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
2-Heptanol	4.58E-02	3.79E-02	8.79E-03	7.42E-03	9.31E-03	9.84E-03	2.11E-02	7.35E-03	4.61E-03	1.95E-02	5.18E-02	3.42E-03	8.29E-03	3.50E-02	1.07E-02	8.05E-02	1.45E-01	1.62E-01
a-Pinene	2.86E-03	3.18E-03	2.66E-03	2.52E-03	2.94E-03	4.51E-03	1.98E-03	2.45E-03	3.09E-03	2.92E-03	1.85E-03	3.76E-03	2.94E-03	3.73E-03	1.49E-03	1.56E-03	3.01E-03	4.82E-03
Unidentified	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Octanone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Hexanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Octanone	1.78E-03	4.15E-03	7.84E-04	2.36E-03	2.08E-03	1.51E-03	9.42E-04	1.95E-03	1.38E-03	2.76E-02	5.38E-02	2.81E-03	1.62E-03	1.45E-03	1.83E-03	4.17E-01	4.36E-01	7.59E-02
Hexanoic acid, ethyl ester	3.89E-03	3.77E-03	3.30E-04	9.31E-04	1.16E-03	1.21E-03	6.17E-04	2.16E-04	1.80E-04	4.02E-04	3.34E-02	1.48E-04	4.03E-04	1.16E-03	5.03E-04	6.38E-02	1.61E-03	1.46E-02
4-Methylanisole	1.13E-04	2.63E-04	2.18E-04	7.02E-04	0.00E+00	1.22E-03	1.34E-04	1.04E-04	1.50E-04	1.69E-03	1.09E-03	6.71E-04	0.00E+00	1.50E-03	3.10E-04	2.50E-03	3.03E-03	9.49E-03
Butanoic acid, 3-methylbutyl ester	3.26E-04	4.15E-04	6.31E-04	9.86E-04	2.05E-03	1.25E-03	3.61E-04	4.67E-04	2.77E-04	1.00E-03	4.47E-03	4.07E-04	1.14E-03	1.02E-03	4.38E-04	1.17E-02	1.83E-03	1.20E-02
8-Nonen-2-one	1.10E-03	6.77E-03	1.25E-03	5.04E-03	1.50E-03	2.27E-03	1.18E-03	2.31E-03	2.05E-03	2.79E-02	4.83E-02	1.56E-03	2.39E-03	2.72E-03	1.44E-03	1.04E+00	1.13E+00	1.53E-01
2-Nonanone	3.46E-02	9.77E-03	8.21E-03	1.18E-02	1.01E-02	2.07E-02	4.47E-02	2.93E-02	3.68E-02	2.67E-01	8.81E-01	2.70E-02	8.62E-03	1.25E-02	2.70E-02	1.03E+01	8.22E+00	1.67E+00
Benzeneethanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Hexanoic acid, butyl ester	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Octanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Decanone	3.00E-04	2.85E-04	0.00E+00	3.16E-04	0.00E+00	5.85E-04	1.02E-03	8.78E-04	4.65E-04	2.29E-03	6.28E-03	6.63E-04	0.00E+00	5.69E-04	3.54E-04	4.18E-02	1.81E-02	2.61E-03
Octanoic acid, ethyl ester	8.06E-04	4.38E-04	1.12E-04	1.78E-04	6.47E-04	2.01E-04	7.13E-04	2.58E-04	4.55E-05	5.63E-05	1.93E-03	4.11E-05	5.94E-04	8.36E-04	8.82E-04	8.21E-04	7.33E-05	1.10E-03
3-Methybutyl hexanoate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Acetic acid, 2-phenylethyl ester	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Undecanone	9.30E-04	4.97E-04	5.95E-04	1.30E-03	5.66E-04	9.35E-04	1.48E-03	1.56E-03	1.35E-03	2.83E-03	4.56E-03	1.51E-03	8.51E-04	3.12E-03	6.59E-04	2.31E-01	7.69E-02	1.03E-02
n-decanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

LRI Suggested Compound	Model inoculum: *Y. lipolytica* trials Milk	Milk	Milk	Spore only	Spore only	Spore only	*K. lactis* trials Milk	Milk	Milk	Spore only	Spore only	Spore only	*D. hansenii* & *T. beigelii* trials Milk	Milk	Milk	Spore only	Spore only	Spore only
Acetaldehyde	7.63E-03	0.00E+00	0.00E+00	2.42E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.18E-03	9.76E-04	1.98E-03	2.86E-03	1.34E-03	2.88E-03
Methanethiol	1.77E-03	1.46E-03	5.58E-03	8.92E-04	2.25E-03	7.36E-04	2.09E-03	1.84E-03	6.55E-04	7.62E-05	1.19E-03	5.61E-04	0.00E+00	3.27E-03	1.39E-03	0.00E+00	0.00E+00	2.82E-04
Ethanol	5.41E-02	1.59E-02	3.65E-02	4.06E-01	3.99E-02	1.01E-01	3.45E-02	5.90E-02	4.75E-02	1.48E-02	2.94E-02	3.38E-02	2.82E-02	1.14E-02	6.86E-03	1.69E-02	2.15E-02	8.06E-03
Acetone	1.37E-01	1.25E-01	1.86E-01	3.09E-02	3.76E-02	7.06E-02	1.44E-01	1.62E-01	1.66E-01	5.26E-02	2.91E-02	2.54E-02	5.69E-01	3.56E-01	3.21E-01	5.66E-01	1.29E-01	1.55E-01
1-propanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl propanal	1.21E-03	3.07E-04	7.72E-04	1.64E-03	0.00E+00	2.38E-04	6.49E-04	6.07E-04	7.26E-04	4.61E-04	1.65E-03	4.00E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	3.20E-03	1.13E-03	4.20E-03	0.00E+00	1.86E-02	1.15E-02	1.41E-03	4.47E-03	4.67E-03	0.00E+00	7.31E-04	0.00E+00	2.72E-02	1.07E-02	1.41E-02	1.16E-02	3.46E-03	2.23E-03
2-Butanone	1.25E-01	1.13E-01	1.35E-01	1.36E-02	1.18E-02	1.59E-02	1.22E-01	1.47E-01	1.49E-01	1.44E-02	1.20E-02	1.62E-02	3.81E-01	2.65E-01	2.28E-01	1.06E-01	5.31E-02	5.22E-02
Ethylacetate	3.10E-01	7.49E-03	1.04E-02	4.89E-03	0.00E+00	3.08E-03	2.54E-03	7.62E-03	4.86E-03	1.12E-03	1.65E-03	2.05E-03	5.81E-03	1.77E-03	1.38E-03	1.78E-03	3.47E-03	1.06E-03
2-Methyl-1-propanol	0.00E+00	0.00E+00	4.20E-03	9.89E-03	3.90E-03	3.44E-03	2.47E-03	0.00E+00	1.20E-03	2.44E-03	2.82E-03	1.78E-03	1.47E-03	5.49E-04	1.02E-03	1.59E-03	1.06E-02	5.95E-03
3-Methyl-butanal	1.13E-03	0.00E+00	1.23E-03	1.24E-02	9.42E-05	1.37E-02	2.12E-04	0.00E+00	0.00E+00	2.44E-03	1.80E-02	4.77E-03	1.42E-03	7.22E-04	1.07E-03	6.15E-03	1.21E-03	7.02E-04
1-Butanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.43E-03	1.21E-03	0.00E+00	1.36E-03	3.27E-04	6.35E-04
2-Methyl-butanal	5.90E-03	8.15E-04	8.38E-03	5.34E-03	2.43E-04	2.53E-03	3.22E-03	1.39E-03	0.00E+00	9.58E-04	4.38E-03	7.33E-04	4.13E-03	4.11E-03	1.59E-03	3.82E-03	9.74E-04	4.91E-04
2-Pentanone	1.05E-02	1.01E-02	2.49E-02	6.72E-01	8.99E-01	1.15E+00	1.10E-02	1.11E-02	1.11E-02	9.94E-02	6.12E-02	1.36E-01	2.32E-02	2.14E-02	1.88E-02	2.32E+00	8.45E-01	1.53E+00
2-Pentanol	1.50E-03	1.98E-03	4.98E-04	3.24E-03	1.25E-03	3.13E-03	2.18E-03	1.53E-03	1.00E-03	6.57E-03	4.96E-03	3.93E-03	0.00E+00	6.32E-03	8.23E-03	4.99E-02	9.09E-03	2.16E-02
3-Hydroxy-2-butanone	6.45E-03	4.59E-03	3.64E-03	1.72E-03	1.12E-02	1.12E-01	3.15E-03	4.42E-03	7.42E-03	3.27E-03	4.12E-04	0.00E+00	3.64E-03	0.00E+00	0.00E+00	9.22E-03	2.56E-03	1.10E-03
Ethyl ester propanoic acid	4.61E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.65E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Methyl-cyclohexane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.76E-02	5.73E-02	5.54E-02	4.62E-02	2.85E-02	2.03E-02
n-Propyl acetate	4.78E-04	0.00E+00	0.00E+00	6.73E-04	3.94E-04	4.98E-04	1.39E-04	0.00E+00	0.00E+00	1.50E-03	4.71E-04	1.78E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-butanol	2.51E-03	0.00E+00	1.92E-03	1.96E-02	5.92E-02	2.70E-02	0.00E+00	5.71E-04	0.00E+00	8.97E-03	7.61E-03	8.16E-03	5.02E-03	5.42E-03	3.23E-03	6.61E-03	9.13E-02	7.18E-02
2-Methyl-1-butanol	2.28E-03	2.95E-04	6.70E-04	9.27E-03	5.92E-03	6.70E-03	0.00E+00	3.64E-04	0.00E+00	2.04E-03	2.45E-03	2.33E-03	3.70E-04	1.34E-04	2.75E-03	7.49E-04	2.13E-02	1.22E-02
Dimethyl-disulfide	7.00E-04	1.55E-03	1.69E-02	1.64E-03	2.74E-03	1.20E-03	1.47E-03	1.14E-03	2.09E-04	4.22E-04	1.31E-03	9.52E-04	1.04E-02	1.47E-02	1.60E-02	3.92E-03	2.80E-03	2.06E-03
3-Methyl-2-pentanone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E-04	0.00E+00	0.00E+00	0.00E+00	4.88E-05	7.63E-05	5.00E-05	6.35E-04	4.44E-04	1.03E-04	1.28E-03	5.21E-04	6.79E-04

LRI Suggested Compound	Model inoculum																	
	Y. lipolytica trials						*K. lactis* trials						*D. hansenii* & *T. beigelii* trials					
	Milk	Milk	Milk	Spore only	Spore only	Spore only	Milk	Milk	Milk	Spore only	Spore only	Spore only	Milk	Milk	Milk	Spore only	Spore only	Spore only
2-Methyl-ethyl ester propanoic acid	2.03E-02	1.18E-02	1.25E-02	6.50E-03	6.03E-03	4.92E-03	2.03E-02	2.08E-02	2.21E-02	1.03E-02	1.31E-02	1.20E-02	1.28E-02	2.47E-02	2.27E-02	1.70E-02	1.04E-02	1.39E-02
2-Methyl-heptane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.94E-02	1.03E-01	9.69E-02	1.09E-01	7.05E-02	1.02E-01
1-Pentanol	2.97E-03	1.83E-03	2.52E-03	1.40E-02	6.00E-03	4.96E-03	2.80E-03	2.50E-03	3.12E-03	7.01E-02	2.46E-02	2.23E-02	6.18E-03	5.93E-03	2.92E-03	4.81E-02	9.32E-03	8.11E-02
Isobutyl acetate	2.69E-02	1.08E-02	1.36E-02	1.33E-02	7.94E-03	4.24E-03	1.74E-02	1.69E-02	1.85E-02	7.68E-03	1.03E-02	6.35E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-heptane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.89E-03	2.85E-03	2.14E-03	3.23E-03	1.91E-03	1.48E-03
2-Hexanone	6.20E-03	1.67E-03	4.75E-03	1.26E-01	1.89E-01	1.97E-01	1.82E-03	1.84E-03	2.27E-03	2.57E-02	1.56E-02	3.56E-02	3.23E-03	1.18E-03	1.70E-03	2.80E-01	1.69E-01	3.14E-01
Octane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.90E-02	6.29E-02	5.74E-02	6.80E-02	4.36E-02	3.86E-02
Butanoic acid	2.33E-02	1.45E-02	1.84E-02	1.27E-02	1.14E-02	7.84E-03	1.91E-02	2.16E-02	3.69E-02	1.18E-02	1.37E-02	1.32E-02	0.00E+00	0.00E+00	0.00E+00	2.00E-02	0.00E+00	0.00E+00
3-Methyl-butanoic acid	0.00E+00	0.00E+00	2.51E-01	0.00E+00	0.00E+00	3.12E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.29E-03	1.23E-03	2.47E-04	2.81E-03	3.17E-04	4.17E-04
2-Methyl-butanoic acid	0.00E+00	0.00E+00	5.00E-04	1.16E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.52E-04	0.00E+00	0.00E+00	2.64E-04
Pentanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.66E-04	2.33E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E-04	1.05E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-1-butanol, acetate	1.63E-03	0.00E+00	2.28E-04	0.00E+00	0.00E+00	3.38E-04	0.00E+00	0.00E+00	3.74E-04	0.00E+00	0.00E+00	3.49E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Heptanone	1.14E-01	1.05E-01	2.28E-01	5.31E+00	8.03E+00	8.98E+00	1.44E-01	1.05E-01	1.35E-01	2.56E+00	1.59E+00	2.74E+00	2.46E-01	1.80E-01	1.32E-01	1.61E+01	1.61E+01	2.11E+01
Styrene	1.09E-02	1.58E-03	4.96E-04	2.34E-03	4.74E-04	8.47E-04	9.47E-04	1.52E-03	2.90E-03	3.99E-03	5.80E-04	5.44E-04	2.07E-03	2.28E-02	1.43E-03	4.24E-03	4.03E-03	3.05E-03
2-Heptanol	0.00E+00	0.00E+00	4.45E-03	1.06E-01	2.00E-02	5.41E-02	0.00E+00	0.00E+00	0.00E+00	1.00E-01	8.87E-02	6.71E-02	6.97E-03	4.58E-03	2.59E-03	1.12E-01	7.39E-02	1.99E-01
a-Pinene	9.89E-04	6.14E-04	6.51E-04	6.26E-04	4.63E-04	5.61E-04	2.11E-03	2.45E-03	4.31E-03	6.05E-04	7.76E-04	1.04E-03	5.94E-03	4.21E-03	2.62E-03	2.50E-03	1.11E-03	1.52E-03
Unidentified	0.00E+00	0.00E+00	2.68E-04	0.00E+00	1.27E-04	0.00E+00	0.00E+00	0.00E+00	2.32E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	0.00E+00	0.00E+00	4.38E-04	1.62E-03	0.00E+00	6.45E-04	0.00E+00	3.77E-04	0.00E+00	2.52E-04	2.36E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Octanone	0.00E+00	0.00E+00	0.00E+00	7.41E-04	1.59E-04	7.37E-05	0.00E+00	0.00E+00	0.00E+00	1.02E-04	2.74E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Hexanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.49E-02	0.00E+00	0.00E+00
2-Octanone	2.22E-03	7.70E-04	1.70E-03	2.03E-01	3.85E-01	5.58E-01	8.99E-04	6.62E-04	8.20E-04	8.95E-02	4.89E-02	7.87E-02	3.94E-03	1.69E-03	2.15E-03	3.85E-01	6.07E-01	1.14E+00
Hexanoic acid, ethyl ester	2.56E-04	1.13E-03	7.34E-04	2.54E-03	3.72E-04	7.99E-04	0.00E+00	0.00E+00	0.00E+00	1.37E-04	3.57E-04	4.47E-04	6.78E-04	2.52E-04	2.16E-05	1.62E-03	2.16E-04	0.00E+00
4-Methylanisole	0.00E+00	0.00E+00	0.00E+00	3.94E-03	2.92E-03	2.94E-03	0.00E+00	3.84E-05	0.00E+00	6.17E-03	3.00E-03	2.17E-03	2.78E-03	2.12E-04	3.24E-04	1.51E-04	1.68E-03	4.78E-03

	Model inoculum																	
	Y. lipolytica trials						*K. lactis* trials						*D. hansenii* & *T. beigelii* trials					
LRI Suggested Compound	Milk	Milk	Milk	Spore only	Spore only	Spore only	Milk	Milk	Milk	Spore only	Spore only	Spore only	Milk	Milk	Milk	Spore only	Spore only	Spore only
Butanoic acid, 3-methylbutyl ester	0.00E+00	1.46E-04	0.00E+00	1.08E-03	1.27E-03	7.91E-04	0.00E+00	2.81E-04	0.00E+00	0.00E+00	1.37E-04	0.00E+00	2.61E-03	1.15E-03	4.48E-04	9.20E-04	3.03E-03	2.48E-03
8-Nonen-2-one	0.00E+00	2.85E-03	2.23E-02	5.95E-01	1.12E+00	1.90E+00	8.54E-03	0.00E+00	0.00E+00	2.47E-01	1.15E-01	1.95E-01	2.14E-03	1.05E-03	9.17E-04	8.68E-01	1.95E+00	3.22E+00
2-Nonanone	2.21E-02	2.65E-02	2.30E-02	3.25E+00	4.44E+00	6.79E+00	4.63E-02	1.68E-02	2.61E-02	1.93E+00	1.17E+00	1.73E+00	2.78E-02	2.18E-02	2.17E-02	7.44E+00	1.00E+01	1.51E+01
Benzeneethanol	4.51E-04	0.00E+00	2.34E-04	1.59E-03	1.31E-03	5.11E-04	2.48E-04	2.18E-04	0.00E+00	2.15E-03	3.19E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Hexanoic acid, butyl ester	0.00E+00	0.00E+00	0.00E+00	9.98E-05	0.00E+00	0.00E+00	7.22E-05	6.42E-05	0.00E+00	1.25E-04	0.00E+00	6.69E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Octanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.74E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Decanone	1.89E-04	1.39E-04	9.38E-05	0.00E+00	0.00E+00	4.63E-02	2.11E-04	0.00E+00	0.00E+00	5.15E-03	0.00E+00	3.31E-03	1.59E-03	7.06E-04	5.20E-04	1.19E-02	5.16E-02	1.08E-01
Octanoic acid, ethyl ester	4.12E-04	1.85E-03	1.96E-03	2.20E-03	1.62E-03	3.31E-03	1.06E-04	0.00E+00	7.46E-05	4.50E-04	1.66E-03	1.18E-03	7.38E-04	3.69E-04	2.28E-04	1.18E-03	3.48E-04	8.93E-05
3-Methybutyl hexanoate	0.00E+00	2.66E-04	5.99E-05	0.00E+00	0.00E+00	2.08E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.33E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Acetic acid, 2-phenylethyl ester	3.31E-03	2.54E-03	4.20E-03	5.31E-03	1.63E-03	1.77E-02	5.98E-03	1.53E-03	0.00E+00	5.30E-03	4.91E-03	1.96E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Undecanone	3.44E-03	2.96E-03	2.40E-03	7.82E-02	2.67E-01	4.11E-01	3.68E-03	2.84E-03	3.89E-03	7.62E-02	3.51E-02	5.90E-02	5.52E-03	2.47E-03	1.02E-03	8.04E-02	3.69E-01	8.52E-01
n-decanoic acid	2.95E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Unidentified	0.00E+00	4.50E-04	1.12E-04	5.37E-04	7.00E-04	1.07E-03	1.62E-04	8.28E-05	0.00E+00	2.67E-04	3.98E-04	1.59E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Appendix 8. ANOVA of aroma compounds generated (Appendix 7) in models inoculatd with *Y. lipolytica* at three concentrations.

Only compounds which distinguish between models are shown

Summary of all pairwise comparisons for Q1 (Fisher (LSD)):

Category	LS means(Methanethiol)	Groups	
10^8	669671.127	A	
Milk	417885.057	A	B
P.roq	183901.908		B
10^5	162679.259		B
10^2	105253.085		B
10^5 + spores	69750.114		B
10^8 + spores	49728.296		B
10^2 + spores	35587.727		B

Category	LS means(Acetone)	Groups			
10^5	49979997.648	A			
10^2	31591857.014		B		
10^8	25053055.535		B	C	
Milk	21200487.196		B	C	
10^8 + spores	18310899.371		B	C	D
10^2 + spores	15786681.761			C	D
10^5 + spores	11848502.131			C	D
P.roq	6591085.699				D

Category	LS means(2-methyl propanal)	Groups		
10^8	2312766.067	A		
10^5	1301295.410	A	B	
10^2	689114.865		B	C
10^8 + spores	287041.361		B	C
Milk	108630.463			C
P.roq	88864.119			C
10^5 + spores	73918.844			C
10^2 + spores	43961.434			C

Category	LS means(2-Butanone)	Groups	
10^2	21850321.441	A	
10^5	21080354.612	A	
Milk	17728754.955	A	
10^8	17476599.056	A	
10^8 + spores	5874754.330		B
10^2 + spores	3174716.352		B
10^5 + spores	3095533.094		B
P.roq	1957668.388		B

Category	LS means(2-Methyl-1-propanol)	Groups			
10^5	2748175.665	A			
10^2	1610743.801		B		
10^8	1394906.942		B	C	
P.roq	816729.605		B	C	D
10^2 + spores	695422.298		B	C	D
10^5 + spores	449213.362			C	D
10^8 + spores	379072.489			C	D
Milk	198844.368				D

Category	LS means(3-Methyl-butanal)	Groups	
10^5	4501966.528	A	
10^8	3922495.298	A	B
10^2	1649092.577	A	B
P.roq	1240750.035	A	B
10^8 + spores	580096.345	A	B
10^2 + spores	413188.798	A	B
10^5 + spores	149732.296		B
Milk	112149.723		B

Category	LS means(2-Methyl-butanal)	Groups		
10^8	4315934.301	A		
10^5	3291135.575	A	B	
10^2	2068750.088	A	B	C
Milk	715592.216		B	C
10^8 + spores	590569.028		B	C
P.roq	384538.104		B	C
10^5 + spores	226834.660			C
10^2 + spores	222954.868			C

Category	LS means(2-Pentanone)	Groups			
10^8 + spores	321362865.778	A			
10^5 + spores	156643438.330		B		
P.roq	128781897.225		B	C	
10^2 + spores	83623881.912			C	
10^5	11943571.874				D
10^8	10667481.717				D
10^2	8433881.792				D
Milk	2153017.267				D

Category	LS means(2-Pentanol)	Groups	
10^5 + spores	5124770.543	A	
10^2 + spores	1356828.110		B
10^8 + spores	367493.788		B
10^8	361000.673		B
P.roq	360960.543		B
10^5	300179.784		B
Milk	188268.165		B
10^2	88977.368		B

Category	LS means(3-Hydroxy-2-butanone)	Groups	
P.roq	5938412.675	A	
10^2 + spores	3146420.079	A	B
Milk	695430.394	A	B
10^2	614268.995	A	B
10^5	576741.437	A	B
10^8	414404.628	A	B
10^8 + spores	70257.015		B
10^5 + spores	26761.210		B

Category	LS means(n-Propyl acetate)	Groups	
P.roq	74144.021	A	
10^2 + spores	68903.770	A	
10^5 + spores	56481.156	A	B
Milk	22640.625	A	B
10^8 + spores	18198.629	A	B
10^5	7429.856	A	B
10^2	6273.120	A	B
10^8	0.000		B

Category	LS means(3-Methyl-butanol)	Groups	
10^5	37316017.431	A	
10^8	12497190.152		B
10^2	10954459.780		B
10^2 + spores	7417264.051		B
P.roq	5011517.936		B
10^5 + spores	4609277.556		B
10^8 + spores	2855525.116		B
Milk	209803.135		B

Category	LS means(2-Methyl-1-butanol)	Groups		
10^5	2930105.206	A		
10^2	1423009.781		B	
10^8	1291613.022		B	C
10^2 + spores	1225976.916		B	C
P.roq	1037427.027		B	C
10^5 + spores	559217.924		B	C
10^8 + spores	358526.630		B	C
Milk	153757.495			C

Category	LS means(Dimethyl-disulfide)	Groups	
10^8	1506211.105	A	
Milk	906743.399	A	B
10^5	475074.921	A	B
10^2	446292.082	A	B
P.roq	264139.057		B
10^5 + spores	135048.977		B
10^2 + spores	118420.062		B
10^8 + spores	36561.573		B

Category	LS means(3-Methyl-2-pentanone)	Groups		
10^5	141856.255	A		
10^8	72193.672		B	
10^5 + spores	59751.819		B	C
10^2	39353.767		B	C
10^8 + spores	34155.495		B	C
10^2 + spores	29563.404		B	C
P.roq	4945.591		B	C
Milk	0.000			C

Category	LS means(2-Methyl-ethyl ester propanoic acid)	Groups			
10^5	2780055.803	A			
10^2	2556145.732	A			
Milk	2112788.836	A	B		
10^8	1911488.472	A	B	C	
10^2 + spores	1118560.652		B	C	D
10^5 + spores	871595.601			C	D
P.roq	826591.095				D
10^8 + spores	711273.767				D

Category	LS means(1-Pentanol)	Groups		
10^2 + spores	2201561.571	A		
10^5 + spores	1539548.794	A	B	
10^5	1534425.205	A	B	
P.roq	1182503.918		B	C
10^2	667833.023		B	C
10^8	656574.721		B	C
10^8 + spores	444115.270			C
Milk	346642.050			C

Category	LS means(Isobutyl acetate)	Groups		
10^5	3169649.341	A		
10^2	2752930.996	A	B	
Milk	2428824.137	A	B	C
10^8	2016421.274	A	B	C
10^5 + spores	1315712.690		B	C
P.roq	1208705.063		B	C
10^2 + spores	967785.233			C
10^8 + spores	921114.860			C

Category	LS means(2-Hexanone)	Groups			
10^8 + spores	67821793.736	A			
10^5 + spores	41903100.839		B		
P.roq	24226634.891			C	
10^2 + spores	18189504.088			C	
10^8	1970330.650				D
10^5	1917433.334				D
10^2	1853275.593				D
Milk	598107.884				D

Category	LS means(Octane)	Groups		
10^2	471193518.392	A		
10^8	447989246.645	A		
10^5	294084908.960	A	B	
10^8 + spores	249500114.018	A	B	C
10^5 + spores	182521671.807		B	C
10^2 + spores	82147800.467		B	C
Milk	0.000			C
P.roq	0.000			C

Category	LS means(Butanoic acid)	Groups	
10^2	4178787.831	A	
10^5	4074624.179	A	
10^8	3296083.033	A	B
Milk	2666051.861	A	B
10^2 + spores	2022203.985		B
10^5 + spores	1902767.226		B
10^8 + spores	1794494.947		B
P.roq	1514860.329		B

Category	LS means(Pentanoic acid)	Groups		
10^2	7490448.820	A		
10^8	7110426.746	A		
10^5	4885906.536	A	B	
10^5 + spores	2328174.709		B	C
10^2 + spores	1095336.639		B	C
P.roq	23674.825			C
10^8 + spores	0.000			C
Milk	0.000			C

Category	LS means(2-Heptanone)	Groups		
10^8 + spores	1985346318.803	A		
10^5 + spores	1594569279.228	A		
P.roq	1057373430.446		B	
10^2 + spores	1036982232.620		B	
10^2	140096031.249			C
10^8	136091160.532			C
10^5	83460705.509			C
Milk	21158647.711			C

Category	LS means(Styrene)	Groups	
10^2	9443676.588	A	
10^5	5944881.361	A	B
10^8	706026.403		B
Milk	616186.728		B
10^5 + spores	289739.422		B
10^8 + spores	260383.931		B
10^2 + spores	255568.128		B
P.roq	173592.054		B

Category	LS means(2-Heptanol)	Groups	
10^5 + spores	180136481.122	A	
10^2 + spores	38731005.310		B
10^5	26535441.502		B
10^8	23200932.013		B
10^2	21894358.188		B
P.roq	8516163.912		B
10^8 + spores	8405137.888		B
Milk	210649.311		B

Category	LS means(a-Pinene)	Groups			
10^2	119273.996	A			
10^8	117714.131	A			
Milk	106784.770	A	B		
10^5	104811.941	A	B		
P.roq	78201.615	A	B	C	
10^2 + spores	69865.194		B	C	
10^5 + spores	48663.453			C	D
10^8 + spores	24232.010				D

Category	LS means(Unidentified)	Groups		
10^8	523346.407	A		
10^2	448740.472	A	B	
10^5	381666.760	A	B	
10^5 + spores	352484.985	A	B	C
10^8 + spores	286765.709	A	B	C
10^2 + spores	121506.112		B	C
P.roq	107132.619		B	C
Milk	20748.083			C

Category	LS means(Hexanoic acid)	Groups		
10^8	511144266.024	A		
10^2	502788594.839	A		
10^5	303273630.589	A	B	
10^8 + spores	269211443.086	A	B	C
10^5 + spores	206912642.865		B	C
10^2 + spores	89261004.237		B	C
Milk	0.000			C
P.roq	0.000			C

Category	LS means(2-Octanone)	Groups	
10^8 + spores	83463016.044	A	
10^5 + spores	75300739.769	A	
P.roq	54303963.922	A	
10^2 + spores	43403413.446	A	B
10^2	1097273.798		B
10^8	1030347.749		B
10^5	771347.340		B
Milk	221849.125		B

Category	LS means(Hexanoic acid, ethyl ester)	Groups		
10^8	8950344.757	A		
10^8 + spores	5246626.377		B	
10^5 + spores	4901840.557		B	
10^2	3642884.554		B	C
10^5	1778021.903		B	C
10^2 + spores	1007369.775			C
P.roq	175802.785			C
Milk	100475.966			C

Category	LS means(4-Methylanisole)	Groups		
P.roq	464212.440	A		
10^2 + spores	75667.373		B	
10^5 + spores	18987.077		B	C
10^8 + spores	11476.446		B	C
10^8	6041.984		B	C
10^5	1613.337			C
Milk	0.000			C
10^2	0.000			C

Category	LS means(Butanoic acid, 3-methylbutyl ester)	Groups	
10^8	1130348.603	A	
10^5	815782.814	A	B
10^2	641700.516	A	B
10^2 + spores	600088.708	A	B
10^8 + spores	545591.024	A	B
10^5 + spores	489196.373	A	B
P.roq	148878.944		B
Milk	6902.773		B

Category	LS means(8-Nonen-2-one)	Groups	
10^8 + spores	253317366.889	A	
10^5 + spores	243777112.676	A	
P.roq	171323418.834	A	
10^2 + spores	136301924.402	A	
10^5	1244422.211		B
Milk	1192402.828		B
10^2	871280.583		B
10^8	233985.970		B

Category	LS means(2-Nonanone)	Groups	
P.roq	685959674.068	A	
10^5 + spores	661315579.830	A	
10^8 + spores	555980551.022	A	
10^2 + spores	454450525.124	A	
10^2	31362665.059		B
10^8	26756657.206		B
10^5	21017007.218		B
Milk	3391391.623		B

Category	LS means(Benzeneethanol)	Groups	
10^5	12285884.155	A	
10^2	3618704.720		B
10^8	2617708.040		B
10^8 + spores	1440927.462		B
10^5 + spores	390632.795		B
10^2 + spores	287761.055		B
P.roq	161488.548		B
Milk	32430.543		B

Category	LS means(Hexanoic acid, butyl ester)	Groups		
10^8	222089.641	A		
10^5	169493.058	A	B	
10^2	151654.105	A	B	C
10^8 + spores	150840.121	A	B	C
10^5 + spores	129668.139	A	B	C
10^2 + spores	53223.383		B	C
P.roq	4731.132			C
Milk	0.000			C

Category	LS means(Octanoic acid)	Groups		
10^2	128139518.881	A		
10^8	124648288.696	A		
10^8 + spores	85483567.157	A	B	
10^5 + spores	73234822.925	A	B	
10^5	62895743.405		B	
10^2 + spores	31319544.095		B	C
Milk	0.000			C
P.roq	0.000			C

Category	LS means(Octanoic acid, ethyl ester)	Groups		
10^8	3683364.880	A		
10^8 + spores	2755933.445	A	B	
10^5 + spores	2614883.593	A	B	
10^2	1750007.801	A	B	C
10^5	1513233.813		B	C
10^2 + spores	1182663.868		B	C
P.roq	337376.435			C
Milk	199694.847			C

Category	LS means(3-Methybutyl hexanoate)	Groups		
10^8	491421.167	A		
10^5	417531.276	A	B	
10^2	287629.287	A	B	C
10^8 + spores	230484.401	A	B	C
10^5 + spores	223828.322	A	B	C
10^2 + spores	96714.341		B	C
Milk	15424.939			C
P.roq	9871.294			C

Category	LS means(Acetic acid, 2-phenylethyl ester)	Groups	
10^8 + spores	4602683.567	A	
10^8	1842749.631		B
10^2 + spores	1724537.027		B
10^5	1268706.309		B
P.roq	1169192.713		B
10^5 + spores	1037722.622		B
10^2	811527.414		B
Milk	476258.338		B

Category	LS means(2-Undecanone)	Groups	
P.roq	35849354.726	A	
10^5 + spores	35223151.848	A	
10^2 + spores	13901901.928		B
10^8 + spores	10082975.527		B
10^2	3531917.735		B
10^8	3045872.711		B
10^5	2323406.121		B
Milk	416814.048		B

Category	LS means(n-decanoic acid)	Groups	
10^2	10681172.684	A	
10^8	9150213.422	A	
10^8 + spores	8499360.914	A	
10^5 + spores	6308358.616	A	B
10^5	6217097.172	A	B
10^2 + spores	1956349.494		B
Milk	139697.635		B
P.roq	0.000		B

Category	LS means(Unidentified)	Groups			
10^8	720025.198	A			
10^8 + spores	617980.456	A	B		
10^5 + spores	576966.095	A	B		
10^2	420417.380	A	B	C	
10^2 + spores	374531.827	A	B	C	D
10^5	310625.151		B	C	D
P.roq	109473.046			C	D
Milk	26597.887				D

Appendix 9. Average aroma compound generation within models following incubation at 25°C for 10 days.

Triplicate samples (Appendix 7).SPME GC-MS signal intensities for compounds are expressed relative to the signal intensity observed from a 5µg/L 2-nonanone standard.

	Model Inoculum (CFU/mL) *Y. lipoltica*															
	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk only		Spore only	
LRI suggested compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Acetaldehyde	8.76E-03	93.90	4.63E-03	141.42	0.00E+00	N/A	0.00E+00	N/A	2.20E-03	141.42	0.00E+00	N/A	2.54E-03	141.42	8.07E-03	141.42
Methanethiol	4.71E-03	61.51	3.50E-04	33.45	1.14E-03	99.82	4.91E-04	79.93	7.40E-04	114.05	2.50E-04	17.48	2.94E-03	63.77	1.29E-03	52.67
Ethanol	1.13E-01	24.66	6.88E-02	16.86	6.66E-02	68.46	1.03E-01	85.50	9.29E-02	39.10	9.79E-02	60.29	3.55E-02	43.94	1.82E-01	87.88
Acetone	1.76E-01	18.77	1.29E-01	8.92	3.52E-01	26.35	8.33E-02	14.00	2.22E-01	23.02	1.11E-01	44.30	1.49E-01	17.91	4.64E-02	37.44
1-propanol	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
2-methyl propanal	1.63E-02	14.14	2.02E-03	60.36	9.15E-03	102.89	5.20E-04	90.64	4.85E-03	50.87	3.09E-04	94.23	7.64E-04	48.47	6.25E-04	115.56
Unidentified	0.00E+00	N/A	0.00E+00	N/A	8.94E-04	141.42	2.19E-04	141.42	3.23E-04	141.42	1.37E-02	127.21	2.84E-03	45.07	1.00E-02	76.47
2-Butanone	1.23E-01	20.28	4.13E-02	24.23	1.48E-01	14.00	2.18E-02	20.52	1.54E-01	27.97	2.23E-02	3.83	1.25E-01	7.32	1.38E-02	12.17
Ethylacetate	7.65E-03	18.30	4.03E-03	38.13	5.72E-03	71.57	5.06E-03	40.06	1.21E-02	101.39	7.91E-03	36.18	1.09E-01	129.84	2.66E-03	75.96
2-Methyl-1-propanol	9.81E-03	15.73	2.67E-03	27.68	1.93E-02	45.11	3.16E-03	33.74	1.13E-02	28.58	4.89E-03	35.96	1.40E-03	141.42	5.75E-03	51.11
3-Methyl-butanal	2.76E-02	19.45	4.08E-03	56.47	3.17E-02	118.02	1.05E-03	87.83	1.16E-02	53.20	2.91E-03	79.56	7.89E-04	70.89	8.73E-03	70.19
2-Methyl-butanal	3.04E-02	22.66	4.15E-03	67.25	2.32E-02	112.60	1.60E-03	62.26	1.46E-02	41.57	1.57E-03	53.08	5.03E-03	62.59	2.70E-03	77.12
2-Pentanone	7.50E-02	21.28	2.26E+00	9.26	8.40E-02	16.68	1.10E+00	14.38	5.93E-02	20.86	5.88E-01	62.52	1.51E-02	45.54	9.06E-01	21.38
2-Pentanol	2.54E-03	30.84	2.59E-03	43.99	2.11E-03	40.65	3.60E-02	42.07	6.26E-04	84.15	9.54E-03	61.02	1.32E-03	46.57	2.54E-03	35.81
3-Hydroxy-2-butanone	2.92E-03	51.37	4.94E-04	71.05	4.06E-03	16.18	1.88E-04	141.42	4.32E-03	33.57	2.21E-02	101.39	4.89E-03	23.86	4.18E-02	119.88
Ethyl ester propanoic acid	8.64E-04	29.60	0.00E+00	N/A	1.66E-04	141.42	1.03E-04	141.42	0.00E+00	N/A	5.03E-05	141.42	1.54E-03	141.42	0.00E+00	N/A
n-Propyl acetate	0.00E+00	N/A	1.28E-04	97.48	5.23E-05	141.42	3.97E-04	77.87	4.41E-05	75.33	4.85E-04	99.81	1.59E-04	141.42	5.22E-04	22.13
3-Methyl-butanol	8.79E-02	19.45	2.01E-02	41.47	2.62E-01	52.84	3.24E-02	49.19	7.71E-02	19.82	5.22E-02	68.45	1.48E-03	72.54	3.53E-02	48.85
2-Methyl-1-butanol	9.09E-03	13.33	2.52E-03	36.63	2.06E-02	41.23	3.93E-03	34.10	1.00E-02	19.41	8.62E-03	83.47	1.08E-03	79.56	7.30E-03	19.62
Dimethyl-disulfide	1.06E-02	59.91	2.57E-04	29.87	3.34E-03	104.72	9.50E-04	43.32	3.14E-03	103.77	8.33E-04	47.79	6.38E-03	116.56	1.86E-03	34.89

Model Inoculum (CFU/mL)

Y. lipoltica

	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk only		Spore only	
LRI suggested compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
3-Methyl-2-pentanone	5.08E-04	34.23	2.40E-04	4.41	9.98E-04	48.02	4.20E-04	57.03	2.77E-04	80.92	2.08E-04	87.46	0.00E+00	N/A	3.48E-05	141.42
2-Methyl-ethyl ester propanoic acid	1.34E-02	8.98	5.00E-03	74.76	1.96E-02	27.02	6.13E-03	33.55	1.80E-02	29.09	7.87E-03	38.36	1.49E-02	26.01	5.81E-03	11.39
1-Pentanol	4.62E-03	41.01	3.12E-03	29.86	1.08E-02	35.16	1.08E-02	31.06	4.70E-03	31.78	1.55E-02	31.07	2.44E-03	19.27	8.32E-03	48.54
Isobutyl acetate	1.42E-02	21.49	6.48E-03	60.96	2.23E-02	48.18	9.26E-03	39.22	1.94E-02	27.91	6.81E-03	70.76	1.71E-02	41.03	8.50E-03	43.86
2-Hexanone	1.39E-02	12.74	4.77E-01	7.37	1.35E-02	46.34	2.95E-01	13.52	1.30E-02	23.27	1.28E-01	53.89	4.21E-03	44.88	1.70E-01	18.67
Octane	3.15E+00	37.94	1.76E+00	21.52	2.07E+00	68.61	1.28E+00	25.41	3.31E+00	34.70	5.78E-01	141.42	0.00E+00	N/A	0.00E+00	N/A
Butanoic acid	2.32E-02	17.26	1.26E-02	38.76	2.87E-02	39.63	1.34E-02	31.56	2.94E-02	28.34	1.42E-02	27.47	1.88E-02	19.26	1.07E-02	19.36
3-Methyl-butanoic acid	5.05E-03	33.05	2.35E-03	11.47	3.95E-02	67.77	5.00E-03	103.52	7.29E-03	12.83	4.35E-03	47.04	8.37E-02	141.42	1.04E-03	141.42
2-Methyl-butanoic acid	3.62E-05	141.42	1.31E-04	70.74	0.00E+00	N/A	3.44E-05	141.42	1.54E-04	71.48	3.22E-05	141.42	1.67E-04	141.42	3.86E-05	141.42
Pentanoic acid	5.00E-02	42.24	0.00E+00	N/A	3.44E-02	56.81	1.64E-02	79.91	5.27E-02	35.74	7.71E-03	141.42	0.00E+00	N/A	1.67E-04	71.17
3-Methyl-1-butanol, acetate	3.61E-04	73.89	0.00E+00	N/A	7.70E-04	84.56	6.67E-04	9.63	0.00E+00	N/A	5.80E-04	44.40	6.18E-04	116.27	1.13E-04	141.42
2-Heptanone	9.57E-01	18.71	1.40E+01	19.79	5.87E-01	53.08	1.12E+01	16.30	9.85E-01	21.53	7.29E+00	40.86	1.49E-01	37.66	7.44E+00	20.91
Styrene	4.97E-03	99.80	1.83E-03	73.10	4.18E-02	50.12	2.04E-03	34.77	6.64E-02	90.90	1.80E-03	69.96	4.33E-03	107.96	1.22E-03	66.10
2-Heptanol	1.63E-01	19.34	5.91E-02	42.88	1.87E-01	31.08	1.27E+00	35.54	1.54E-01	26.90	2.72E-01	34.05	1.48E-03	141.42	5.99E-02	58.70
a-Pinene	8.28E-04	19.72	1.70E-04	71.32	7.37E-04	3.16	3.42E-04	33.68	8.39E-04	33.91	4.91E-04	10.66	7.51E-04	22.46	5.50E-04	12.24
Unidentified	2.69E-04	71.17	0.00E+00	N/A	5.68E-04	141.42	6.34E-05	141.42	4.16E-05	141.42	2.95E-04	141.42	8.92E-05	141.42	4.22E-05	141.42
Unidentified	3.68E-03	23.31	2.02E-03	52.89	2.68E-03	94.50	2.48E-03	31.60	3.16E-03	39.71	8.55E-04	39.41	1.46E-04	141.42	7.54E-04	88.10
3-Octanone	0.00E+00	N/A	0.00E+00	N/A	5.75E-05	141.42	0.00E+00	N/A	0.00E+00	N/A	2.94E-03	141.42	0.00E+00	N/A	3.25E-04	91.36
Hexanoic acid	3.60E+00	36.37	1.89E+00	20.36	2.13E+00	76.25	1.46E+00	31.51	3.54E+00	26.62	6.28E-01	141.42	0.00E+00	N/A	0.00E+00	N/A
2-Octanone	7.25E-03	17.71	5.87E-01	50.71	5.43E-03	58.76	5.30E-01	19.05	7.72E-03	5.69	3.05E-01	71.33	1.56E-03	38.34	3.82E-01	37.89
Hexanoic acid, ethyl ester	6.30E-02	22.18	3.69E-02	27.66	1.25E-02	93.20	3.45E-02	69.19	2.56E-02	41.90	7.09E-03	45.11	7.07E-04	50.56	1.24E-03	75.77
4-Methylanisole	4.25E-05	126.28	8.07E-05	141.42	1.13E-05	141.42	1.34E-04	141.42	0.00E+00	N/A	5.32E-04	83.40	0.00E+00	N/A	3.27E-03	14.62
Butanoic acid, 3-methylbutyl ester	7.95E-03	29.52	3.84E-03	17.47	5.74E-03	118.19	3.44E-03	37.60	4.51E-03	19.09	4.22E-03	106.58	4.86E-05	141.42	1.05E-03	18.90
8-Nonen-2-one	1.65E-03	104.30	1.78E+00	46.67	8.75E-03	114.11	1.71E+00	14.87	6.13E-03	110.90	9.59E-01	76.00	8.39E-03	118.18	1.21E+00	44.36

Model Inoculum (CFU/mL)

Y. lipoltica

	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk only		Spore only	
LRI suggested compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
2-Nonanone	1.88E-01	19.76	3.91E+00	35.34	1.48E-01	61.32	4.65E+00	9.45	2.21E-01	7.37	3.20E+00	49.65	2.39E-02	7.98	4.83E+00	30.47
Benzeneethanol	1.84E-02	44.66	1.01E-02	23.15	8.64E-02	68.30	2.75E-03	18.59	2.55E-02	44.00	2.02E-03	81.70	2.28E-04	80.65	1.14E-03	40.19
Hexanoic acid, butyl ester	1.56E-03	41.37	1.06E-03	48.07	1.19E-03	99.80	9.12E-04	13.61	1.07E-03	11.29	3.74E-04	111.93	0.00E+00	N/A	3.33E-05	141.42
Octanoic acid	8.77E-01	30.88	6.01E-01	16.55	4.42E-01	75.08	5.15E-01	24.15	9.01E-01	25.99	2.20E-01	107.72	0.00E+00	N/A	0.00E+00	N/A
2-Decanone	2.91E-04	74.78	1.26E-03	141.42	3.86E-04	119.58	4.79E-03	141.42	5.61E-04	70.76	2.19E-03	71.51	1.41E-04	27.63	1.54E-02	141.42
Octanoic acid, ethyl ester	2.59E-02	20.96	1.94E-02	13.57	1.06E-02	83.81	1.84E-02	75.80	1.23E-02	36.65	8.32E-03	37.66	1.40E-03	50.09	2.37E-03	29.53
3-Methybutyl hexanoate	3.46E-03	32.45	1.62E-03	10.87	2.94E-03	115.38	1.57E-03	34.04	2.02E-03	16.48	6.80E-04	70.73	1.09E-04	104.81	6.94E-05	141.42
Acetic acid, 2-phenylethyl ester	1.30E-02	20.85	3.24E-02	66.00	8.92E-03	74.52	7.30E-03	60.87	5.71E-03	49.50	1.21E-02	34.08	3.35E-03	20.30	8.22E-03	83.72
2-Undecanone	2.14E-02	25.14	7.09E-02	37.44	1.63E-02	62.85	2.48E-01	5.21	2.48E-02	11.03	9.78E-02	56.87	2.93E-03	14.56	2.52E-01	54.02
n-decanoic acid	6.44E-02	42.29	5.98E-02	29.62	4.37E-02	75.18	4.44E-02	45.43	7.51E-02	40.31	1.38E-02	108.15	9.83E-04	141.42	0.00E+00	N/A
Unidentified	5.06E-03	25.28	4.35E-03	7.83	2.19E-03	77.84	4.06E-03	52.61	2.96E-03	18.79	2.63E-03	59.02	1.87E-04	102.14	7.70E-04	29.18

Model Inoculum (CFU/mL)

K. lactis

	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
LRI suggested compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Acetaldehyde	4.72E-02	79.65	3.82E-01	64.37	2.13E-01	90.60	3.47E-01	40.14	2.70E-01	37.75	2.90E-01	52.04	0.00E+00	N/A	0.00E+00	N/A
Methanethiol	7.45E-04	141.42	9.89E-04	128.63	1.00E-03	87.50	6.35E-04	141.42	2.88E-04	141.42	0.00E+00	N/A	1.53E-03	4.10E+01	6.08E-04	7.47E+01
Ethanol	5.86E+00	13.01	5.04E+00	4.10	5.02E+00	4.01	4.76E+00	10.60	5.32E+00	18.98	2.41E+00	50.15	4.70E-02	2.13E+01	2.60E-02	3.12E+01
Acetone	1.46E-03	74.73	5.67E-03	40.10	4.93E-03	27.97	1.12E-02	5.62	6.29E-03	25.87	1.70E-02	8.63	1.57E-01	6.29E+00	3.57E-02	3.37E+01
1-propanol	1.53E-02	72.11	2.42E-02	13.27	2.09E-02	2.94	1.85E-02	35.11	2.59E-02	50.96	1.17E-02	54.88	0.00E+00	N/A	0.00E+00	N/A
2-methyl propanal	3.25E-03	50.59	5.19E-03	24.42	4.25E-03	18.99	1.45E-02	17.03	8.41E-03	54.97	2.61E-02	31.90	6.61E-04	7.45E+00	8.38E-04	6.89E+01
Unidentified	1.00E-02	78.87	1.48E-02	93.55	2.00E-02	63.20	3.05E-02	77.25	3.18E-02	92.31	2.68E-02	54.08	3.52E-03	4.25E+01	2.44E-04	1.41E+02

Model Inoculum (CFU/mL)

K. lactis

	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
LRI suggested compound	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**
2-Butanone	2.81E-03	17.30	7.27E-03	41.72	8.50E-03	28.43	1.01E-02	19.97	1.19E-02	27.94	1.06E-02	13.57	1.40E-01	8.84E+00	1.42E-02	1.20E+01
Ethylacetate	7.15E+00	10.11	7.10E+00	5.69	6.87E+00	8.77	7.49E+00	12.85	7.12E+00	7.97	8.52E+00	5.99	5.01E-03	4.15E+01	1.61E-03	2.37E+01
2-Methyl-1-propanol	3.71E-01	33.15	2.33E-01	13.10	2.42E-01	4.95	2.31E-01	42.74	3.41E-01	62.46	1.33E-01	86.95	1.22E-03	8.25E+01	2.35E-03	1.82E+01
3-Methyl-butanal	9.17E-04	71.40	1.53E-03	17.50	9.58E-04	19.71	1.30E-02	43.70	1.90E-03	49.38	1.80E-02	55.44	7.07E-05	1.41E+02	8.39E-03	8.15E+01
2-Methyl-butanal	6.17E-03	20.55	7.44E-03	30.61	3.83E-03	19.52	6.90E-02	42.76	8.62E-03	34.29	5.26E-02	64.30	1.54E-03	8.58E+01	2.02E-03	8.24E+01
2-Pentanone	1.26E-03	26.62	1.37E-03	19.65	2.30E-03	6.27	1.92E-02	37.44	2.94E-03	51.15	8.40E-02	30.75	1.11E-02	3.83E-01	9.90E-02	3.10E+01
2-Pentanol	4.98E-04	76.09	3.49E-04	75.04	3.62E-04	78.87	2.49E-03	29.75	1.88E-04	72.35	3.57E-03	4.15	1.57E-03	3.06E+01	5.15E-03	2.11E+01
3-Hydroxy-2-butanone	4.99E-04	141.42	1.16E-02	121.08	8.36E-03	45.65	4.06E-02	33.83	2.35E-02	45.14	7.63E-02	31.91	5.00E-03	3.58E+01	1.23E-03	1.18E+02
Ethyl ester propanoic acid	3.72E-01	2.67	3.55E-01	8.07	3.27E-01	7.30	3.36E-01	22.72	3.17E-01	78.20	3.61E-01	19.41	0.00E+00	N/A	3.22E-05	1.41E+02
n-Propyl acetate	5.06E-02	12.95	5.19E-02	9.64	4.17E-02	4.87	3.39E-02	29.36	4.70E-02	32.27	1.05E-01	12.63	4.62E-05	1.41E+02	7.16E-04	7.92E+01
3-Methyl-butanol	1.88E+00	0.71	1.68E+00	6.59	1.74E+00	4.24	2.01E+00	12.41	1.88E+00	22.93	2.42E+00	27.30	1.90E-04	1.41E+02	8.25E-03	6.75E+00
2-Methyl-1-butanol	7.34E-01	14.34	7.57E-01	7.17	6.46E-01	4.61	7.42E-01	10.40	7.57E-01	30.88	5.04E-01	52.32	1.21E-04	1.41E+02	2.27E-03	7.59E+00
Dimethyl-disulfide	7.58E-04	72.24	6.50E-04	126.22	9.28E-04	80.51	2.39E-04	110.16	2.68E-04	141.42	3.81E-05	141.42	9.38E-04	5.68E+01	8.94E-04	4.07E+01
3-Methyl-2-pentanone	0.00E+00	N/A	0.00E+00	N/A	1.19E-05	141.42	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	5.84E-05	2.17E+01
2-Methyl-ethyl ester propanoic acid	1.49E-01	3.94	1.31E-01	5.52	7.60E-02	10.83	5.65E-02	31.68	9.21E-02	37.65	2.54E-02	45.87	2.11E-02	3.48E+00	1.18E-02	9.99E+00
1-Pentanol	4.64E-03	37.09	4.17E-03	33.09	2.92E-03	31.22	4.15E-03	66.67	4.55E-03	4.15	7.02E-03	73.68	2.81E-03	8.89E+00	3.90E-02	5.65E+01
Isobutyl acetate	1.79E-01	6.45	1.70E-01	9.95	1.47E-01	11.44	2.25E-01	40.14	1.44E-01	35.94	3.36E-01	3.14	1.76E-02	3.74E+00	8.11E-03	2.02E+01
2-Hexanone	7.37E-04	12.72	7.02E-04	19.39	8.97E-04	18.83	6.77E-03	40.00	1.10E-03	42.45	3.44E-02	35.53	1.98E-03	1.04E+01	2.56E-02	3.18E+01
Octane	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
Butanoic acid	1.04E-02	8.11	9.37E-03	10.95	1.07E-02	18.34	9.51E-03	29.06	1.40E-02	45.70	8.37E-03	31.45	2.59E-02	3.04E+01	1.29E-02	6.11E+00
3-Methyl-butanoic acid	0.00E+00	N/A	0.00E+00	N/A	9.20E-04	141.42	3.30E-04	141.42	4.87E-05	141.42	2.75E-03	94.03	0.00E+00	N/A	0.00E+00	N/A
2-Methyl-butanoic acid	2.53E-04	20.88	1.10E-04	72.98	9.81E-05	70.93	1.74E-04	43.21	3.04E-05	141.42	9.09E-04	96.27	0.00E+00	N/A	0.00E+00	N/A
Pentanoic acid	5.82E-05	141.42	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	6.76E-05	141.42	0.00E+00	N/A	0.00E+00	N/A	8.91E-05	7.53E+01
3-Methyl-1-butanol, acetate	2.54E-01	13.20	2.53E-01	10.67	1.86E-01	15.93	2.62E-01	21.93	1.96E-01	29.42	6.68E-01	38.12	1.25E-04	1.41E+02	1.16E-04	1.41E+02

Model Inoculum (CFU/mL)

K. lactis

	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
LRI suggested compound	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**
2-Heptanone	5.80E-02	11.29	6.06E-02	19.60	5.54E-02	12.04	7.91E-01	31.22	7.36E-02	10.20	3.08E+00	41.01	1.28E-01	1.30E+01	2.30E+00	2.20E+01
Styrene	1.03E-03	28.23	1.06E-03	38.05	1.17E-03	9.81	1.40E-03	44.79	1.52E-03	62.73	2.70E-03	92.92	1.79E-03	4.58E+01	1.70E-03	9.48E+01
2-Heptanol	3.05E-02	11.12	2.77E-02	17.40	2.90E-02	12.23	3.92E-01	40.06	2.89E-02	24.44	1.85E-01	51.52	0.00E+00	N/A	8.53E-02	1.61E+01
a-Pinene	1.47E-03	9.39	8.31E-04	7.68	1.16E-03	15.36	8.87E-04	34.86	1.17E-03	39.75	6.69E-04	27.04	2.96E-03	3.28E+01	8.07E-04	2.23E+01
Unidentified	7.47E-05	141.42	0.00E+00	N/A	3.85E-05	141.42	2.65E-04	91.83	0.00E+00	N/A	4.09E-04	84.05	7.73E-05	1.41E+02	0.00E+00	N/A
Unidentified	1.32E-03	4.30	1.16E-03	5.23	8.15E-04	48.74	1.69E-02	36.41	1.12E-03	15.29	2.36E-02	91.98	1.26E-04	1.41E+02	1.63E-04	7.08E+01
3-Octanone	0.00E+00	N/A	2.61E-05	141.42	1.95E-05	141.42	2.64E-03	89.26	0.00E+00	N/A	5.86E-04	94.96	0.00E+00	N/A	1.25E-04	9.01E+01
Hexanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
2-Octanone	5.59E-04	30.65	4.54E-04	77.14	6.37E-04	30.68	1.78E-02	29.33	1.48E-04	141.42	1.30E-01	57.69	7.94E-04	1.24E+01	7.24E-02	2.38E+01
Hexanoic acid, ethyl ester	5.44E-02	7.50	5.39E-02	13.02	4.13E-02	20.39	1.17E-01	26.71	4.83E-02	26.45	6.86E-02	90.01	0.00E+00	N/A	3.14E-04	4.15E+01
4-Methylanisole	0.00E+00	N/A	0.00E+00	N/A	3.10E-05	141.42	0.00E+00	N/A	0.00E+00	N/A	4.13E-03	46.80	1.28E-05	1.41E+02	3.78E-03	4.55E+01
Butanoic acid, 3-methylbutyl ester	7.47E-04	31.93	7.62E-04	24.23	1.18E-03	21.32	2.34E-02	34.04	1.13E-03	23.52	4.19E-02	48.05	9.38E-05	1.41E+02	4.57E-05	1.41E+02
8-Nonen-2-one	5.17E-03	51.64	4.89E-03	61.13	3.31E-03	88.25	5.28E-02	39.82	6.66E-03	71.98	3.29E-01	56.03	2.85E-03	1.41E+02	1.86E-01	2.93E+01
2-Nonanone	3.43E-02	48.43	3.71E-02	49.63	2.93E-02	60.83	4.12E-01	24.95	5.91E-02	50.48	2.23E+00	44.78	2.97E-02	4.16E+01	1.61E+00	1.99E+01
Benzeneethanol	1.44E-03	36.23	1.78E-03	52.21	7.69E-04	47.96	6.48E-03	43.60	1.58E-03	52.60	3.87E-03	102.28	1.55E-04	7.11E+01	8.24E-04	1.15E+02
Hexanoic acid, butyl ester	9.53E-05	93.03	6.68E-05	76.05	8.10E-05	71.51	5.19E-04	38.98	9.95E-05	81.36	6.81E-04	87.33	4.55E-05	7.11E+01	6.40E-05	7.99E+01
Octanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	2.58E-05	1.41E+02
2-Decanone	0.00027	96.96	0.00021	123.50	0.00024	73.34	0.00114	28.52	0.00032	141.42	0.00866	47.35	0.00007	1.41E+02	0.00282	7.56E+01
Octanoic acid, ethyl ester	4.39E-02	17.52	3.95E-02	17.86	4.38E-02	11.82	5.68E-02	42.44	4.32E-02	30.35	2.26E-02	94.85	6.01E-05	7.38E+01	1.10E-03	4.54E+01
3-Methybutyl hexanoate	1.65E-04	81.68	1.68E-04	78.25	6.72E-05	141.42	8.40E-04	69.76	0.00E+00	N/A	1.40E-03	54.97	0.00E+00	N/A	2.78E-05	1.41E+02
Acetic acid, 2-phenylethyl ester	2.84E-01	5.46	2.77E-01	18.45	2.18E-01	12.47	6.03E-01	33.11	2.18E-01	34.44	9.57E-01	17.85	2.50E-03	1.01E+02	9.94E-03	6.88E+01
2-Undecanone	3.24E-03	34.53	3.14E-03	39.01	2.49E-03	31.35	8.90E-03	22.95	5.03E-03	32.65	9.46E-02	59.43	3.47E-03	1.30E+01	5.68E-02	2.97E+01
n-decanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A

Model Inoculum (CFU/mL)

K. lactis

	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
LRI suggested compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Unidentified	8.34E-03	23.02	6.78E-03	25.82	7.21E-03	12.76	1.38E-02	54.85	6.33E-03	34.90	4.43E-03	98.61	8.16E-05	8.11E+01	2.75E-04	3.56E+01

Model Inoculum (CFU/mL)

D. hansenii

	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
LRI suggested compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Acetaldehyde	1.02E-03	6.54E+00	2.10E-03	5.59E+01	1.13E-03	3.51E+01	2.02E-02	1.27E+02	1.06E-03	5.76E+01	6.75E-03	9.78E+01	1.71E-03	3.08E+01	2.36E-03	3.06E+01
Methanethiol	3.29E-03	2.77E+01	8.43E-05	1.41E+02	2.87E-03	3.92E+01	0.00E+00	N/A	2.30E-03	2.03E+01	2.04E-04	7.16E+01	1.55E-03	8.63E+01	9.39E-05	1.41E+02
Ethanol	4.84E-02	8.75E+01	1.10E-01	7.48E+01	2.01E-02	7.74E+00	6.73E-02	8.11E+01	2.64E-02	5.76E+01	2.08E-01	1.11E+02	1.55E-02	5.94E+01	1.55E-02	3.61E+01
Acetone	3.16E-01	1.22E+01	1.53E-01	4.55E+01	3.39E-01	7.17E+00	2.38E-01	7.14E+01	3.33E-01	1.32E+01	1.71E-01	3.92E+01	4.15E-01	2.64E+01	2.84E-01	7.06E+01
Unidentified	1.06E-02	2.95E+01	4.11E-03	1.41E+01	1.10E-02	1.62E+01	1.40E-02	4.71E+01	2.01E-02	4.56E+01	7.40E-03	5.88E+01	1.73E-02	4.10E+01	5.75E-03	7.20E+01
2-Butanone	2.23E-01	1.58E+01	5.81E-02	4.75E+01	2.43E-01	9.35E+00	1.16E-01	8.97E+01	2.28E-01	1.21E+01	6.17E-02	2.25E+01	2.92E-01	2.24E+01	7.05E-02	3.57E+01
Ethylacetate	2.53E-03	3.56E+01	3.73E-03	9.30E+01	2.69E-03	4.44E+01	1.73E-03	7.07E+01	2.76E-03	1.74E+01	1.87E-03	5.36E+01	2.99E-03	6.70E+01	2.10E-03	4.82E+01
2-Methyl-1-propanol	1.00E-02	4.02E+01	7.38E-03	7.23E+01	2.30E-03	4.17E+01	3.29E-03	7.61E+01	3.91E-03	3.57E+01	1.93E-02	8.39E+01	1.02E-03	3.72E+01	6.05E-03	6.09E+01
3-Methyl-butanal	4.98E-04	3.72E+01	5.35E-03	1.27E+02	6.32E-04	4.40E+01	5.90E-03	7.16E+01	6.61E-04	4.63E+01	4.49E-02	1.18E+02	1.07E-03	2.66E+01	2.69E-03	9.14E+01
1-Butanol	8.34E-04	1.41E+02	6.29E-04	9.44E+01	6.15E-04	8.39E+01	5.49E-05	1.41E+02	9.40E-04	3.15E+01	7.48E-04	8.27E+01	8.80E-04	7.15E+01	7.74E-04	5.60E+01
2-Methyl-butanal	2.53E-03	4.46E+01	1.64E-03	8.57E+01	1.74E-03	9.10E+00	5.03E-03	1.02E+02	1.70E-03	5.84E+01	1.05E-02	1.04E+02	3.28E-03	3.64E+01	1.76E-03	8.34E+01
2-Pentanone	2.67E-02	1.62E+01	1.16E+00	2.96E+01	2.20E-02	1.36E+01	6.94E-01	1.64E+01	2.10E-02	1.31E+01	6.87E-01	6.11E+01	2.11E-02	8.49E+00	1.56E+00	3.85E+01
2-Pentanol	6.91E-03	3.04E+01	1.05E-02	1.60E+01	5.44E-03	1.48E+01	9.99E-03	2.77E+01	6.08E-03	2.67E+01	1.38E-02	2.14E+01	4.85E-03	7.25E+01	2.69E-02	6.36E+01
3-Hydroxy-2-butanone	5.42E-04	1.41E+02	1.92E-03	1.39E+01	6.63E-04	7.09E+01	2.15E-03	4.56E+01	0.00E+00	N/A	2.09E-03	3.74E+01	1.21E-03	1.41E+02	4.29E-03	8.23E+01
Methyl-cyclohexane	6.43E-02	2.34E+01	2.50E-02	1.39E+01	6.30E-02	1.32E+01	5.01E-02	3.96E+01	6.49E-02	1.41E+01	4.31E-02	1.73E+01	5.01E-02	1.77E+01	3.16E-02	3.41E+01
3-Methyl-butanol	3.38E-02	3.40E+01	8.89E-02	4.59E+01	6.43E-03	5.52E+01	5.11E-02	7.19E+01	5.54E-03	2.87E+01	3.09E-01	1.01E+02	4.56E-03	2.09E+01	5.66E-02	6.40E+01
2-Methyl-1-butanol	8.53E-03	1.70E+01	1.23E-02	5.49E+01	3.13E-03	1.83E+01	7.73E-03	2.91E+01	3.25E-03	2.57E+01	4.30E-02	6.38E+01	1.09E-03	1.09E+02	1.14E-02	7.36E+01

Model Inoculum (CFU/mL)

D. hansenii

LRI suggested compound	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Dimethyl-disulfide	2.01E-02	4.51E+01	5.76E-03	2.79E+01	1.35E-02	2.69E+01	2.20E-03	8.07E+01	1.77E-02	2.43E+01	3.12E-03	6.74E+01	1.37E-02	1.77E+01	2.93E-03	2.61E+01
3-Methyl-2-pentanone	7.06E-04	1.95E+01	5.57E-04	3.41E+01	2.19E-04	4.01E+01	5.17E-04	1.24E+02	1.32E-04	3.75E+01	3.80E-04	2.90E+01	3.94E-04	5.58E+01	8.27E-04	3.95E+01
Methy-ethyl ester propanoic acid	1.88E-02	3.38E+01	7.77E-03	1.50E+01	1.88E-02	1.25E+01	1.90E-02	2.78E+01	2.53E-02	1.73E+01	1.82E-02	3.13E+01	2.00E-02	2.59E+01	1.38E-02	1.94E+01
2-Methyl heptane	8.95E-02	1.98E+01	4.51E-02	8.29E+00	9.63E-02	8.89E+00	9.21E-02	2.80E+01	1.13E-01	1.08E+01	9.20E-02	2.61E+01	8.30E-02	2.88E+01	9.38E-02	1.79E+01
1-Pentanol	5.62E-03	3.68E+01	6.19E-03	3.87E+01	7.35E-03	1.60E+01	9.21E-03	3.00E+01	6.32E-03	1.85E+01	1.88E-02	1.15E+01	5.01E-03	2.96E+01	4.62E-02	6.36E+01
3-Methyl heptane	1.67E-03	7.55E+01	1.34E-03	2.50E+01	2.81E-03	1.04E+01	2.82E-03	3.67E+01	2.96E-03	1.76E+01	1.43E-03	1.91E+01	2.63E-03	1.32E+01	2.21E-03	3.39E+01
2-Hexanone	1.64E-03	4.44E+01	1.61E-01	2.26E+01	1.26E-03	2.96E+01	9.81E-02	3.57E+01	1.95E-03	2.61E+01	1.31E-01	7.27E+01	2.04E-03	4.28E+01	2.54E-01	2.43E+01
Butanoic acid	0.00E+00	N/A	5.46E-04	1.41E+02	0.00E+00	N/A	5.76E-01	1.41E+02	0.00E+00	N/A	5.47E-04	1.41E+02	0.00E+00	N/A	6.67E-03	1.41E+02
Octane	5.79E-02	1.54E+01	3.42E-02	9.95E+00	5.79E-02	2.96E+00	6.33E-02	3.13E+01	6.25E-02	1.36E+01	5.63E-02	9.09E+00	4.65E-02	4.21E+01	5.01E-02	2.56E+01
3-Methyl butanoic acid	1.13E-03	6.09E+01	2.44E-04	2.88E+01	1.25E-04	1.40E+01	2.48E-03	9.04E+01	7.64E-04	8.42E+01	1.78E-03	1.18E+02	1.59E-03	7.97E+01	1.18E-03	9.76E+01
2-Methyl butanoic acid	3.67E-04	3.95E+01	1.04E-04	1.41E+02	1.18E-04	7.08E+01	1.85E-04	1.41E+02	4.12E-04	1.41E+02	5.01E-04	1.55E+01	1.17E-04	1.41E+02	8.78E-05	1.41E+02
2-Heptanone	2.47E-01	1.01E+01	1.69E+01	9.47E+00	1.75E-01	2.24E+01	1.21E+01	2.15E+01	1.50E-01	2.18E+01	1.27E+01	4.05E+01	1.86E-01	2.52E+01	1.78E+01	1.34E+01
Styrene	4.57E-03	5.66E+01	3.48E-02	1.19E+02	2.39E-03	3.86E+01	5.83E-02	7.99E+01	3.75E-03	1.14E+01	4.17E-03	4.74E+01	8.76E-03	1.13E+02	3.77E-03	1.38E+01
2-Heptanol (solvent GCMS)	4.74E-03	1.91E+01	1.08E-01	4.45E+01	2.39E-03	9.65E+00	1.13E-01	4.28E+01	3.77E-03	7.02E+01	9.54E-02	3.51E+01	4.72E-03	3.80E+01	1.28E-01	4.06E+01
a-Pinene	2.93E-03	2.57E+01	1.79E-03	2.57E+01	1.57E-03	1.33E+01	2.80E-03	1.84E+01	2.80E-03	2.47E+01	2.51E-03	3.37E+01	4.26E-03	3.19E+01	1.71E-03	3.40E+01
Hexanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	4.79E-01	1.41E+02	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	4.97E-03	1.41E+02
2-Octanone	2.09E-03	2.22E+01	8.57E-01	1.23E+01	2.77E-03	7.48E+00	3.52E-01	5.37E+01	1.64E-03	2.84E+01	4.44E-01	6.08E+01	2.59E-03	3.75E+01	7.12E-01	4.47E+01
Hexanoic acid ethyl ester	4.21E-03	9.36E+01	7.42E-03	9.22E+01	7.44E-05	7.08E+01	7.81E-03	6.43E+01	4.02E-04	5.31E+01	1.14E-03	5.59E+01	3.17E-04	8.57E+01	6.11E-04	1.17E+02
4-Methylanisole	2.48E-04	7.08E+01	2.51E-03	3.98E+01	1.01E-04	1.41E+02	1.50E-03	6.87E+01	7.02E-04	9.66E+01	2.69E-03	4.59E+01	1.10E-03	1.07E+02	2.20E-03	8.73E+01
Butanoic acid 3-methylbutyl ester	1.02E-03	4.75E+01	9.02E-03	6.42E+01	5.99E-04	5.88E+01	7.52E-03	5.41E+01	3.38E-04	7.68E+01	9.19E-03	9.38E+01	1.40E-03	6.41E+01	2.14E-03	4.17E+01
8-Nonen-2-one	1.53E-03	2.62E+01	2.20E+00	1.31E+01	1.73E-03	3.82E+01	9.06E-01	5.69E+01	1.85E-03	3.01E+01	1.18E+00	6.40E+01	1.37E-03	3.98E+01	2.01E+00	4.78E+01
2-Nonanone	4.09E-02	8.95E+00	1.16E+01	7.97E+00	2.98E-02	5.54E+01	6.71E+00	4.44E+01	8.87E-03	1.96E+01	7.69E+00	4.32E+01	2.38E-02	1.21E+01	1.09E+01	2.94E+01
Octanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	2.00E-01	1.41E+02	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
2-Decanone	8.32E-04	7.34E+01	6.57E-02	2.56E+01	9.04E-04	2.90E+01	2.58E-02	8.45E+01	7.38E-04	1.06E+02	2.54E-02	8.83E+01	9.39E-04	4.97E+01	5.71E-02	6.90E+01

Model Inoculum (CFU/mL)

D. hansenii

LRI suggested compound	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Octanoic acid ethyl ester	4.90E-04	9.01E+01	4.07E-04	2.98E+01	4.14E-04	7.19E+01	4.65E-04	6.33E+01	2.45E-04	4.97E+01	3.82E-04	4.72E+01	4.45E-04	4.83E+01	5.39E-04	8.63E+01
2-Undecanone	1.76E-03	1.84E+01	4.68E-01	3.05E+01	1.31E-03	3.04E+01	1.13E-01	7.60E+01	1.99E-03	4.80E+01	1.73E-01	1.09E+02	3.00E-03	6.25E+01	4.34E-01	7.34E+01

Model Inoculum (CFU/mL)

T. beigelii

LRI suggested compound	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Acetaldehyde	2.72E-03	7.30E+01	4.13E-03	3.87E+01	2.77E-03	7.79E+01	1.35E-02	1.21E+02	5.66E-03	8.20E+01	2.04E-03	2.94E+01	1.71E-03	3.08E+01	2.36E-03	3.06E+01
Methanethiol	1.01E-04	7.07E+01	0.00E+00	N/A	5.21E-05	1.41E+02	5.05E-05	1.41E+02	1.53E-04	7.67E+01	3.32E-05	1.41E+02	1.55E-03	8.63E+01	9.39E-05	1.41E+02
Ethanol	2.49E-01	2.77E+01	1.31E-01	8.75E+01	5.60E-02	4.87E+00	3.00E-01	1.32E+02	3.92E-01	1.24E+02	1.96E-01	5.85E+01	1.55E-02	5.94E+01	1.55E-02	3.61E+01
Acetone	2.72E-01	2.15E+00	2.78E-01	2.41E+01	2.46E-01	1.78E+01	1.76E-01	1.82E+01	2.73E-01	5.47E+01	1.42E-01	4.22E+01	4.15E-01	2.64E+01	2.84E-01	7.06E+01
Unidentified	8.06E-03	6.19E+01	8.94E-03	3.26E+01	3.38E-03	4.75E+01	9.31E-03	2.08E+01	2.22E-02	2.89E+01	6.37E-03	3.93E+01	1.73E-02	4.10E+01	5.75E-03	7.20E+01
2-Butanone	1.28E-01	1.08E+01	7.76E-02	7.64E+01	7.16E-02	6.57E+01	4.21E-02	3.60E+01	1.41E-01	6.52E+01	3.48E-02	4.48E+00	2.92E-01	2.24E+01	7.05E-02	3.57E+01
Ethylacetate	3.12E-03	3.22E+01	4.77E-03	3.10E+01	1.65E-03	1.89E+01	7.14E-03	1.03E+02	5.82E-03	6.65E+01	4.63E-03	3.55E+01	2.99E-03	6.70E+01	2.10E-03	4.82E+01
2-Methyl-1-propanol	2.30E-03	3.45E+01	6.44E-02	7.07E+01	2.23E-02	7.22E+01	1.14E-02	1.08E+02	1.62E-01	1.39E+02	7.18E-03	8.56E+01	1.02E-03	3.72E+01	6.05E-03	6.09E+01
3-Methyl-butanal	1.47E-03	5.03E+01	8.40E-04	4.61E+01	3.94E-04	7.84E+01	5.90E-03	1.32E+02	9.57E-04	2.56E+01	5.64E-03	8.65E+01	1.07E-03	2.66E+01	2.69E-03	9.14E+01
1-Butanol	7.50E-04	2.34E+01	4.99E-04	5.42E+01	8.88E-04	3.78E+01	1.35E-01	1.41E+02	3.67E-01	1.41E+02	1.03E-03	2.13E+01	8.80E-04	7.15E+01	7.74E-04	5.60E+01
2-Methyl-butanal	1.86E-03	6.14E+01	2.00E-03	3.78E+01	6.30E-04	5.28E+01	5.22E-03	1.22E+02	1.34E-03	7.10E+01	1.88E-03	5.96E+01	3.28E-03	3.64E+01	1.76E-03	8.34E+01
2-Pentanone	5.59E-02	6.47E+01	8.55E-02	4.34E+01	1.37E-01	2.26E+01	1.70E-01	3.28E+01	4.08E-02	1.72E+01	4.65E-01	4.10E+01	2.11E-02	8.49E+00	1.56E+00	3.85E+01
2-Pentanol	6.45E-03	1.02E+01	1.71E-02	2.70E+01	1.10E-02	9.80E+00	1.12E-02	3.51E+01	5.91E-03	3.70E+01	1.53E-02	2.43E+01	4.85E-03	7.25E+01	2.69E-02	6.36E+01
3-Hydroxy-2-butanone	1.87E-03	2.46E+01	3.11E-03	4.19E+01	2.80E-03	4.95E+01	9.23E-01	1.41E+02	8.48E-04	7.10E+01	1.56E-03	3.28E+01	1.21E-03	1.41E+02	4.29E-03	8.23E+01
Methyl-cyclohexane	4.78E-02	4.25E+01	6.09E-02	1.64E+01	3.58E-02	2.82E+01	4.20E-02	7.36E+00	5.36E-02	3.02E+01	5.03E-02	2.18E+01	5.01E-02	1.77E+01	3.16E-02	3.41E+01
3-Methyl-butanol	1.68E-02	2.98E+00	1.37E-01	5.82E+01	3.02E-02	5.12E+01	4.45E-02	8.90E+01	7.60E-02	1.27E+02	6.31E-02	6.75E+01	4.56E-03	2.09E+01	5.66E-02	6.40E+01

Model Inoculum (CFU/mL)

T. beigelii

	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
LRI suggested compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
2-Methyl-1-butanol	3.19E-03	4.95E+01	4.73E-02	6.73E+01	1.87E-02	6.22E+01	8.26E-03	6.54E+01	7.73E-03	1.09E+02	8.68E-03	6.45E+01	1.09E-03	1.09E+02	1.14E-02	7.36E+01
Dimethyl-disulfide	6.00E-04	5.70E+01	3.71E-04	3.57E+01	1.27E-04	6.01E+01	1.84E-03	1.25E+02	2.17E-03	6.76E+01	5.63E-04	6.89E+01	1.37E-02	1.77E+01	2.93E-03	2.61E+01
3-Methyl-2-pentanone	2.25E-04	1.51E+01	3.61E-04	2.24E+01	1.25E-04	3.71E+01	2.69E-04	5.23E+01	1.90E-04	9.60E+01	5.70E-04	5.72E+01	3.94E-04	5.58E+01	8.27E-04	3.95E+01
Methy-ethyl ester propanoic acid	1.47E-02	2.21E+01	2.06E-02	2.44E+01	1.37E-02	1.94E+01	1.48E-02	3.98E+00	1.79E-02	4.93E+01	1.67E-02	2.50E+01	2.00E-02	2.59E+01	1.38E-02	1.94E+01
2-Methyl heptane	7.46E-02	4.24E+01	1.19E-01	2.42E+01	5.13E-02	2.06E+01	7.32E-02	5.85E+00	8.98E-02	4.45E+01	1.00E-01	2.26E+01	8.30E-02	2.88E+01	9.38E-02	1.79E+01
1-Pentanol	6.94E-03	5.85E+01	8.34E-03	4.16E+01	3.37E-03	3.96E+01	4.66E-03	2.53E+01	3.81E-03	3.62E+01	7.86E-03	9.14E+00	5.01E-03	2.96E+01	4.62E-02	6.36E+01
3-Methyl heptane	2.11E-03	3.29E+01	2.82E-03	2.23E+01	1.28E-03	7.25E+01	1.63E-03	9.32E+00	2.10E-03	2.40E+01	2.06E-03	3.91E+01	2.63E-03	1.32E+01	2.21E-03	3.39E+01
2-Hexanone	1.17E-03	1.15E+01	2.02E-03	5.23E+01	1.44E-03	3.72E+01	1.16E-02	7.47E+01	2.31E-03	4.07E+01	6.98E-02	5.09E+01	2.04E-03	4.28E+01	2.54E-01	2.43E+01
Butanoic acid	0.00E+00	N/A	0.00E+00	N/A	3.20E-04	1.41E+02	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	6.67E-03	1.41E+02
Octane	4.68E-02	3.78E+01	6.76E-02	1.83E+01	3.22E-02	2.15E+01	4.30E-02	3.34E+00	5.26E-02	2.83E+01	6.14E-02	1.62E+01	4.65E-02	4.21E+01	5.01E-02	2.56E+01
3-Methyl butanoic acid	6.04E-04	2.82E+01	7.22E-02	1.37E+02	1.03E-03	6.18E+01	8.44E-04	1.17E+02	9.60E-04	4.34E+01	6.84E-03	9.65E+01	1.59E-03	7.97E+01	1.18E-03	9.76E+01
2-Methyl butanoic acid	5.08E-05	1.41E+02	1.40E-02	1.39E+02	4.38E-04	6.42E+01	1.28E-04	9.49E+01	4.82E-04	7.93E+01	2.25E-03	1.27E+02	1.17E-04	1.41E+02	8.78E-05	1.41E+02
2-Heptanone	1.20E-01	9.37E+00	1.08E-01	2.85E+01	9.49E-02	6.96E+01	1.79E+00	6.86E+01	1.06E-01	2.39E+01	9.31E+00	4.37E+01	1.86E-01	2.52E+01	1.78E+01	1.34E+01
Styrene	2.31E-03	2.25E+01	1.25E-02	5.18E+01	3.63E-03	3.87E+01	8.89E-02	6.22E+01	1.97E-03	3.48E+01	2.46E-01	2.40E+01	8.76E-03	1.13E+02	3.77E-03	1.38E+01
2-Heptanol (solvent GCMS)	3.08E-02	5.16E+01	8.86E-03	1.17E+01	1.10E-02	6.55E+01	2.49E-02	8.08E+01	1.80E-02	6.71E+01	1.29E-01	2.71E+01	4.72E-03	3.80E+01	1.28E-01	4.06E+01
a-Pinene	2.90E-03	7.39E+00	3.33E-03	2.58E+01	2.51E-03	1.82E+01	2.84E-03	2.76E+01	2.72E-03	3.41E+01	3.13E-03	4.25E+01	4.26E-03	3.19E+01	1.71E-03	3.40E+01
Hexanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	4.97E-03	1.41E+02
2-Octanone	2.24E-03	6.31E+01	1.99E-03	1.78E+01	1.43E-03	2.89E+01	2.81E-02	7.42E+01	1.64E-03	9.49E+00	3.09E-01	5.34E+01	2.59E-03	3.75E+01	7.12E-01	4.47E+01
Hexanoic acid ethyl ester	2.66E-03	6.20E+01	1.10E-03	1.10E+01	3.37E-04	5.87E+01	1.13E-02	1.38E+02	6.88E-04	4.87E+01	2.67E-02	1.01E+02	3.17E-04	8.57E+01	6.11E-04	1.17E+02
4-Methylanisole	1.98E-04	3.16E+01	6.41E-04	7.80E+01	1.29E-04	1.46E+01	1.15E-03	3.63E+01	6.05E-04	1.07E+02	5.01E-03	6.35E+01	1.10E-03	1.07E+02	2.20E-03	8.73E+01
Butanoic acid 3-methylbutyl ester	4.57E-04	2.80E+01	1.43E-03	3.17E+01	3.68E-04	2.11E+01	1.96E-03	9.14E+01	8.67E-04	3.55E+01	8.53E-03	5.55E+01	1.40E-03	6.41E+01	2.14E-03	4.17E+01
8-Nonen-2-one	3.04E-03	8.68E+01	2.94E-03	5.17E+01	1.85E-03	2.60E+01	2.59E-02	7.38E+01	2.18E-03	2.48E+01	7.75E-01	5.69E+01	1.37E-03	3.98E+01	2.01E+00	4.78E+01
2-Nonanone	1.75E-02	6.89E+01	1.42E-02	3.29E+01	3.69E-02	1.71E+01	3.92E-01	9.19E+01	1.61E-02	4.94E+01	6.73E+00	5.46E+01	2.38E-02	1.21E+01	1.09E+01	2.94E+01
Octanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A

	Model Inoculum (CFU/mL)															
	T. beigelii															
	10^8		10^8 + spores		10^5		10^5 + spores		10^2		10^2 + spores		Milk		Spore only	
LRI suggested compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
2-Decanone	1.95E-04	7.08E+01	3.00E-04	7.96E+01	7.87E-04	2.99E+01	3.08E-03	7.66E+01	3.08E-04	7.62E+01	2.08E-02	7.73E+01	9.39E-04	4.97E+01	5.71E-02	6.90E+01
Octanoic acid ethyl ester	4.52E-04	6.27E+01	3.42E-04	6.30E+01	3.39E-04	8.21E+01	6.75E-04	1.31E+02	7.71E-04	1.64E+01	6.66E-04	6.53E+01	4.45E-04	4.83E+01	5.39E-04	8.63E+01
2-Undecanone	6.74E-04	2.75E+01	9.32E-04	3.20E+01	1.46E-03	6.00E+00	2.97E-03	4.22E+01	1.54E-03	7.24E+01	1.06E-01	8.71E+01	3.00E-03	6.25E+01	4.34E-01	7.34E+01

Appendix 10. ANOVA of amounts of compounds generated in models inoculated at three concentrations of *K. lactis* (Appendix 7) and incubated at 25°C for 10 days.

Only compounds which distinguish between models are shown

Summary of all pairwise comparisons for Q1 (Fisher (LSD)):

Category	LS means(Acetaldehyde)	Groups	
10^8 + spores	54320954.798	A	
10^5 + spores	49275843.056	A	
10^2 + spores	41284042.511	A	B
10^2	38408664.405	A	B
10^5	30257214.437	A	B
10^8	6702797.866		B
Milk	0.000		B
P.roq	0.000		B

Category	LS means(Ethanol)	Groups		
10^8	833556798.037	A		
10^2	756550547.250	A		
10^8 + spores	717182219.328	A		
10^5	713360677.376	A		
10^5 + spores	676861460.405	A		
10^2 + spores	343210885.429		B	
Milk	6680277.821			C
P.roq	3700314.235			C

Category	LS means(Acetone)	Groups			
Milk	22372350.409	A			
P.roq	5078502.898		B		
10^2 + spores	2417831.155			C	
10^5 + spores	1592991.697			C	D
10^2	894762.116			C	D
10^8 + spores	806608.697			C	D
10^5	700738.290				D
10^8	206842.563				D

Category	LS means(1-propanol)	Groups	
10^2	3680694.177	A	
10^8 + spores	3446720.786	A	
10^5	2975791.518	A	
10^5 + spores	2631215.756	A	
10^8	2173155.839	A	
10^2 + spores	1656497.469	A	B
Milk	0.000		B
P.roq	0.000		B

Category	LS means(2-methyl propanal)	Groups			
10^2 + spores	3703686.976	A			
10^5 + spores	2055619.483		B		
10^2	1195199.644		B	C	
10^8 + spores	737618.337			C	D
10^5	603955.342			C	D
10^8	462529.255			C	D
P.roq	119169.465				D
Milk	93909.921				D

Category	LS means(2-Butanone)	Groups		
Milk	19846363.020	A		
P.roq	2018261.644		B	
10^2	1697715.383		B	C
10^2 + spores	1513313.643		B	C
10^5 + spores	1440435.826		B	C
10^5	1208847.821		B	C
10^8 + spores	1033777.864		B	C
10^8	400046.233			C

Category	LS means(Ethylacetate)	Groups		
10^2 + spores	1211710167.225	A		
10^5 + spores	1064959601.459	A	B	
10^8	1016140421.357		B	
10^2	1012693093.146		B	
10^8 + spores	1009277854.427		B	
10^5	977099865.836		B	
Milk	711570.441			C
P.roq	228164.486			C

Category	LS means(2-Methyl-1-propanol)	Groups		
10^8	52730993.068	A		
10^2	48484969.388	A	B	
10^5	34346727.688	A	B	
10^8 + spores	33137056.740	A	B	
10^5 + spores	32798105.761	A	B	
10^2 + spores	18879152.323		B	C
P.roq	333516.983			C
Milk	173898.427			C

Category	LS means(3-Methyl-butanal)	Groups	
10^2 + spores	2564338.018	A	
10^5 + spores	1848402.465	A	
P.roq	1192907.074	A	B
10^2	270008.179		B
10^8 + spores	216991.727		B
10^5	136157.399		B
10^8	130371.550		B
Milk	10056.401		B

Category	LS means(2-Methyl-butanal)	Groups	
10^5 + spores	9805133.670	A	
10^2 + spores	7479331.049	A	
10^2	1225352.867		B
10^8 + spores	1058066.592		B
10^8	877451.780		B
10^5	543772.726		B
P.roq	287550.510		B
Milk	218445.840		B

Category	LS means(2-Pentanone)	Groups	
P.roq	14076753.452	A	
10^2 + spores	11942369.229	A	
10^5 + spores	2733957.408		B
Milk	1576463.893		B
10^2	417374.668		B
10^5	327650.708		B
10^8 + spores	194530.134		B
10^8	179235.451		B

Category	LS means(2-Pentanol)	Groups				
P.roq	732566.868	A				
10^2 + spores	507094.135		B			
10^5 + spores	353426.425		B	C		
Milk	223156.664			C	D	
10^8	70813.479				D	E
10^5	51404.140					E
10^8 + spores	49651.223					E
10^2	26659.982					E

Category	LS means(3-Hydroxy-2-butanone)	Groups		
10^2 + spores	10841118.534	A		
10^5 + spores	5770070.740		B	
10^2	3344278.312		B	C
10^8 + spores	1651719.860			C
10^5	1188506.409			C
Milk	710204.013			C
P.roq	174313.366			C
10^8	70893.196			C

Category	LS means(Ethyl ester propanoic acid)	Groups	
10^8	52858266.322	A	
10^2 + spores	51334378.705	A	
10^8 + spores	50417124.909	A	
10^5 + spores	47735466.437	A	
10^5	46505542.591	A	
10^2	44994305.082	A	
P.roq	4574.401		B
Milk	0.000		B

Category	LS means(n-Propyl acetate)	Groups		
10^2 + spores	14996992.985	A		
10^8 + spores	7383436.127		B	
10^8	7197323.872		B	
10^2	6682315.003		B	
10^5	5928904.638		B	
10^5 + spores	4822376.310		B	
P.roq	101845.298			C
Milk	6566.048			C

Category	LS means(3-Methyl-butanol)	Groups		
10^2 + spores	343433011.008	A		
10^5 + spores	285661291.197	A	B	
10^8	267147178.963	A	B	
10^2	266786038.043	A	B	
10^5	247838021.854		B	
10^8 + spores	238920487.022		B	
P.roq	1172565.736			C
Milk	27050.701			C

Category	LS means(2-Methyl-1-butanol)	Groups	
10^8 + spores	107591801.157	A	
10^2	107585497.368	A	
10^5 + spores	105416704.265	A	
10^8	104361909.832	A	
10^5	91806392.857	A	
10^2 + spores	71664998.090	A	
P.roq	322936.909		B
Milk	17263.851		B

Category	LS means(3-Methyl-2-pentanone)	Groups	
P.roq	8296.499	A	
10^5	1694.920		B
10^2 + spores	0.000		B
10^5 + spores	0.000		B
10^2	0.000		B
10^8	0.000		B
10^8 + spores	0.000		B
Milk	0.000		B

Category	LS means(2-Methyl-ethyl ester propanoic acid)	Groups				
10^8	21151874.917	A				
10^8 + spores	18680621.056	A				
10^2	13096838.648		B			
10^5	10809897.176		B	C		
10^5 + spores	8035204.899			C	D	
10^2 + spores	3611937.537				D	E
Milk	2998884.623					E
P.roq	1677223.407					E

Category	LS means(1-Pentanol)	Groups	
P.roq	5547438.060	A	
10^2 + spores	998092.645		B
10^8	659533.171		B
10^2	646655.232		B
10^8 + spores	592183.925		B
10^5 + spores	590601.016		B
10^5	414789.987		B
Milk	399209.083		B

Category	LS means(Isobutyl acetate)	Groups			
10^2 + spores	47716503.226	A			
10^5 + spores	32004519.356		B		
10^8	25457772.784		B	C	
10^8 + spores	24170969.237		B	C	
10^5	20930249.622		B	C	
10^2	20471712.535			C	
Milk	2496639.356				D
P.roq	1152942.026				D

Category	LS means(2-Hexanone)	Groups	
10^2 + spores	4894915.578	A	
P.roq	3642013.823	A	
10^5 + spores	963031.477		B
Milk	280861.837		B
10^2	155999.321		B
10^5	127543.205		B
10^8	104820.174		B
10^8 + spores	99751.229		B

Category	LS means(Butanoic acid)	Groups	
Milk	3677912.585	A	
10^2	1994150.484		B
P.roq	1832998.950		B
10^5	1522885.682		B
10^8	1485240.829		B
10^5 + spores	1351483.525		B
10^8 + spores	1332523.142		B
10^2 + spores	1190191.879		B

Category	LS means(3-Methyl-butanoic acid)	Groups	
10^2 + spores	390902.558	A	
10^5	130751.362	A	B
10^5 + spores	46891.157		B
10^2	6920.255		B
10^8	0.000		B
10^8 + spores	0.000		B
Milk	0.000		B
P.roq	0.000		B

Category	LS means(2-Methyl-butanoic acid)	Groups	
10^2 + spores	129206.099	A	
10^8	35914.811	A	B
10^5 + spores	24760.561		B
10^8 + spores	15704.257		B
10^5	13950.891		B
10^2	4315.295		B
Milk	0.000		B
P.roq	0.000		B

Category	LS means(3-Methyl-1-butanol, acetate)	Groups		
10^2 + spores	95022892.753	A		
10^5 + spores	37302277.853		B	
10^8	36090098.476		B	
10^8 + spores	35993452.619		B	
10^2	27877075.912		B	C
10^5	26441498.169		B	C
Milk	17708.556			C
P.roq	16550.048			C

Category	LS means(2-Heptanone)	Groups	
10^2 + spores	438260419.024	A	
P.roq	326547535.756	A	
10^5 + spores	112438421.601		B
Milk	18233695.483		B
10^2	10458606.290		B
10^8 + spores	8620319.554		B
10^8	8245393.473		B
10^5	7875784.056		B

Category	LS means(2-Heptanol)	Groups		
10^5 + spores	55658386.210	A		
10^2 + spores	26326632.950		B	
P.roq	12132424.330		B	C
10^8	4340141.774			C
10^5	4118304.652			C
10^2	4113159.103			C
10^8 + spores	3936214.224			C
Milk	0.000			C

Category	LS means(a-Pinene)	Groups	
Milk	420080.219	A	
10^8	209649.603		B
10^2	166563.995		B
10^5	165302.045		B
10^5 + spores	126148.764		B
10^8 + spores	118063.641		B
P.roq	114764.356		B
10^2 + spores	95111.783		B

Category	LS means(Unidentified)	Groups	
10^2 + spores	58086.076	A	
10^5 + spores	37608.374	A	B
Milk	10991.560	A	B
10^8	10616.206	A	B
10^5	5477.891		B
10^2	0.000		B
10^8 + spores	0.000		B
P.roq	0.000		B

Category	LS means(Unidentified)	Groups	
10^2 + spores	3358977.045	A	
10^5 + spores	2404503.738	A	B
10^8	186999.059		B
10^8 + spores	165266.508		B
10^2	158629.583		B
10^5	115841.786		B
P.roq	23120.791		B
Milk	17864.256		B

Category	LS means(3-Octanone)	Groups	
10^5 + spores	375194.299	A	
10^2 + spores	83271.094		B
P.roq	17809.750		B
10^8 + spores	3713.624		B
10^5	2767.835		B
Milk	0.000		B
10^2	0.000		B
10^8	0.000		B

Category	LS means(2-Octanone)	Groups		
10^2 + spores	18471828.770	A		
P.roq	10288714.639	A	B	
10^5 + spores	2524530.382		B	C
Milk	112816.287			C
10^5	90577.447			C
10^8	79447.645			C
10^8 + spores	64579.278			C
10^2	20981.752			C

Category	LS means(Hexanoic acid, ethyl ester)	Groups		
10^5 + spores	16579094.484	A		
10^2 + spores	9749325.251	A	B	
10^8	7727030.385		B	
10^8 + spores	7659656.806		B	
10^2	6867123.835		B	C
10^5	5872724.345		B	C
P.roq	44582.873			C
Milk	0.000			C

Category	LS means(4-Methylanisole)	Groups	
10^2 + spores	587733.386	A	
P.roq	537673.157	A	
10^5	4413.277		B
Milk	1821.946		B
10^2	0.000		B
10^5 + spores	0.000		B
10^8	0.000		B
10^8 + spores	0.000		B

Category	LS means(Butanoic acid, 3-methylbutyl ester)	Groups		
10^2 + spores	5953921.483	A		
10^5 + spores	3320821.538		B	
10^5	167249.584			C
10^2	161237.665			C
10^8 + spores	108271.170			C
10^8	106181.100			C
Milk	13336.748			C
P.roq	6498.369			C

Category	LS means(8-Nonen-2-one)	Groups		
10^2 + spores	46741139.055	A		
P.roq	26380754.612	A	B	
10^5 + spores	7503441.786		B	C
10^2	946208.080			C
10^8	734594.229			C
10^8 + spores	695346.169			C
10^5	471024.022			C
Milk	404810.280			C

Category	LS means(2-Nonanone)	Groups	
10^2 + spores	317234593.070	A	
P.roq	228953239.952	A	
10^5 + spores	58554808.381		B
10^2	8407683.822		B
10^8 + spores	5272250.231		B
10^8	4874128.028		B
Milk	4225903.174		B
10^5	4171743.974		B

Category	LS means(Benzeneethanol)	Groups	
10^5 + spores	921657.538	A	
10^2 + spores	550842.681	A	B
10^8 + spores	253587.652		B
10^2	224948.985		B
10^8	204041.480		B
P.roq	117156.164		B
10^5	109340.495		B
Milk	22078.556		B

Category	LS means(Hexanoic acid, butyl ester)	Groups	
10^2 + spores	96863.834	A	
10^5 + spores	73713.325	A	B
10^2	14147.580		B
10^8	13553.498		B
10^5	11511.386		B
10^8 + spores	9496.231		B
P.roq	9100.214		B
Milk	6465.197		B

Category	LS means(2-Decanone)	Groups	
10^2 + spores	1230457.969	A	
P.roq	401070.639		B
10^5 + spores	161628.349		B
10^2	45469.365		B
10^8	38657.738		B
10^5	33886.671		B
10^8 + spores	29605.671		B
Milk	9995.961		B

Category	LS means(Octanoic acid, ethyl ester)	Groups		
10^5 + spores	8076457.938	A		
10^8	6238128.435	A	B	
10^5	6229638.825	A	B	
10^2	6137649.013	A	B	
10^8 + spores	5611163.515	A	B	
10^2 + spores	3218353.923		B	C
P.roq	155848.352			C
Milk	8550.650			C

Category	LS means(3-Methybutyl hexanoate)	Groups		
10^2 + spores	198851.731	A		
10^5 + spores	119463.476	A	B	
10^8 + spores	23890.937		B	C
10^8	23525.135		B	C
10^5	9552.433			C
P.roq	3946.365			C
Milk	0.000			C
10^2	0.000			C

Category	LS means(Acetic acid, 2-phenylethyl ester)	Groups				
10^2 + spores	136032062.783	A				
10^5 + spores	85773881.046		B			
10^8	40367247.901			C		
10^8 + spores	39385372.621			C		
10^2	31037161.662			C	D	
10^5	31033076.805			C	D	
P.roq	1412672.260				D	E
Milk	355969.457					E

Category	LS means(2-Undecanone)	Groups	
10^2 + spores	13451171.856	A	
P.roq	8069595.371	A	
10^5 + spores	1265062.411		B
10^2	715672.814		B
Milk	493262.027		B
10^8	461234.090		B
10^8 + spores	446851.591		B
10^5	353873.586		B

Category	LS means(Unidentified)	Groups			
10^5 + spores	1959270.445	A			
10^8	1185802.104	A	B		
10^5	1025559.657	A	B	C	
10^8 + spores	963814.177	A	B	C	D
10^2	900416.529		B	C	D
10^2 + spores	629443.120		B	C	D
P.roq	39025.620			C	D
Milk	11605.364				D

Appendix 11. ANOVA of amounts of compounds generated in models inoculated at three concentrations of *D. hansenii* (Appendix 7) and incubated at 25°C for 10 days.

Only compounds which distinguish between models are shown

Summary of all pairwise comparisons for Q1 (Fisher (LSD)):

Category	LS means(1.63_methanethiol)	Groups			
10^8 (D_10^8)	162359.700	A			
10^5 (D_10^5)	141445.664	A	B		
10^2 (D_10^2)	113352.657	A	B		
Milk	76596.849		B	C	
10^2 + spores (SD_10^2)	10076.491			C	D
P. roq (S)	4629.975			C	D
10^8 + spores (SD_10^8)	4154.200			C	D
10^5 + spores (SD_10^5)	0.000				D

Category	LS means(1.78_ethanol)	Groups	
SD_10^2	10269374.555	A	
SD_10^8	5418728.214	A	B
SD_10^5	3317598.997	A	B
D_10^8	2383247.010	A	B
D_10^2	1300771.167	A	B
D_10^5	991858.790	A	B
Milk	762974.822		B
S	762916.920		B

Category	LS means(2.08_acetone)	Groups	
Milk	20461392.923	A	
D_10^5	16722327.140	A	B
D_10^2	16425894.405	A	B
D_10^8	15597475.118	A	B
S	13976006.547	A	B
SD_10^5	11707602.918	A	B
SD_10^2	8405863.476		B
SD_10^8	7526166.643		B

Category	LS means(2.93_unidentified_3)	Groups		
D_10^2	991083.814	A		
Milk	854104.995	A	B	
SD_10^5	687680.707	A	B	C
D_10^5	543990.576	A	B	C
D_10^8	524929.593	A	B	C
SD_10^2	364784.063		B	C
S	283602.325			C
SD_10^8	202610.102			C

Category	LS means(3.40_2-butanone)	Groups	
Milk	14368674.250	A	
D_10^5	11957085.375	A	
D_10^2	11235508.558	A	
D_10^8	11009453.050	A	
SD_10^5	5728897.104		B
S	3473455.631		B
SD_10^2	3042596.198		B
SD_10^8	2864647.881		B

Category	LS means(3.95_2-methyl-1-propanol)	Groups	
SD_10^2	953340.392	A	
D_10^8	494478.780	A	B
SD_10^8	363851.982	A	B
S	298351.064	A	B
D_10^2	192954.369		B
SD_10^5	161975.313		B
D_10^5	113390.570		B
Milk	50029.381		B

Category	LS means(4.50_3-methyl-butanal)	Groups		
SD_10^2	2213818.753	A		
SD_10^5	290805.541	A	B	
SD_10^8	263922.373	A	B	
S	132491.320		B	
Milk	52751.276		B	
D_10^2	32559.711		B	
D_10^5	31135.538		B	
D_10^8	24558.220		B	

Category	LS means(5.19_2-pentanone)	Groups		
S	77014221.844	A		
SD_10^8	57092814.498	A	B	
SD_10^5	34190177.546		B	
SD_10^2	33843836.648		B	
D_10^8	1316529.306			C
D_10^5	1084141.703			C
Milk	1040605.634			C
D_10^2	1037255.589			C

Category	LS means(5.43_2-pentanol)	Groups	
S	1324415.539	A	
SD_10^2	678874.474	A	B
SD_10^8	518379.190		B
SD_10^5	492559.581		B
D_10^8	340722.163		B
D_10^2	299908.921		B
D_10^5	268303.901		B
Milk	239170.520		B

Category	LS means(5.70_3-hydroxy-2-butanone)	Groups	
S	211672.912	A	
SD_10^5	105959.888	A	B
SD_10^2	103050.285	A	B
SD_10^8	94560.568	A	B
Milk	59836.880	A	B
D_10^5	32701.603		B
D_10^8	26693.244		B
D_10^2	0.000		B

Category	LS means(6.08_methyl-cyclohexane)	Groups		
D_10^2	3201153.271	A		
D_10^8	3171039.732	A		
D_10^5	3107712.446	A		
SD_10^5	2471086.281	A	B	
Milk	2470040.509	A	B	
SD_10^2	2124135.267	A	B	C
S	1559323.162		B	C
SD_10^8	1234417.100			C

Category	LS means(6.26_3-methyl-butanol)	Groups	
SD_10^2	15209234.788	A	
SD_10^8	4379989.573	A	B
S	2788517.105		B
SD_10^5	2519778.928		B
D_10^8	1665004.032		B
D_10^5	317043.230		B
D_10^2	273169.412		B
Milk	224767.787		B

Category	LS means(6.35_2-methyl-1-butanol)	Groups		
SD_10^2	2117231.136	A		
SD_10^8	605908.023		B	
S	563211.633		B	
D_10^8	420642.879		B	
SD_10^5	380938.684		B	
D_10^2	159973.762		B	
D_10^5	154413.153		B	
Milk	53507.572		B	

Category	LS means(6.60_dimethyl-disulfide)	Groups		
D_10^8	992095.503	A		
D_10^2	873491.769	A		
Milk	675840.601	A	B	
D_10^5	666403.821	A	B	
SD_10^8	283665.265		B	C
SD_10^2	153967.573			C
S	144284.522			C
SD_10^5	108390.544			C

Category	LS means(6.72_3-methyl-2-pentanone)	Groups		
S	40753.685	A		
D_10^8	34800.091	A	B	
SD_10^8	27439.013	A	B	
SD_10^5	25458.400	A	B	
Milk	19420.464	A	B	
SD_10^2	18723.785	A	B	
D_10^5	10772.855		B	
D_10^2	6499.887		B	

Category	LS means(6.79_methy-ethyl_ester_propanoic_acid)	Groups		
D_10^2	1246503.266	A		
Milk	987977.300	A	B	
SD_10^5	938548.157	A	B	
D_10^5	927054.407	A	B	
D_10^8	924381.627	A	B	
SD_10^2	895794.729	A	B	
S	678136.288		B	C
SD_10^8	383136.023			C

Category	LS means(6.99_2-methyl_heptane)	Groups	
D_10^2	5564460.944	A	
D_10^5	4745587.478	A	
S	4622885.440	A	
SD_10^5	4541381.275	A	
SD_10^2	4535661.809	A	
D_10^8	4410003.950	A	
Milk	4090306.071	A	B
SD_10^8	2221371.922		B

Category	LS means(7.03_1pentanol)	Groups	
S	2276054.501	A	
SD_10^2	928637.722		B
SD_10^5	453993.836		B
D_10^5	362471.806		B
D_10^2	311584.909		B
SD_10^8	304988.737		B
D_10^8	276978.534		B
Milk	246934.098		B

Category	LS means(7.18_3-methyl_heptane)	Groups		
D_10^2	145916.286	A		
SD_10^5	139242.763	A	B	
D_10^5	138332.528	A	B	C
Milk	129600.690	A	B	C
S	108716.507	A	B	C
D_10^8	82228.969	A	B	C
SD_10^2	70570.202		B	C
SD_10^8	66289.985			C

Category	LS means(7.56_2-hexanone)	Groups		
S	12537109.493	A		
SD_10^8	7925013.269		B	
SD_10^2	6464812.798		B	
SD_10^5	4835464.648		B	
Milk	100506.883			C
D_10^2	96155.594			C
D_10^8	81005.165			C
D_10^5	61961.888			C

Category	LS means(7.86_octane)	Groups	
SD_10^5	3120208.598	A	
D_10^2	3078489.063	A	
D_10^8	2856148.635	A	B
D_10^5	2854196.356	A	B
SD_10^2	2772938.189	A	B
S	2468491.246	A	B
Milk	2289544.775	A	B
SD_10^8	1685636.629		B

Category	LS means(9.95_2-heptanone)	Groups		
S	875401183.927	A		
SD_10^8	831742482.894	A	B	
SD_10^2	627682367.852		B	
SD_10^5	595960524.616		B	
D_10^8	12167857.446			C
Milk	9170691.909			C
D_10^5	8617079.690			C
D_10^2	7403496.633			C

Category	LS means(10.11_styrene)	Groups	
SD_10^5	2871598.781	A	
SD_10^8	1717177.796	A	B
Milk	431567.747		B
D_10^8	225022.130		B
SD_10^2	205467.172		B
S	186024.008		B
D_10^2	184871.083		B
D_10^5	117882.734		B

Category	LS means(10.16_2-heptanol_(solvent_GCMS))	Groups	
S	6319892.911	A	
SD_10^5	5549165.192	A	
SD_10^8	5317055.396	A	
SD_10^2	4703820.692	A	
D_10^8	233681.922		B
Milk	232496.083		B
D_10^2	185598.946		B
D_10^5	117919.944		B

Category	LS means(11.14_a-pinene)	Groups	
Milk	209802.305	A	
D_10^8	144653.899	A	B
D_10^2	138128.695	A	B
SD_10^5	138094.415	A	B
SD_10^2	123653.596		B
SD_10^8	88119.983		B
S	84383.425		B
D_10^5	77367.541		B

Category	LS means(12.23_2-octanone)	Groups			
SD_10^8	42259499.333	A			
S	35098529.349	A	B		
SD_10^2	21893941.832		B	C	
SD_10^5	17340880.868			C	D
D_10^5	136339.877				D
Milk	127864.146				D
D_10^8	102964.405				D
D_10^2	81070.627				D

Category	LS means(12.36_hexanoic_acid_ethyl_ester)	Groups		
SD_10^5	385031.952	A		
SD_10^8	365829.653	A	B	
D_10^8	207756.442	A	B	C
SD_10^2	56259.870	A	B	C
S	30134.207		B	C
D_10^2	19797.963		B	C
Milk	15636.720			C
D_10^5	3666.523			C

Category	LS means(13.03_4-methylanisole)	Groups		
SD_10^2	132794.849	A		
SD_10^8	123578.098	A	B	
S	108649.531	A	B	C
SD_10^5	74109.186	A	B	C
Milk	54444.732	A	B	C
D_10^2	34610.678	A	B	C
D_10^8	12221.886		B	C
D_10^5	4968.470			C

Category	LS means(13.59_butanoic_acid_3_methylbutyl_ester)	Groups		
SD_10^2	452811.444	A		
SD_10^8	444690.863	A	B	
SD_10^5	370679.273	A	B	C
S	105670.458	A	B	C
Milk	69113.835	A	B	C
D_10^8	50185.571	A	B	C
D_10^5	29508.664		B	C
D_10^2	16648.422			C

Category	LS means(14.21_8-nonen-2-one)	Groups		
SD_10^8	108529493.707	A		
S	99178689.088	A		
SD_10^2	58359175.662	A	B	
SD_10^5	44664729.340		B	C
D_10^2	91204.740			C
D_10^5	85251.322			C
D_10^8	75232.222			C
Milk	67469.205			C

Category	LS means(14.38_2-nonanone)	Groups		
SD_10^8	573687921.707	A		
S	535265688.253	A	B	
SD_10^2	378802614.866	A	B	
SD_10^5	330654971.863		B	
D_10^8	2016226.528			C
D_10^5	1469128.492			C
Milk	1172133.624			C
D_10^2	436957.921			C

Category	LS means(16.42_2-decanone)	Groups		
SD_10^8	3240527.002	A		
S	2812703.660	A	B	
SD_10^5	1269875.079		B	C
SD_10^2	1254031.563		B	C
Milk	46268.539			C
D_10^5	44541.896			C
D_10^8	41023.673			C
D_10^2	36363.972			C

Category	LS means(18.29_2-undecanone)	Groups	
SD_10^8	23079190.258	A	
S	21388682.236	A	
SD_10^2	8542952.159	A	B
SD_10^5	5568917.401		B
Milk	147902.352		B
D_10^2	98315.487		B
D_10^8	86757.884		B
D_10^5	64508.220		B

Appendix 12. ANOVA of amounts of compounds generated in models inoculated at three concentrations of *T. beigelii* (Appendix 7) and incubated at 25°C for 10 days.

Only compounds which discriminate between models shown

Summary of all pairwise comparisons for Q1 (Fisher (LSD)):

Category	LS means(1.63_methanethiol)	Groups	
Milk	76596.849	A	
10^2 (T_10^2)	7564.943		B
10^8 (T_10^8)	4958.970		B
P. roq. (S)	4629.975		B
10^5 (T_10^5)	2567.158		B
10^5 + spores (ST_10^5)	2486.752		B
10^2 + spores (ST_10^2)	1635.154		B
10^8 + spores (ST_10^8)	0.000		B

Category	LS means(2.08_acetone)	Groups	
Milk	20461392.923	A	
S	13976006.547	A	B
ST_10^8	13726567.464	A	B
T_10^2	13439567.441	A	B
T_10^8	13411446.828	A	B
T_10^5	12130125.585	A	B
ST_10^5	8677710.418		B
ST_10^2	6997111.494		B

Category	LS means(2.93_unidentified_3)	Groups		
T_10^2	1092842.740	A		
Milk	854104.995	A	B	
ST_10^5	458702.372		B	C
ST_10^8	440779.750		B	C
T_10^8	397380.165		B	C
ST_10^2	314091.537			C
S	283602.325			C
T_10^5	166578.772			C

Category	LS means(3.40_2-butanone)	Groups		
Milk	14368674.250	A		
T_10^2	6957099.609		B	
T_10^8	6321058.670		B	C
ST_10^8	3826749.258		B	C
T_10^5	3530122.176		B	C
S	3473455.631		B	C
ST_10^5	2075011.180		B	C
ST_10^2	1717107.293			C

Category	LS means(5.19_2-pentanone)	Groups	
S	77014221.844	A	
ST_10^2	22936114.866		B
ST_10^5	8355633.732		B
T_10^5	6731334.018		B
ST_10^8	4214983.435		B
T_10^8	2753752.747		B
T_10^2	2012553.099		B
Milk	1040605.634		B

Category	LS means(5.43_2-pentanol)	Groups	
S	1324415.539	A	
ST_10^8	844459.547	A	B
ST_10^2	754311.384	A	B
ST_10^5	550287.579		B
T_10^5	540436.881		B
T_10^8	317885.914		B
T_10^2	291122.273		B
Milk	239170.520		B

Category	LS means(6.08_methyl-cyclohexane)	Groups	
ST_10^8	3003128.693	A	
T_10^2	2640018.519	A	B
ST_10^2	2477269.535	A	B
Milk	2470040.509	A	B
T_10^8	2355045.637	A	B
ST_10^5	2070468.973	A	B
T_10^5	1764088.166	A	B
S	1559323.162		B

Category	LS means(6.26_3-methyl-butanol)	Groups	
ST_10^8	6751541.505	A	
T_10^2	3743956.029	A	B
ST_10^2	3112198.408	A	B
S	2788517.105	A	B
ST_10^5	2192605.040	A	B
T_10^5	1486719.490	A	B
T_10^8	830494.956		B
Milk	224767.787		B

Category	LS means(6.35_2-methyl-1-butanol)	Groups	
ST_10^8	2333611.186	A	
T_10^5	922223.741		B
S	563211.633		B
ST_10^2	427831.038		B
ST_10^5	407208.296		B
T_10^2	381255.036		B
T_10^8	157464.310		B
Milk	53507.572		B

Category	LS means(6.60_dimethyl-disulfide)	Groups	
Milk	675840.601	A	
S	144284.522		B
T_10^2	107097.794		B
ST_10^5	90451.411		B
T_10^8	29572.030		B
ST_10^2	27738.874		B
ST_10^8	18305.552		B
T_10^5	6237.390		B

Category	LS means(6.72_3-methyl-2-pentanone)	Groups		
S	40753.685	A		
ST_10^2	28091.320	A	B	
Milk	19420.464		B	C
ST_10^8	17801.805		B	C
ST_10^5	13256.527		B	C
T_10^8	11101.431		B	C
T_10^2	9378.714		B	C
T_10^5	6141.589			C

Category	LS means(6.99_2-methyl_heptane)	Groups	
ST_10^8	5880525.969	A	
ST_10^2	4935115.424	A	B
S	4622885.440	A	B
T_10^2	4427748.200	A	B
Milk	4090306.071	A	B
T_10^8	3676135.442	A	B
ST_10^5	3609712.578	A	B
T_10^5	2527014.830		B

Category	LS means(7.03_1pentanol)	Groups	
S	2276054.501	A	
ST_10^8	411277.993		B
ST_10^2	387471.064		B
T_10^8	341833.122		B
Milk	246934.098		B
ST_10^5	229735.444		B
T_10^2	187914.181		B
T_10^5	166114.764		B

Category	LS means(7.18_3-methyl_heptane)	Groups	
ST_10^8	139225.081	A	
Milk	129600.690	A	B
S	108716.507	A	B
T_10^8	104183.106	A	B
T_10^2	103723.648	A	B
ST_10^2	101760.759	A	B
ST_10^5	80494.480	A	B
T_10^5	63294.253		B

Category	LS means(7.56_2-hexanone)	Groups		
S	12537109.493	A		
ST_10^2	3439879.693		B	
ST_10^5	570152.736			C
T_10^2	113825.457			C
Milk	100506.883			C
ST_10^8	99794.524			C
T_10^5	70913.462			C
T_10^8	57499.986			C

Category	LS means(7.86_octane)	Groups	
ST_10^8	3330498.760	A	
ST_10^2	3027803.914	A	
T_10^2	2592358.385	A	B
S	2468491.246	A	B
T_10^8	2307951.935	A	B
Milk	2289544.775	A	B
ST_10^5	2120620.450	A	B
T_10^5	1585053.238		B

Category	LS means(9.95_2-heptanone)	Groups		
S	875401183.927	A		
ST_10^2	458665370.869		B	
ST_10^5	88409252.130			C
Milk	9170691.909			C
T_10^8	5913254.675			C
ST_10^8	5340544.684			C
T_10^2	5212264.634			C
T_10^5	4677767.143			C

Category	LS means(10.11_styrene)	Groups		
ST_10^2	12123268.641	A		
ST_10^5	4382679.564		B	
ST_10^8	616384.376			C
Milk	431567.747			C
S	186024.008			C
T_10^5	179126.108			C
T_10^8	114054.501			C
T_10^2	97027.964			C

Category	LS means(10.16_2-heptanol_(solvent_GCMS))	Groups	
ST_10^2	6350535.161	A	
S	6319892.911	A	
T_10^8	1518801.354		B
ST_10^5	1228844.389		B
T_10^2	887287.976		B
T_10^5	542977.818		B
ST_10^8	436621.319		B
Milk	232496.083		B

Category	LS means(11.14_a-pinene)	Groups	
Milk	209802.305	A	
ST_10^8	163928.327	A	B
ST_10^2	154322.785	A	B
T_10^8	143130.188	A	B
ST_10^5	140147.442	A	B
T_10^2	134196.533	A	B
T_10^5	123585.011	A	B
S	84383.425		B

Category	LS means(12.23_2-octanone)	Groups		
S	35098529.349	A		
ST_10^2	15253421.187		B	
ST_10^5	1383653.685			C
Milk	127864.146			C
T_10^8	110343.207			C
ST_10^8	97929.005			C
T_10^2	80678.730			C
T_10^5	70249.614			C

Category	LS means(12.36_hexanoic_acid_ethyl_ester)	Groups	
ST_10^2	1313785.057	A	
ST_10^5	557486.856	A	B
T_10^8	131301.414		B
ST_10^8	54206.577		B
T_10^2	33902.926		B
S	30134.207		B
T_10^5	16632.300		B
Milk	15636.720		B

Category	LS means(13.03_4-methylanisole)	Groups	
ST_10^2	246766.448	A	
S	108649.531	A	B
ST_10^5	56600.151		B
Milk	54444.732		B
ST_10^8	31593.342		B
T_10^2	29818.698		B
T_10^8	9758.462		B
T_10^5	6369.332		B

Category	LS means(13.59_butanoic_acid_3_methylbutyl_ester)	Groups	
ST_10^2	420206.439	A	
S	105670.458		B
ST_10^5	96637.434		B
ST_10^8	70512.825		B
Milk	69113.835		B
T_10^2	42722.159		B
T_10^8	22547.275		B
T_10^5	18155.745		B

Category	LS means(14.21_8-nonen-2-one)	Groups	
S	99178689.088	A	
ST_10^2	38175712.259		B
ST_10^5	1278671.294		B
T_10^8	149858.395		B
ST_10^8	144862.120		B
T_10^2	107670.642		B
T_10^5	91073.821		B
Milk	67469.205		B

Category	LS means(14.38_2-nonanone)	Groups		
S	535265688.253	A		
ST_10^2	331540216.653		B	
ST_10^5	19309670.131			C
T_10^5	1820043.979			C
Milk	1172133.624			C
T_10^8	863413.554			C
T_10^2	791584.164			C
ST_10^8	700174.602			C

Category	LS means(16.42_2-decanone)	Groups	
S	2812703.660	A	
ST_10^2	1026483.186		B
ST_10^5	151678.940		B
Milk	46268.539		B
T_10^5	38804.784		B
T_10^2	15173.735		B
ST_10^8	14804.056		B
T_10^8	9611.109		B

Category	LS means(18.29_2-undecanone)	Groups	
S	21388682.236	A	
ST_10^2	5229373.502		B
Milk	147902.352		B
ST_10^5	146206.996		B
T_10^2	76042.564		B
T_10^5	72188.206		B
ST_10^8	45947.662		B
T_10^8	33207.745		B

Appendix 13. Aroma compounds generated in models following incubation at 5°C or 15°C for 20days.

SPME GC-MS signal intensities for compounds are expressed relative to the signal intensity observed from a 5μg/L 2-nonanone standard.

	Yeast inoculum (CFU mL-1) Y. lipolytica											
	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Acetaldehyde	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.55E-04	0.00E+00	0.00E+00	0.00E+00
Methanethiol	0.00E+00	1.66E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.22E-05
Ethanol	1.90E-04	5.25E-04	1.83E-04	3.72E-05	5.35E-04	2.19E-03	4.52E-03	4.19E-03	3.91E-03	3.21E-03	2.62E-03	2.23E-03
Acetone	1.37E-02	1.66E-02	1.29E-02	1.28E-02	1.20E-02	1.08E-02	1.74E-02	1.66E-02	1.74E-02	1.69E-02	1.56E-02	1.32E-02
1-Propanol	8.44E-03	5.88E-03	7.58E-03	7.24E-03	8.55E-03	9.94E-03	1.07E-02	1.01E-02	1.31E-02	1.07E-02	1.03E-02	9.29E-03
2-Methyl propanal	0.00E+00	6.94E-06	0.00E+00	0.00E+00	0.00E+00	1.47E-05	1.33E-04	2.37E-04	1.27E-03	4.21E-04	7.23E-05	1.07E-05
2-Butanone	9.33E-03	1.03E-02	9.07E-03	2.14E-03	2.20E-03	1.04E-03	8.96E-03	9.31E-03	9.63E-03	4.41E-03	3.43E-03	1.47E-03
Ethylacetate	0.00E+00	2.39E-04	0.00E+00	1.06E-04	5.28E-04	5.06E-04	2.40E-04	3.58E-04	2.04E-04	4.90E-04	3.58E-04	7.54E-04
2-Methyl-1-propanol	2.83E-04	2.70E-04	3.70E-04	5.72E-05	2.36E-04	8.94E-04	5.22E-04	3.58E-04	2.75E-04	4.21E-04	2.20E-04	1.48E-04
3-Methyl-butanal	0.00E+00	0.00E+00	2.21E-05	1.36E-05	1.28E-05	0.00E+00	9.96E-05	2.97E-04	3.93E-03	9.92E-04	1.00E-04	0.00E+00
2-Methyl-butanal	2.64E-04	5.84E-05	5.65E-05	0.00E+00	6.42E-06	0.00E+00	2.18E-04	2.41E-04	4.65E-03	1.30E-03	1.68E-04	0.00E+00
2-Pentanone	1.17E-03	1.72E-03	1.18E-03	3.31E-02	4.72E-02	2.21E-02	4.56E-03	4.11E-03	4.73E-03	3.33E-02	2.93E-02	1.19E-01
2-Pentanol	0.00E+00	3.99E-05	0.00E+00	5.04E-04	8.39E-04	4.76E-04	1.26E-04	9.54E-05	1.34E-04	1.09E-03	6.56E-04	6.71E-04
3-Hydroxy-2-butanone	1.58E-04	1.27E-04	1.25E-04	6.78E-05	5.10E-05	1.27E-04	1.10E-04	1.29E-04	1.75E-04	1.28E-04	1.32E-04	0.00E+00
Ethyl ester propanoic acid	1.75E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.08E-05	1.31E-05	0.00E+00	2.65E-05	0.00E+00	0.00E+00
n-Propyl acetate	5.26E-06	0.00E+00	6.07E-06	1.69E-05	4.91E-05	7.64E-06	1.05E-05	9.11E-06	0.00E+00	1.10E-05	2.12E-05	7.90E-05
3-Methyl-butanol	3.54E-04	6.26E-04	5.97E-04	5.51E-05	8.57E-04	1.64E-03	1.85E-03	1.53E-03	1.89E-03	2.68E-03	1.80E-03	1.48E-03
2-Methyl-1-butanol	1.28E-04	1.67E-04	1.91E-04	3.60E-05	2.64E-04	3.61E-04	4.81E-04	2.50E-04	2.92E-04	4.47E-04	2.76E-04	1.53E-04
Dimethyl-disulfide	0.00E+00	5.09E-05	0.00E+00	5.50E-06	4.95E-06	6.29E-05	1.96E-05	9.48E-05	8.73E-04	1.52E-04	2.66E-05	3.54E-05

Yeast inoculum (CFU mL-1)

Y. lipolytica

	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
3-Methyl-2-pentanone	6.28E-06	0.00E+00	0.00E+00	0.00E+00	2.06E-05	2.66E-05	2.92E-05	5.49E-05	1.66E-05	8.50E-05	3.92E-05	1.96E-05
Methy-ethyl ester propanoic acid	6.34E-04	8.19E-04	8.13E-04	1.56E-04	0.00E+00	2.79E-04	1.57E-03	1.45E-03	9.76E-04	5.56E-04	3.53E-04	1.45E-04
1-Pentanol	3.87E-04	5.74E-04	3.72E-04	3.61E-04	6.22E-03	7.74E-04	6.65E-04	5.66E-04	4.92E-04	9.64E-04	9.01E-04	9.67E-04
Isobutyl acetate	9.51E-04	1.12E-03	8.43E-04	5.08E-04	1.04E-03	1.26E-03	1.92E-03	1.61E-03	1.32E-03	0.00E+00	2.14E-03	8.02E-04
2-Hexanone	1.20E-04	1.44E-04	7.43E-05	5.61E-03	1.20E-02	5.56E-03	9.25E-04	8.58E-04	1.15E-03	6.00E-03	5.54E-03	2.72E-02
Butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.41E-01	1.32E-01	1.50E-01	5.95E-02	3.90E-02	2.55E-02
Octane	9.48E-04	1.35E-03	9.40E-04	4.61E-04	7.31E-04	1.04E-03	2.69E-03	1.86E-03	1.89E-03	9.41E-04	1.25E-03	4.17E-04
3-Methyl-butanoic acid	1.35E-05	0.00E+00	0.00E+00	1.63E-05	1.81E-05	3.95E-05	2.90E-04	1.89E-04	2.50E-04	1.95E-04	0.00E+00	0.00E+00
2-Methyl butanoic acid	0.00E+00	0.00E+00	2.16E-06	0.00E+00	0.00E+00	4.18E-06	0.00E+00	3.18E-06	4.00E-06	0.00E+00	0.00E+00	0.00E+00
Pentanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.11E-05	4.69E-05	1.66E-03	2.14E-03	2.33E-03	6.42E-04	5.01E-04	0.00E+00
3-Methyl-1-butanol acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.57E-05	2.98E-05	0.00E+00	0.00E+00	0.00E+00	6.08E-05	2.87E-05	1.80E-04
2-Heptanone	3.27E-03	3.77E-03	2.06E-03	6.75E-02	3.92E-01	2.45E-01	4.56E-02	3.62E-02	5.88E-02	2.04E-01	3.02E-01	1.39E+00
Styrene	1.42E-04	6.95E-05	9.86E-05	4.82E-05	3.76E-04	1.31E-04	2.03E-03	1.02E-03	6.26E-04	1.63E-04	9.74E-04	3.37E-05
2-Heptanol (solvent GCMS)	9.71E-04	1.56E-03	1.01E-03	3.35E-02	9.04E-02	8.15E-02	9.20E-03	8.23E-03	6.07E-03	6.56E-02	6.83E-02	5.51E-02
a-Pinene	1.28E-04	9.00E-05	9.12E-05	1.18E-04	1.31E-04	1.19E-04	4.63E-05	2.22E-04	5.11E-05	1.21E-04	3.15E-05	3.64E-05
2-Octanone	1.67E-05	2.27E-05	3.38E-05	3.40E-04	7.93E-03	5.54E-03	4.02E-04	3.64E-04	4.35E-04	3.91E-03	7.50E-03	8.50E-02
Hexanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.70E-01	1.52E-01	1.87E-01	7.93E-02	6.05E-02	1.79E-02
3-Octanone	5.64E-05	1.36E-05	2.31E-05	4.24E-05	1.06E-04	1.20E-04	3.83E-04	4.97E-04	7.24E-04	5.48E-04	5.08E-04	7.25E-05
Hexanoic acid ethyl ester	3.20E-06	2.45E-05	5.33E-06	6.31E-06	1.00E-05	5.33E-05	4.89E-04	5.82E-04	1.16E-03	5.95E-04	5.93E-04	8.45E-05
4-Methylanisole	3.17E-06	3.97E-06	0.00E+00	2.14E-05	0.00E+00	1.24E-05	0.00E+00	6.15E-06	0.00E+00	6.00E-06	5.46E-06	4.99E-06
Butanoic acid 3-methylbutyl ester	0.00E+00	0.00E+00	0.00E+00	1.60E-05	3.18E-05	1.54E-05	6.45E-05	6.06E-05	1.09E-04	4.14E-05	1.36E-04	5.74E-05
8-Nonen-2-one	3.56E-05	2.03E-04	1.49E-04	1.25E-03	3.02E-02	1.53E-02	1.86E-04	1.04E-04	1.49E-04	1.10E-02	2.00E-02	2.57E-01
2-Nonanone	7.05E-04	1.59E-03	1.44E-03	3.94E-03	1.49E-01	9.11E-02	9.49E-03	8.30E-03	1.16E-02	1.14E-01	1.64E-01	8.77E-01

	Yeast inoculum (CFU mL-1) Y. lipolytica											
	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Benzeneethanol	3.71E-04	3.81E-04	1.90E-04	3.55E-04	4.82E-05	1.22E-04	2.54E-04	2.35E-04	1.56E-04	1.40E-04	8.67E-05	1.64E-04
Hexanoic acid butyl ester	0.00E+00	6.49E-06	0.00E+00	6.10E-06	1.06E-05	0.00E+00	0.00E+00	2.11E-05	1.90E-05	6.58E-05	2.14E-05	0.00E+00
Octanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.28E-03	4.31E-02	4.07E-02	4.25E-02	2.81E-02	2.44E-02	1.11E-02
2-Decanone	1.23E-05	0.00E+00	1.74E-05	2.21E-05	5.66E-04	2.81E-04	3.56E-05	7.22E-05	6.89E-05	4.59E-04	6.87E-04	7.03E-03
Octanoic acid ethyl ester	5.74E-06	7.93E-05	0.00E+00	6.09E-06	2.01E-05	3.12E-04	7.49E-04	8.19E-04	7.37E-04	2.12E-04	2.13E-04	4.24E-04
3-methybutyl hexanoate	1.29E-05	0.00E+00	0.00E+00	1.33E-05	0.00E+00	1.83E-05	4.30E-05	2.89E-05	4.31E-05	6.97E-05	2.48E-05	5.23E-05
Acetic acid 2-phenylethyl ester	1.67E-05	5.53E-04	2.85E-05	4.27E-04	1.30E-04	6.09E-04	3.05E-04	2.70E-04	4.34E-04	2.92E-04	1.25E-04	2.74E-03
2-Undecanone	9.46E-05	1.16E-04	8.94E-05	2.98E-04	4.10E-03	1.58E-03	1.01E-03	7.97E-04	1.14E-03	3.49E-03	4.38E-03	3.32E-02
n-Decanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.15E-03	1.86E-03	3.00E-03	1.33E-03	1.62E-03	8.31E-04

	Yeast inoculum (CFU mL-1) Y. lipolytica											
	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Acetaldehyde	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Methanethiol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethanol	2.16E-04	4.15E-04	7.18E-05	2.37E-03	0.00E+00	2.83E-03	1.81E-03	3.57E-03	1.86E-01	6.99E-04	2.33E-03	3.46E-04
Acetone	1.29E-02	1.32E-02	2.01E-02	6.74E-03	7.61E-03	2.28E-03	1.58E-02	1.90E-02	8.16E-03	5.94E-03	9.12E-03	1.65E-02
1-Propanol	8.37E-03	1.06E-02	3.72E-03	1.50E-02	4.99E-03	1.34E-02	9.21E-03	1.09E-02	7.43E-03	8.37E-03	1.10E-02	2.32E-03
2-Methyl propanal	0.00E+00	2.24E-05	0.00E+00	1.05E-04	8.09E-06	8.05E-05	0.00E+00	2.10E-04	2.36E-04	0.00E+00	4.40E-05	5.94E-06
2-Butanone	1.02E-02	1.12E-02	1.02E-02	1.24E-03	2.16E-03	9.64E-04	9.00E-03	1.03E-02	3.88E-03	1.23E-03	1.62E-03	3.24E-03

	Yeast inoculum (CFU mL-1)											
	Y. lipolytica											
	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Ethylacetate	2.48E-04	3.32E-04	0.00E+00	1.75E-04	8.25E-05	9.74E-05	3.00E-04	0.00E+00	2.10E-02	3.39E-04	4.02E-04	4.09E-04
2-Methyl-1-propanol	4.35E-04	0.00E+00	1.32E-04	5.46E-04	0.00E+00	2.99E-04	2.40E-04	3.88E-04	9.91E-03	3.95E-04	3.68E-04	3.67E-04
3-Methyl-butanal	1.92E-05	0.00E+00	1.59E-05	7.99E-05	3.80E-06	1.58E-04	4.52E-05	1.74E-04	3.71E-04	1.95E-05	1.42E-04	5.00E-05
2-Methyl-butanal	3.84E-05	5.13E-05	1.39E-04	1.05E-04	0.00E+00	7.18E-05	5.31E-05	1.46E-04	3.74E-04	1.66E-04	5.87E-05	3.34E-04
2-Pentanone	1.10E-03	1.09E-03	2.71E-03	9.07E-03	8.30E-02	5.23E-04	3.55E-03	3.18E-03	1.62E-03	4.23E-02	2.97E-02	9.27E-02
2-Pentanol	3.58E-05	0.00E+00	8.75E-05	2.02E-04	7.10E-04	7.94E-05	5.83E-05	5.87E-05	2.58E-05	1.86E-03	1.59E-03	1.91E-03
3-Hydroxy-2-butanone	6.52E-05	2.21E-04	1.26E-04	1.72E-04	6.03E-05	8.32E-05	1.24E-04	1.40E-04	1.33E-01	1.81E-05	7.70E-05	8.14E-05
Ethyl ester propanoic acid	0.00E+00	0.00E+00	0.00E+00	2.10E-05	0.00E+00	0.00E+00	3.57E-05	0.00E+00	8.27E-04	0.00E+00	0.00E+00	5.09E-05
n-Propyl acetate	7.87E-06	0.00E+00	0.00E+00	1.46E-05	2.27E-05	0.00E+00	0.00E+00	1.19E-05	1.56E-04	3.75E-05	4.16E-05	1.91E-05
3-Methyl-butanol	4.66E-04	2.31E-04	6.20E-04	1.00E-03	4.14E-05	8.68E-04	2.64E-03	1.28E-03	1.36E-01	1.17E-03	3.41E-03	1.92E-03
2-Methyl-1-butanol	1.65E-04	1.47E-04	1.28E-04	2.12E-04	2.75E-05	2.05E-04	3.32E-04	2.99E-04	4.87E-03	2.24E-04	4.44E-04	3.13E-04
Dimethyl-disulfide	8.65E-06	1.56E-05	0.00E+00	2.94E-05	0.00E+00	1.26E-04	4.17E-05	1.39E-04	1.20E-04	0.00E+00	2.55E-05	0.00E+00
3-Methyl-2-pentanone	2.09E-05	5.66E-06	2.68E-05	4.62E-05	8.54E-06	0.00E+00	1.03E-05	1.06E-05	0.00E+00	5.91E-05	5.41E-05	1.17E-04
Methy-ethyl ester propanoic acid	7.17E-04	6.90E-04	5.08E-04	5.68E-04	8.19E-05	6.01E-04	7.29E-04	6.49E-04	8.59E-04	4.60E-04	7.25E-04	5.29E-04
1-Pentanol	3.19E-04	3.53E-04	2.68E-04	1.88E-03	3.33E-04	1.46E-03	8.66E-04	3.04E-04	5.85E-04	2.46E-03	6.74E-04	1.83E-03
Isobutyl acetate	7.56E-04	8.82E-04	1.30E-03	1.30E-03	1.85E-03	9.48E-04	1.14E-03	8.91E-04	1.32E-03	2.95E-03	1.85E-03	3.51E-03
2-Hexanone	8.14E-05	9.48E-05	2.64E-04	3.15E-03	2.89E-02	1.46E-04	5.24E-04	3.17E-04	4.04E-04	6.84E-03	7.02E-03	1.17E-02
Butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.89E-02	3.06E-02	0.00E+00	2.21E-02	2.81E-02	8.65E-03
Octane	8.48E-04	1.21E-03	1.17E-03	1.26E-03	5.84E-04	1.87E-03	1.31E-03	9.34E-04	1.35E-03	1.06E-03	1.44E-03	1.60E-03
3-Methyl-butanoic acid	0.00E+00	0.00E+00	2.81E-05	0.00E+00	0.00E+00	1.20E-05	1.21E-03	8.49E-05	0.00E+00	1.33E-03	2.74E-04	4.39E-04
2-Methyl butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.40E-06	8.68E-06	0.00E+00	9.07E-06	9.47E-06	0.00E+00	6.90E-06
Pentanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.62E-04	0.00E+00	0.00E+00	3.21E-04	3.35E-04	0.00E+00
3-Methyl-1-butanol acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.01E-04	6.92E-05	7.58E-05	1.44E-04

Yeast inoculum (CFU mL-1)

Y. lipolytica

	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
2-Heptanone	1.96E-03	3.63E-03	6.81E-03	3.36E-01	1.23E+00	2.66E-02	1.97E-02	1.85E-02	2.55E-02	3.15E-01	4.31E-01	3.84E-01
Styrene	0.00E+00	4.70E-04	8.74E-04	0.00E+00	0.00E+00	1.94E-05	1.16E-03	1.10E-03	3.86E-04	1.08E-04	1.17E-04	9.01E-05
2-Heptanol (solvent GCMS)	7.44E-04	1.03E-03	2.05E-03	9.54E-03	2.72E-01	2.39E-03	5.24E-03	5.33E-03	1.87E-03	1.09E-01	9.62E-02	2.16E-01
a-Pinene	6.13E-05	1.83E-04	3.39E-04	3.50E-05	3.60E-05	7.36E-05	5.82E-05	2.94E-04	5.17E-05	7.20E-05	2.76E-05	1.17E-04
2-Octanone	3.32E-05	5.26E-05	7.09E-05	9.85E-03	4.96E-02	6.91E-04	1.43E-04	1.77E-04	1.55E-04	6.85E-03	9.46E-03	8.73E-03
Hexanoic acid	0.00E+00	0.00E+00	3.13E-03	0.00E+00	0.00E+00	0.00E+00	3.94E-02	3.39E-02	3.01E-02	0.00E+00	4.18E-02	5.81E-03
3-Octanone	1.71E-04	1.47E-04	9.97E-05	9.01E-05	4.40E-05	5.00E-05	1.54E-04	1.92E-04	1.15E-02	8.94E-05	3.46E-04	1.35E-04
Hexanoic acid ethyl ester	2.04E-05	2.26E-05	9.71E-06	5.28E-05	1.98E-05	2.01E-05	5.70E-05	1.01E-04	1.67E-02	1.62E-05	3.43E-04	3.21E-05
4-Methylanisole	4.55E-06	3.43E-06	0.00E+00	3.91E-05	2.80E-05	1.91E-05	0.00E+00	0.00E+00	0.00E+00	3.54E-05	1.51E-05	0.00E+00
Butanoic acid 3-methylbutyl ester	2.56E-05	0.00E+00	3.06E-05	1.34E-05	0.00E+00	0.00E+00	4.84E-05	2.88E-05	4.17E-04	2.86E-05	1.60E-04	0.00E+00
8-Nonen-2-one	1.06E-04	3.17E-05	9.70E-04	2.39E-02	2.12E-01	1.78E-03	1.67E-04	9.55E-05	9.18E-05	1.93E-02	2.29E-02	2.75E-02
2-Nonanone	8.15E-04	9.17E-04	4.65E-03	1.81E-01	5.48E-01	2.58E-02	3.21E-03	4.89E-03	3.98E-03	1.28E-01	1.41E-01	1.46E-01
Benzeneethanol	2.93E-04	1.21E-05	4.48E-03	2.97E-05	1.92E-04	1.01E-05	7.89E-04	9.45E-05	3.79E-03	8.93E-04	2.76E-04	3.90E-03
Hexanoic acid butyl ester	0.00E+00	0.00E+00	1.19E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.81E-04	1.03E-05	2.47E-05	1.74E-05
Octanoic acid	0.00E+00	0.00E+00	5.14E-04	7.57E-04	0.00E+00	0.00E+00	9.45E-03	1.23E-02	1.03E-02	2.67E-03	2.09E-02	2.66E-03
2-Decanone	1.01E-05	1.45E-05	3.84E-05	8.27E-04	3.08E-03	4.29E-05	2.76E-05	2.47E-05	7.14E-05	4.18E-04	4.83E-04	5.27E-04
Octanoic acid ethyl ester	0.00E+00	2.35E-05	8.13E-05	9.29E-05	1.42E-04	1.28E-04	8.59E-05	1.64E-04	1.16E-02	1.65E-05	3.34E-04	1.86E-04
3-methybutyl hexanoate	0.00E+00	1.41E-05	0.00E+00	8.24E-06	0.00E+00	7.68E-06	1.53E-05	1.12E-05	1.21E-04	2.26E-05	1.89E-05	2.15E-05
Acetic acid 2-phenylethyl ester	3.79E-05	4.35E-04	2.45E-04	1.28E-03	1.57E-03	1.85E-04	1.96E-03	4.45E-04	1.61E-03	1.31E-04	9.34E-04	1.83E-03
2-Undecanone	1.05E-04	1.10E-04	2.01E-04	3.69E-03	1.74E-02	4.40E-04	4.97E-04	4.25E-04	4.74E-04	4.71E-03	3.27E-03	5.21E-03
n-Decanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.15E-04	0.00E+00	0.00E+00	0.00E+00	7.38E-04	0.00E+00

	Yeast inoculum (CFU mL-1)											
	K. lactis											
	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Acetaldehyde	2.92E-02	2.30E-02	1.76E-02	2.32E-02	1.50E-02	1.46E-02	5.93E-03	7.03E-03	2.20E-02	3.83E-02	2.28E-02	1.84E-02
Methanethiol	0.00E+00	1.34E-05	2.13E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethanol	3.69E-01	3.30E-01	3.15E-01	4.02E-01	3.55E-01	3.22E-01	5.42E-01	5.05E-01	4.60E-01	3.96E-01	4.30E-01	3.79E-01
Acetone	1.03E-03	1.04E-03	9.41E-04	1.47E-03	5.82E-04	9.31E-04	2.49E-04	2.13E-04	3.11E-04	1.16E-03	8.78E-04	7.23E-04
1-Propanol	4.15E-03	4.20E-03	5.48E-03	1.02E-02	2.26E-03	4.85E-03	1.83E-02	9.49E-03	8.11E-03	4.62E-03	9.30E-03	5.26E-03
2-Methyl propanal	2.38E-03	1.92E-03	2.21E-03	2.29E-03	2.71E-04	2.30E-03	3.27E-04	3.57E-04	6.60E-04	8.65E-04	1.17E-03	1.35E-03
2-Butanone	1.05E-03	1.08E-03	8.96E-04	1.58E-03	5.58E-04	1.10E-03	3.74E-04	2.99E-04	6.75E-04	1.02E-03	7.59E-04	7.48E-04
Ethylacetate	7.59E-01	6.86E-01	8.92E-01	5.25E-01	7.29E-01	7.02E-01	6.44E-01	4.89E-01	4.75E-01	6.47E-01	5.96E-01	6.25E-01
2-Methyl-1-propanol	1.31E-02	1.13E-02	8.74E-03	1.60E-02	1.41E-02	1.65E-02	2.35E-02	1.66E-02	1.40E-02	1.32E-02	1.66E-02	1.85E-02
3-Methyl-butanal	5.52E-04	4.62E-04	5.40E-04	4.60E-04	1.07E-04	7.39E-04	1.26E-04	9.77E-05	3.57E-04	3.61E-04	2.62E-03	1.10E-03
2-Methyl-butanal	1.78E-03	1.28E-03	1.59E-03	1.65E-03	5.62E-04	2.15E-03	4.44E-04	4.95E-04	6.69E-03	3.40E-03	1.78E-02	6.37E-03
2-Pentanone	2.56E-04	2.47E-04	1.83E-04	4.25E-03	2.92E-03	2.98E-03	2.43E-04	2.05E-04	1.91E-04	2.77E-03	2.89E-03	1.62E-03
2-Pentanol	2.22E-05	1.97E-05	7.64E-06	1.40E-04	2.50E-04	1.00E-04	4.04E-05	4.11E-05	2.59E-05	1.53E-04	3.66E-04	1.23E-04
3-Hydroxy-2-butanone	1.08E-02	1.17E-02	7.07E-03	7.49E-03	3.46E-03	7.06E-03	5.41E-04	0.00E+00	1.49E-03	6.20E-03	2.31E-03	2.51E-03
Ethyl ester propanoic acid	3.27E-02	3.67E-02	4.12E-02	1.50E-02	3.29E-02	2.75E-02	2.73E-02	2.35E-02	2.73E-02	2.90E-02	2.10E-02	2.16E-02
n-Propyl acetate	4.17E-03	4.26E-03	1.11E-02	9.92E-04	4.43E-03	5.12E-03	2.00E-03	1.78E-03	1.72E-03	1.58E-03	1.16E-03	1.86E-03
3-Methyl-butanol	1.28E-01	1.37E-01	1.20E-01	1.08E-01	1.48E-01	1.51E-01	1.18E-01	1.17E-01	1.24E-01	1.26E-01	1.44E-01	1.60E-01
2-Methyl-1-butanol	3.69E-02	3.86E-02	2.83E-02	3.61E-02	4.11E-02	4.12E-02	5.36E-02	5.22E-02	6.02E-02	6.84E-02	6.94E-02	7.97E-02
Dimethyl-disulfide	0.00E+00	5.93E-06	4.95E-06	0.00E+00	0.00E+00	0.00E+00	6.89E-05	2.64E-04	8.66E-05	2.16E-05	1.39E-04	8.74E-06
3-Methyl-2-pentanone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.52E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Methy-ethyl ester propanoic acid	3.63E-03	3.48E-03	3.46E-03	1.59E-03	3.22E-03	2.39E-03	5.16E-03	4.79E-03	4.32E-03	3.43E-03	2.97E-03	2.24E-03
1-Pentanol	4.61E-04	3.30E-04	3.64E-04	6.88E-04	4.34E-04	4.35E-04	5.50E-04	5.92E-04	8.32E-04	5.47E-04	4.50E-04	3.93E-04
Isobutyl acetate	1.18E-02	1.31E-02	2.23E-02	4.20E-03	1.83E-02	1.24E-02	9.54E-03	7.60E-03	6.72E-03	8.48E-03	8.94E-03	9.45E-03

	Yeast inoculum (CFU mL-1)											
	K. lactis											
	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
2-Hexanone	7.48E-05	7.78E-05	1.07E-04	8.50E-04	9.07E-04	1.23E-03	7.96E-05	6.23E-05	9.39E-05	6.63E-04	6.13E-04	5.14E-04
Butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Octane	9.50E-04	1.02E-03	6.02E-04	1.09E-03	9.06E-04	9.31E-04	1.30E-03	1.19E-03	1.26E-03	1.08E-03	8.48E-04	9.69E-04
3-Methyl-butanoic acid	1.88E-05	2.12E-05	0.00E+00	0.00E+00	0.00E+00	4.69E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.27E-05	0.00E+00
2-Methyl butanoic acid	1.35E-05	2.96E-05	7.04E-06	5.75E-06	0.00E+00	4.69E-06	1.52E-05	1.74E-05	0.00E+00	3.27E-05	1.55E-05	0.00E+00
Pentanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-1-butanol acetate	1.33E-02	1.82E-02	2.37E-02	3.69E-03	2.88E-02	1.32E-02	1.74E-02	1.73E-02	1.57E-02	1.71E-02	1.43E-02	1.97E-02
2-Heptanone	6.46E-03	7.87E-03	5.90E-03	6.14E-02	7.62E-02	8.97E-02	4.46E-03	4.05E-03	5.65E-03	5.19E-02	4.68E-02	5.70E-02
Styrene	2.88E-04	1.37E-03	4.11E-05	1.38E-04	0.00E+00	4.66E-05	4.55E-04	3.03E-04	1.64E-03	3.13E-04	1.97E-05	1.40E-03
2-Heptanol (solvent GCMS)	1.54E-03	1.38E-03	7.32E-04	1.20E-02	2.16E-02	1.19E-02	2.57E-03	2.76E-03	2.87E-03	2.43E-02	3.39E-02	2.77E-02
a-Pinene	1.72E-04	2.01E-04	2.57E-05	7.71E-05	5.12E-05	6.93E-05	7.09E-05	1.59E-05	7.00E-05	4.47E-05	4.21E-05	6.09E-05
2-Octanone	6.08E-05	5.54E-05	6.66E-05	1.03E-03	1.49E-03	1.30E-03	6.97E-05	3.48E-05	7.02E-05	1.10E-03	1.05E-03	1.24E-03
Hexanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Octanone	1.25E-03	1.77E-03	9.79E-04	6.74E-04	2.68E-03	1.09E-03	3.18E-03	3.86E-03	3.08E-03	4.60E-03	3.27E-03	4.27E-03
Hexanoic acid ethyl ester	1.77E-03	2.36E-03	1.41E-03	9.91E-04	3.87E-03	1.55E-03	4.83E-03	5.16E-03	4.09E-03	6.10E-03	4.62E-03	5.87E-03
4-Methylanisole	9.09E-06	0.00E+00	4.77E-06	5.64E-06	6.41E-06	0.00E+00	0.00E+00	3.56E-06	1.21E-05	0.00E+00	3.59E-06	0.00E+00
Butanoic acid 3-methylbutyl ester	2.88E-05	9.35E-05	6.02E-05	1.96E-04	6.14E-04	1.56E-04	9.70E-05	6.19E-05	6.65E-05	7.37E-04	8.59E-04	7.48E-04
8-Nonen-2-one	8.37E-05	3.77E-04	8.43E-05	3.04E-03	4.42E-03	3.49E-03	1.43E-04	4.27E-05	4.29E-04	2.80E-03	2.87E-03	3.75E-03
2-Nonanone	1.51E-03	3.17E-03	1.26E-03	4.05E-02	4.71E-02	3.98E-02	3.75E-03	1.32E-03	4.72E-03	3.72E-02	3.63E-02	4.21E-02
Benzeneethanol	5.00E-05	3.46E-05	1.88E-05	3.54E-05	1.63E-04	3.45E-05	1.45E-04	7.33E-05	2.47E-04	9.94E-05	1.15E-03	3.37E-04
Hexanoic acid butyl ester	9.85E-06	2.05E-05	1.87E-05	1.29E-05	5.62E-05	0.00E+00	1.37E-05	1.93E-05	1.74E-05	4.55E-05	2.71E-05	4.42E-05
Octanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Decanone	3.74E-05	4.57E-05	1.00E-05	8.79E-05	2.64E-04	9.42E-05	3.30E-05	3.33E-05	4.46E-05	1.78E-04	1.79E-04	1.52E-04

							Yeast inoculum (CFU mL-1) K. lactis					
	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores	10^5	10^5	10^5	10^5 + spores	10^5 + spores	10^5 + spores
							Incubation temperature (°C)					
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Octanoic acid ethyl ester	2.22E-03	2.95E-03	1.62E-03	1.79E-04	3.24E-03	1.31E-03	4.85E-03	5.46E-03	5.37E-03	2.89E-03	7.76E-04	3.27E-03
3-methybutyl hexanoate	2.23E-05	2.83E-05	9.59E-06	0.00E+00	5.56E-05	2.49E-05	0.00E+00	1.09E-05	0.00E+00	2.56E-05	2.36E-05	2.49E-05
Acetic acid 2-phenylethyl ester	1.98E-02	2.37E-02	1.95E-02	1.12E-02	4.41E-02	1.82E-02	2.30E-02	2.25E-02	2.59E-02	5.43E-02	6.73E-02	1.17E-01
2-Undecanone	1.28E-04	2.40E-04	1.69E-04	1.40E-03	1.52E-03	9.92E-04	1.91E-04	9.24E-05	3.25E-04	1.19E-03	1.29E-03	1.18E-03
n-Decanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

							Yeast inoculum (CFU mL-1) K. lactis					
	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
							Incubation temperature (°C)					
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Acetaldehyde	2.04E-02	8.13E-03	1.93E-02	2.69E-04	0.00E+00	0.00E+00	1.77E-04	0.00E+00	0.00E+00	4.30E-02	3.50E-02	2.20E-02
Methanethiol	0.00E+00	1.73E-05	1.83E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.41E-05
Ethanol	3.37E-01	3.14E-01	3.36E-01	1.40E-02	1.92E-02	3.04E-02	1.56E-03	9.81E-04	8.89E-04	3.54E-01	3.27E-01	3.17E-01
Acetone	2.22E-03	7.86E-04	1.24E-03	2.38E-03	3.84E-03	2.54E-03	1.04E-02	1.25E-02	9.29E-03	9.35E-04	8.95E-04	9.12E-04
1-Propanol	1.58E-02	3.10E-03	5.31E-03	1.09E-02	1.16E-02	1.25E-02	1.30E-02	1.08E-02	1.13E-02	6.84E-03	6.76E-03	5.12E-03
2-Methyl propanal	4.65E-03	1.10E-03	2.70E-03	1.32E-04	1.27E-04	2.24E-04	4.70E-05	4.39E-05	0.00E+00	1.53E-03	1.55E-03	1.63E-03
2-Butanone	4.33E-03	8.89E-04	1.20E-03	9.66E-04	1.14E-03	8.99E-04	8.83E-03	9.61E-03	7.03E-03	3.93E-04	4.25E-04	5.82E-04
Ethylacetate	3.73E-01	7.51E-01	7.74E-01	3.56E-03	2.12E-02	1.78E-03	1.82E-04	2.31E-04	1.09E-04	6.32E-01	4.52E-01	7.27E-01
2-Methyl-1-propanol	1.59E-02	1.20E-02	1.40E-02	4.61E-04	8.69E-04	8.83E-04	0.00E+00	0.00E+00	6.78E-05	2.18E-02	1.80E-02	1.53E-02
3-Methyl-butanal	1.08E-03	3.57E-04	1.03E-03	6.22E-04	2.96E-04	6.22E-04	2.80E-05	4.88E-06	4.39E-04	2.42E-03	9.47E-04	1.77E-03
2-Methyl-butanal	3.57E-03	7.34E-04	2.74E-03	2.25E-04	1.93E-04	2.88E-04	7.92E-05	5.23E-05	3.66E-04	9.38E-03	3.85E-03	7.01E-03

	Yeast inoculum (CFU mL-1)											
	K. lactis											
	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
2-Pentanone	8.70E-04	1.95E-04	2.63E-04	2.33E-04	4.71E-04	2.92E-04	9.72E-04	9.08E-04	6.44E-03	2.13E-03	1.17E-03	1.68E-03
2-Pentanol	0.00E+00	0.00E+00	1.49E-05	8.45E-05	1.11E-04	4.85E-05	1.07E-04	1.87E-04	2.09E-05	1.32E-04	7.72E-05	1.55E-04
3-Hydroxy-2-butanone	5.34E-03	8.22E-03	1.49E-02	8.60E-05	7.12E-05	1.47E-04	1.73E-04	2.13E-04	9.41E-05	6.39E-03	7.23E-03	7.63E-03
Ethyl ester propanoic acid	1.89E-02	3.59E-02	3.44E-02	1.50E-05	6.68E-05	0.00E+00	1.71E-05	8.05E-06	9.34E-06	1.82E-02	1.94E-02	2.40E-02
n-Propyl acetate	1.05E-03	6.31E-03	6.96E-03	1.41E-05	5.36E-05	3.32E-06	4.47E-06	0.00E+00	6.57E-06	2.45E-03	3.52E-03	2.88E-03
3-Methyl-butanol	1.27E-01	1.40E-01	1.58E-01	2.48E-03	2.03E-03	3.81E-03	5.33E-05	3.11E-05	3.02E-04	2.35E-01	2.24E-01	2.18E-01
2-Methyl-1-butanol	3.96E-02	3.84E-02	4.31E-02	3.81E-04	4.25E-04	5.51E-04	4.88E-05	3.31E-05	5.17E-05	7.74E-02	6.15E-02	7.65E-02
Dimethyl-disulfide	0.00E+00	3.33E-06	0.00E+00	3.44E-04	2.16E-04	2.02E-04	4.79E-04	8.82E-04	1.00E-04	1.25E-05	7.04E-06	2.85E-05
3-Methyl-2-pentanone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.30E-06	0.00E+00	0.00E+00	0.00E+00
Methy-ethyl ester propanoic acid	3.32E-03	3.47E-03	3.03E-03	1.26E-03	1.61E-03	1.01E-03	8.81E-04	8.80E-04	7.51E-04	2.18E-03	1.89E-03	2.44E-03
1-Pentanol	4.88E-04	3.24E-04	4.06E-04	1.57E-03	1.85E-03	9.24E-04	4.42E-04	4.37E-04	3.59E-04	8.46E-04	8.10E-04	6.76E-04
Isobutyl acetate	2.35E-03	1.51E-02	1.37E-02	1.42E-03	1.71E-03	1.03E-03	1.16E-03	1.09E-03	1.04E-03	1.71E-02	1.82E-02	1.52E-02
2-Hexanone	2.33E-04	8.80E-05	9.98E-05	8.22E-05	2.56E-04	1.38E-04	1.25E-04	1.35E-04	2.60E-03	8.81E-04	5.21E-04	7.07E-04
Butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Octane	1.53E-03	1.04E-03	9.79E-04	2.52E-03	2.43E-03	2.24E-03	1.26E-03	1.66E-03	1.41E-03	1.37E-03	1.25E-03	1.42E-03
3-Methyl-butanoic acid	0.00E+00	3.60E-05	3.70E-05	0.00E+00	5.08E-06	6.10E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.11E-05
2-Methyl butanoic acid	9.16E-06	3.48E-05	3.24E-05	3.40E-06	0.00E+00	7.59E-06	0.00E+00	0.00E+00	0.00E+00	1.15E-05	4.24E-06	0.00E+00
Pentanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.77E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-1-butanol acetate	1.86E-03	1.92E-02	1.57E-02	0.00E+00	0.00E+00	2.29E-05	0.00E+00	0.00E+00	0.00E+00	2.52E-02	2.32E-02	2.98E-02
2-Heptanone	1.15E-02	7.54E-03	8.63E-03	1.50E-02	2.75E-02	1.66E-02	7.02E-03	7.31E-03	4.33E-01	8.44E-02	5.04E-02	6.51E-02
Styrene	4.00E-04	2.40E-04	5.00E-05	1.62E-04	6.37E-05	5.55E-05	2.26E-04	9.83E-05	0.00E+00	5.38E-04	8.13E-04	1.47E-03
2-Heptanol (solvent GCMS)	9.60E-04	9.71E-04	1.13E-03	1.25E-03	1.48E-03	1.27E-03	0.00E+00	0.00E+00	1.90E-03	1.71E-02	1.08E-02	1.98E-02
a-Pinene	6.79E-05	2.27E-04	2.61E-05	3.87E-05	3.52E-05	4.55E-05	4.25E-05	5.48E-05	7.00E-05	1.67E-04	1.74E-04	1.91E-05

	Yeast inoculum (CFU mL-1)											
	K. lactis											
	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores	10^2	10^2	10^2	10^2 + spores	10^2 + spores	10^2 + spores
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
2-Octanone	1.32E-04	5.39E-05	1.09E-04	3.56E-04	5.31E-04	3.30E-04	7.00E-05	9.42E-05	1.82E-02	2.46E-03	1.31E-03	1.82E-03
Hexanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Octanone	5.97E-04	1.64E-03	1.19E-03	6.22E-05	5.01E-05	3.92E-05	1.34E-04	6.89E-05	2.89E-04	5.50E-03	3.53E-03	5.69E-03
Hexanoic acid ethyl ester	6.21E-04	2.14E-03	1.76E-03	1.45E-05	1.16E-05	4.10E-05	3.66E-06	1.76E-05	1.87E-04	8.17E-03	5.16E-03	7.40E-03
4-Methylanisole	0.00E+00	1.12E-05	0.00E+00	2.30E-05	5.29E-06	2.21E-05	0.00E+00	4.12E-06	7.18E-06	3.00E-05	1.60E-04	1.28E-05
Butanoic acid 3-methylbutyl ester	4.28E-05	1.20E-04	4.61E-05	2.08E-05	1.46E-05	1.64E-05	0.00E+00	0.00E+00	3.30E-05	4.77E-03	3.24E-03	2.60E-03
8-Nonen-2-one	5.76E-05	3.09E-04	9.77E-05	9.77E-04	1.50E-03	7.66E-04	4.69E-05	3.45E-05	4.33E-02	4.45E-03	2.19E-03	4.18E-03
2-Nonanone	2.08E-03	2.34E-03	2.05E-03	1.67E-02	2.29E-02	1.37E-02	1.18E-03	1.99E-03	2.88E-01	5.15E-02	2.85E-02	4.52E-02
Benzeneethanol	4.11E-05	6.94E-05	3.21E-05	0.00E+00	1.24E-05	1.06E-05	7.76E-06	1.27E-05	0.00E+00	3.00E-04	2.78E-04	5.78E-04
Hexanoic acid butyl ester	0.00E+00	0.00E+00	1.47E-05	2.81E-06	0.00E+00	7.93E-06	0.00E+00	4.93E-06	0.00E+00	1.33E-04	6.74E-05	7.52E-05
Octanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Decanone	3.27E-05	2.71E-05	3.44E-05	2.26E-05	6.18E-05	2.53E-05	1.53E-05	8.88E-06	1.59E-03	1.64E-04	9.24E-05	1.01E-04
Octanoic acid ethyl ester	4.07E-04	3.06E-03	1.88E-03	1.16E-04	7.15E-05	1.74E-04	6.58E-06	8.55E-05	6.35E-05	2.27E-03	1.53E-03	3.05E-03
3-methybutyl hexanoate	0.00E+00	0.00E+00	2.06E-05	0.00E+00	1.70E-05	5.51E-06	0.00E+00	2.30E-05	1.24E-05	1.23E-04	7.68E-05	6.94E-05
Acetic acid 2-phenylethyl ester	8.71E-03	2.61E-02	1.80E-02	4.47E-04	1.37E-04	4.49E-04	2.19E-04	1.25E-04	4.48E-04	8.40E-02	6.67E-02	1.22E-01
2-Undecanone	2.34E-04	2.21E-04	1.17E-04	3.24E-04	3.59E-04	2.34E-04	1.02E-04	1.43E-04	1.07E-02	1.35E-03	7.70E-04	1.40E-03
n-Decanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Model Inoculum

Y. lipolytica and *K. lactis* trials

	Milk	Milk	Milk	Spore only	Spore only	Spore only	Milk	Milk	Milk	Spore only	Spore only	Spore only
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Acetaldehyde	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Methanethiol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.28E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethanol	5.92E-04	1.38E-03	4.40E-04	9.89E-04	1.01E-03	4.82E-04	2.30E-03	1.96E-03	1.37E-03	1.39E-04	3.98E-04	3.55E-02
Acetone	9.31E-03	1.17E-02	1.31E-02	1.91E-03	1.90E-03	1.93E-03	1.57E-02	1.17E-02	4.81E-03	3.95E-03	2.46E-03	3.15E-03
1-Propanol	1.12E-02	1.01E-02	1.17E-02	1.19E-02	1.32E-02	1.10E-02	1.04E-02	1.01E-02	9.58E-03	5.87E-03	1.04E-02	1.06E-02
2-Methyl propanal	3.37E-05	4.85E-05	2.83E-05	1.38E-05	1.29E-04	1.00E-04	2.87E-04	0.00E+00	1.08E-04	0.00E+00	0.00E+00	7.45E-06
2-Butanone	6.72E-03	5.74E-03	1.03E-02	8.88E-04	6.79E-04	7.77E-04	8.83E-03	7.16E-03	2.01E-03	2.32E-04	2.00E-04	1.54E-03
Ethylacetate	8.17E-05	3.41E-04	0.00E+00	0.00E+00	1.01E-04	8.67E-05	5.68E-04	1.45E-04	1.44E-04	1.70E-04	1.87E-04	1.99E-04
2-Methyl-1-propanol	2.25E-04	0.00E+00	0.00E+00	2.24E-04	1.73E-04	1.14E-04	2.03E-04	3.20E-04	1.08E-04	6.91E-04	5.43E-04	7.49E-04
3-Methyl-butanal	4.65E-05	5.71E-05	2.69E-05	1.75E-04	7.34E-04	3.26E-04	4.07E-04	1.75E-05	3.15E-04	1.73E-05	1.88E-05	6.59E-05
2-Methyl-butanal	2.33E-04	7.75E-05	1.20E-04	7.15E-05	2.46E-04	1.30E-04	1.36E-03	2.95E-05	9.97E-05	1.49E-05	1.05E-05	1.03E-04
2-Pentanone	1.87E-03	2.73E-03	9.85E-04	2.23E-04	1.74E-04	2.21E-04	1.86E-03	9.31E-04	7.82E-03	2.15E-04	4.89E-04	7.34E-03
2-Pentanol	5.39E-05	4.51E-05	8.37E-05	9.63E-05	1.05E-04	9.01E-05	1.43E-05	0.00E+00	5.67E-04	1.17E-04	1.40E-04	1.51E-04
3-Hydroxy-2-butanone	1.02E-04	2.54E-04	1.97E-04	8.26E-04	6.24E-05	5.92E-05	2.97E-04	6.16E-05	7.58E-05	0.00E+00	8.50E-05	8.00E-04
Ethyl ester propanoic acid	6.75E-06	0.00E+00	2.53E-05	0.00E+00	1.72E-05	0.00E+00	1.89E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.25E-05
n-Propyl acetate	1.17E-05	0.00E+00	4.73E-06	7.16E-06	0.00E+00	0.00E+00	2.54E-05	0.00E+00	0.00E+00	1.53E-05	3.68E-05	0.00E+00
3-Methyl-butanol	6.92E-05	1.20E-04	3.84E-05	9.13E-04	6.60E-04	2.89E-04	4.47E-04	1.41E-04	3.34E-04	3.82E-03	2.09E-03	1.43E-03
2-Methyl-1-butanol	2.04E-05	5.41E-05	3.55E-05	1.57E-04	1.24E-04	8.32E-05	9.36E-05	6.92E-05	1.37E-04	6.71E-04	4.53E-04	1.13E-03
Dimethyl-disulfide	2.81E-04	1.13E-04	4.81E-04	0.00E+00	2.00E-04	2.04E-04	2.51E-03	7.90E-03	6.91E-04	3.09E-05	1.21E-04	5.11E-06
3-Methyl-2-pentanone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.29E-05	0.00E+00	1.37E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Methy-ethyl ester propanoic acid	6.29E-04	5.18E-04	5.69E-04	6.28E-04	4.23E-04	5.17E-04	5.00E-04	6.44E-04	5.71E-04	3.49E-04	3.21E-04	3.11E-04
1-Pentanol	4.67E-04	4.66E-04	2.31E-04	1.40E-03	1.28E-03	1.42E-03	7.75E-04	4.21E-04	1.25E-03	7.92E-04	2.51E-03	9.48E-04
Isobutyl acetate	8.90E-04	7.18E-04	9.81E-04	9.21E-04	8.01E-04	8.73E-04	8.94E-04	1.04E-03	1.07E-03	7.00E-04	5.89E-04	4.56E-04

Model Inoculum

Y. lipolytica and *K. lactis* trials

	Milk	Milk	Milk	Spore only	Spore only	Spore only	Milk	Milk	Milk	Spore only	Spore only	Spore only
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
2-Hexanone	4.71E-04	6.49E-04	1.29E-04	1.18E-04	1.40E-04	6.87E-05	3.62E-04	1.37E-04	2.34E-03	1.18E-04	2.25E-04	1.83E-03
Butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Octane	1.28E-03	1.31E-03	1.25E-03	1.44E-03	1.17E-03	1.25E-03	1.50E-03	1.52E-03	1.54E-03	1.07E-03	9.72E-04	8.87E-04
3-Methyl-butanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.43E-05	5.62E-05	5.24E-06	2.03E-05	4.65E-06	0.00E+00	0.00E+00
2-Methyl butanoic acid	3.88E-06	4.64E-06	1.94E-06	2.72E-06	0.00E+00	0.00E+00	6.93E-06	0.00E+00	0.00E+00	0.00E+00	4.87E-06	7.87E-06
Pentanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Methyl-1-butanol acetate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.05E-05	0.00E+00
2-Heptanone	3.99E-02	4.94E-02	7.40E-03	1.72E-02	1.96E-02	1.54E-02	6.18E-02	6.88E-03	1.58E-01	8.17E-03	2.19E-02	1.72E-01
Styrene	2.74E-04	8.52E-05	1.22E-04	4.02E-05	6.92E-05	1.44E-05	3.30E-05	2.53E-04	1.00E-04	3.32E-04	1.48E-03	4.44E-05
2-Heptanol (solvent GCMS)	1.05E-04	2.71E-04	0.00E+00	1.42E-03	1.44E-03	1.36E-03	1.29E-04	2.93E-05	2.03E-03	1.29E-03	1.53E-03	5.83E-03
a-Pinene	8.62E-05	5.88E-05	4.29E-05	3.71E-05	3.48E-05	3.48E-05	1.14E-04	4.56E-05	4.35E-05	6.11E-05	1.65E-04	5.88E-05
2-Octanone	7.31E-04	8.83E-04	9.37E-05	4.06E-04	4.57E-04	3.93E-04	2.17E-03	3.54E-05	2.71E-03	1.88E-04	4.94E-04	5.39E-03
Hexanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-Octanone	2.45E-05	8.86E-05	3.98E-05	8.63E-05	0.00E+00	6.83E-05	1.35E-04	5.15E-05	6.62E-05	4.91E-05	7.31E-05	1.06E-04
Hexanoic acid ethyl ester	4.05E-07	5.28E-05	5.76E-06	5.02E-05	1.55E-05	7.58E-06	3.44E-05	2.77E-05	1.47E-05	2.02E-05	3.76E-05	5.26E-05
4-Methylanisole	0.00E+00	0.00E+00	8.02E-06	2.69E-05	4.29E-05	6.81E-06	0.00E+00	3.22E-06	1.33E-05	2.53E-03	6.88E-04	1.01E-04
Butanoic acid 3-methylbutyl ester	1.50E-05	2.46E-05	1.76E-05	1.41E-05	0.00E+00	0.00E+00	0.00E+00	7.59E-06	0.00E+00	0.00E+00	0.00E+00	1.36E-05
8-Nonen-2-one	1.62E-03	1.72E-03	1.17E-04	8.35E-04	1.29E-03	9.99E-04	4.90E-03	1.16E-04	5.89E-03	6.17E-04	1.22E-03	8.08E-03
2-Nonanone	1.75E-02	2.07E-02	2.97E-03	1.19E-02	1.62E-02	1.51E-02	5.66E-02	1.31E-03	5.87E-02	6.64E-03	1.64E-02	8.45E-02
Benzeneethanol	0.00E+00	1.51E-05	1.02E-05	6.52E-06	8.92E-06	1.27E-05	1.09E-05	0.00E+00	6.47E-06	1.30E-04	2.63E-05	1.04E-05
Hexanoic acid butyl ester	0.00E+00	0.00E+00	0.00E+00	6.85E-06	7.00E-06	0.00E+00	2.05E-05	0.00E+00	8.94E-06	0.00E+00	0.00E+00	1.36E-05
Octanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Decanone	2.11E-05	2.36E-05	9.37E-06	3.72E-05	3.93E-05	3.47E-05	8.81E-05	0.00E+00	1.85E-04	3.50E-05	5.69E-05	3.06E-04

	Model Inoculum											
	Y. lipolytica and K. lactis trials											
	Milk	Milk	Milk	Spore only	Spore only	Spore only	Milk	Milk	Milk	Spore only	Spore only	Spore only
	Incubation temperature (°C)											
LRI Suggested Compound	5	5	5	5	5	5	15	15	15	15	15	15
Octanoic acid ethyl ester	1.11E-05	2.07E-04	9.51E-05	8.05E-05	1.78E-05	7.97E-06	5.60E-05	1.40E-05	1.05E-04	5.51E-05	8.48E-05	1.30E-05
3-methybutyl hexanoate	0.00E+00	0.00E+00	0.00E+00	8.30E-06	8.87E-06	0.00E+00	1.56E-05	5.33E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Acetic acid 2-phenylethyl ester	2.40E-05	8.40E-04	1.23E-04	3.75E-04	3.63E-04	9.87E-05	1.23E-03	9.68E-04	3.52E-04	1.68E-03	2.33E-03	4.67E-04
2-Undecanone	2.53E-04	2.45E-04	1.33E-04	2.45E-04	3.44E-04	2.96E-04	6.98E-04	1.08E-04	1.79E-03	3.85E-04	1.01E-03	2.07E-03
n-Decanoic acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Appendix 14. Average aroma compound generation within models following incubation at 5°C or 15°C for 20 days.

Triplicate samples (Appendix 13). SPME GC-MS signal intensities for compounds are expressed relative to the signal intensity observed from a 5µg/L 2-nonanone standard.

	Yeast inoculum (CFU mL-1) *Y. lipolytica*																
	10^5				10^2				10^5 + spores				10^2 + spores				
	Incubation temperature (°C)																
	5		15		5		15		5		15		5		15		
LRI Suggested Compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	
Acetaldehyde	0	N/A	1.85E-04	1.41E+02	0	N/A	0	N/A	0	N/A	0	N/A	0	N/A	0	N/A	
Methanethiol	5.53E-06	1.41E+02	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	4.06E-06	1.41E+02	0.00E+00	N/A	0.00E+00	N/A	
Ethanol	3.00E-04	5.33E+01	4.21E-03	5.99E+00	2.34E-04	6.01E+01	6.39E-02	1.35E+02	9.22E-04	1.00E+02	2.69E-03	1.51E+01	1.74E-03	7.15E+01	1.13E-03	7.68E+01	
Acetone	1.44E-02	1.11E+01	1.72E-02	2.20E+00	1.54E-02	2.18E+01	1.43E-02	3.17E+01	1.19E-02	6.84E+00	1.52E-02	1.00E+01	5.54E-03	4.21E+01	1.05E-02	4.22E+01	
1-Propanol	7.30E-03	1.46E+01	1.13E-02	1.13E+01	7.57E-03	3.79E+01	9.18E-03	1.54E+01	8.58E-03	1.29E+01	1.01E-02	5.98E+00	1.11E-02	3.94E+01	7.22E-03	5.02E+01	
2-Methyl propanal	2.31E-06	1.41E+02	5.46E-04	9.39E+01	7.48E-06	1.41E+02	1.49E-04	7.10E+01	4.91E-06	1.41E+02	1.68E-04	1.08E+02	6.46E-05	6.38E+01	1.66E-05	1.17E+02	
2-Butanone	9.56E-03	5.45E+00	9.30E-03	2.96E+00	1.05E-02	4.75E+00	7.72E-03	3.58E+01	1.79E-03	2.99E+01	3.10E-03	3.94E+01	1.45E-03	3.52E+01	2.03E-03	4.29E+01	
Ethylacetate	7.98E-05	1.41E+02	2.67E-04	2.45E+01	1.93E-04	7.29E+01	7.09E-03	1.38E+02	3.80E-04	5.11E+01	5.34E-04	3.09E+01	1.18E-04	3.44E+01	3.83E-04	8.20E+00	
2-Methyl-1-propanol	3.08E-04	1.43E+01	3.85E-04	2.67E+01	1.89E-04	9.63E+01	3.51E-03	1.29E+02	3.96E-04	9.09E+01	2.63E-04	4.39E+01	2.82E-04	7.93E+01	3.77E-04	3.50E+00	
3-Methyl-butanal	7.36E-06	1.41E+02	1.44E-03	1.22E+02	1.17E-05	7.17E+01	1.97E-04	6.81E+01	8.81E-06	7.08E+01	3.64E-04	1.22E+02	8.06E-05	7.81E+01	7.05E-05	7.38E+01	
2-Methyl-butanal	1.26E-04	7.72E+01	1.70E-03	1.22E+02	7.62E-05	5.85E+01	1.91E-04	7.07E+01	2.14E-06	1.41E+02	4.88E-04	1.18E+02	5.90E-05	7.44E+01	1.86E-04	6.08E+01	
2-Pentanone	1.36E-03	1.90E+01	4.47E-03	5.87E+00	1.63E-03	4.66E+01	2.79E-03	3.00E+01	3.41E-02	3.00E+01	6.06E-02	6.85E+01	3.09E-02	1.20E+02	5.49E-02	4.95E+01	
2-Pentanol	1.33E-05	1.41E+02	1.18E-04	1.39E+01	4.11E-05	8.74E+01	4.76E-05	3.24E+01	6.06E-04	2.72E+01	8.06E-04	2.49E+01	3.30E-04	8.26E+01	1.79E-03	7.99E+00	
3-Hydroxy-2-butanone	1.37E-04	1.11E+01	1.38E-04	1.97E+01	1.37E-04	4.66E+01	4.43E-02	1.41E+02	8.20E-05	3.98E+01	8.65E-05	7.07E+01	1.05E-04	4.59E+01	5.88E-05	4.90E+01	
Ethyl ester propanoic acid	5.83E-06	1.41E+02	1.13E-05	7.60E+01	0.00E+00	N/A	2.88E-04	1.33E+02	0.00E+00	N/A	8.83E-06	1.41E+02	7.01E-06	1.41E+02	1.70E-05	1.41E+02	
n-Propyl acetate	3.78E-06	7.12E+01	6.53E-06	7.12E+01	2.62E-06	1.41E+02	5.60E-05	1.27E+02	2.45E-05	7.24E+01	3.70E-05	8.08E+01	1.24E-05	7.56E+01	3.27E-05	2.98E+01	
3-Methyl-butanol	5.26E-04	2.32E+01	1.76E-03	9.02E+00	4.39E-04	3.65E+01	4.68E-02	1.35E+02	8.52E-04	7.61E+01	1.99E-03	2.54E+01	6.37E-04	6.67E+01	2.17E-03	4.29E+01	
2-Methyl-1-butanol	1.62E-04	1.62E+01	3.41E-04	2.94E+01	1.47E-04	1.02E+01	1.83E-03	1.17E+02	2.20E-04	6.19E+01	2.92E-04	4.14E+01	1.48E-04	5.76E+01	3.27E-04	2.76E+01	
Dimethyl-disulfide	1.70E-05	1.41E+02	3.29E-04	1.17E+02	8.08E-06	7.89E+01	1.00E-04	4.20E+01	2.45E-05	1.11E+02	7.15E-05	8.02E+01	5.19E-05	1.04E+02	8.51E-06	1.41E+02	

	Yeast inoculum (CFU mL-1)															
	Y. lipolytica															
	10^5				10^2				10^5 + spores				10^2 + spores			
	Incubation temperature (°C)															
	5		15		5		15		5		15		5		15	
LRI Suggested Compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
3-Methyl-2-pentanone	2.09E-06	1.41E+02	3.36E-05	4.75E+01	1.78E-05	5.01E+01	6.99E-06	7.07E+01	1.57E-05	7.24E+01	4.79E-05	5.72E+01	1.83E-05	1.10E+02	7.68E-05	3.73E+01
Methy-ethyl ester propanoic acid	7.55E-04	1.14E+01	1.34E-03	1.94E+01	6.39E-04	1.45E+01	7.45E-04	1.16E+01	1.45E-04	7.87E+01	3.51E-04	4.77E+01	4.17E-04	5.69E+01	5.71E-04	1.96E+01
1-Pentanol	4.44E-04	2.07E+01	5.74E-04	1.23E+01	3.13E-04	1.11E+01	5.85E-04	3.92E+01	2.45E-03	1.09E+02	9.44E-04	3.24E+00	1.22E-03	5.33E+01	1.65E-03	4.47E+01
Isobutyl acetate	9.70E-04	1.16E+01	1.62E-03	1.52E+01	9.79E-04	2.37E+01	1.12E-03	1.58E+01	9.37E-04	3.38E+01	9.82E-04	9.00E+01	1.37E-03	2.73E+01	2.77E-03	2.48E+01
2-Hexanone	1.13E-04	2.57E+01	9.77E-04	1.27E+01	1.47E-04	5.67E+01	4.15E-04	2.04E+01	7.74E-03	3.94E+01	1.29E-02	7.82E+01	1.07E-02	1.20E+02	8.52E-03	2.65E+01
Butanoic acid	0.00E+00	N/A	1.41E-01	5.00E+00	0.00E+00	N/A	2.32E-02	7.22E+01	0.00E+00	N/A	4.14E-02	3.38E+01	0.00E+00	N/A	1.96E-02	4.14E+01
Octane	1.08E-03	1.78E+01	2.14E-03	1.80E+01	1.08E-03	1.51E+01	1.20E-03	1.57E+01	7.45E-04	3.20E+01	8.69E-04	3.95E+01	1.24E-03	4.24E+01	1.37E-03	1.66E+01
3-Methyl-butanoic acid	4.51E-06	1.41E+02	2.43E-04	1.70E+01	9.38E-06	1.41E+02	4.33E-04	1.28E+02	2.46E-05	4.27E+01	6.51E-05	1.41E+02	4.00E-06	1.41E+02	6.80E-04	6.80E+01
2-Methyl butanoic acid	7.21E-07	1.41E+02	2.39E-06	7.21E+01	0.00E+00	N/A	5.92E-06	7.08E+01	1.39E-06	1.41E+02	0.00E+00	N/A	1.13E-06	1.41E+02	5.46E-06	7.33E+01
Pentanoic acid	0.00E+00	N/A	2.04E-03	1.37E+01	0.00E+00	N/A	1.54E-04	1.41E+02	1.93E-05	1.03E+02	3.81E-04	7.23E+01	0.00E+00	N/A	2.18E-04	7.08E+01
3-Methyl-1-butanol acetate	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	2.34E-04	1.41E+02	3.51E-05	8.86E+01	9.00E-05	7.25E+01	0.00E+00	N/A	9.63E-05	3.51E+01
2-Heptanone	3.04E-03	2.36E+01	4.69E-02	1.98E+01	4.13E-03	4.87E+01	2.12E-02	1.44E+01	2.35E-01	5.65E+01	6.34E-01	8.52E+01	5.30E-01	9.61E+01	3.76E-01	1.27E+01
Styrene	1.03E-04	2.89E+01	1.22E-03	4.82E+01	4.48E-04	7.97E+01	8.83E-04	3.99E+01	1.85E-04	7.52E+01	3.90E-04	1.07E+02	6.45E-06	1.41E+02	1.05E-04	1.06E+01
2-Heptanol (solvent GCMS)	1.18E-03	2.27E+01	7.83E-03	1.67E+01	1.28E-03	4.40E+01	4.15E-03	3.87E+01	6.85E-02	3.65E+01	6.30E-02	9.01E+00	9.47E-02	1.33E+02	1.40E-01	3.81E+01
a-Pinene	1.03E-04	1.73E+01	1.07E-04	7.68E+01	1.94E-04	5.84E+01	1.35E-04	8.38E+01	1.23E-04	4.89E+00	6.30E-05	6.54E+01	4.82E-05	3.73E+01	7.23E-05	5.07E+01
2-Octanone	2.44E-05	2.91E+01	4.00E-04	7.26E+00	5.22E-05	2.95E+01	1.58E-04	9.06E+00	4.60E-03	6.88E+01	3.21E-02	1.16E+02	2.01E-02	1.06E+02	8.34E-03	1.32E+01
Hexanoic acid	0.00E+00	N/A	1.69E-01	8.46E+00	1.04E-03	1.41E+02	3.45E-02	1.12E+01	0.00E+00	N/A	5.25E-02	4.89E+01	0.00E+00	N/A	1.59E-02	1.17E+02
3-Octanone	3.10E-05	5.92E+01	5.35E-04	2.65E+01	1.39E-04	2.12E+01	3.96E-03	1.35E+02	8.92E-05	3.76E+01	3.76E-04	5.72E+01	6.14E-05	3.34E+01	1.90E-04	5.88E+01
Hexanoic acid ethyl ester	1.10E-05	8.69E+01	7.43E-04	3.99E+01	1.76E-05	3.21E+01	5.61E-03	1.39E+02	2.32E-05	9.19E+01	4.24E-04	5.66E+01	3.09E-05	5.02E+01	1.30E-04	1.15E+02
4-Methylanisole	2.38E-06	7.20E+01	2.05E-06	1.41E+02	2.66E-06	7.28E+01	0.00E+00	N/A	1.13E-05	7.80E+01	5.48E-06	7.55E+00	2.88E-05	2.85E+01	1.68E-05	8.63E+01
Butanoic acid 3-methylbutyl ester	0.00E+00	N/A	7.81E-05	2.82E+01	1.87E-05	7.16E+01	1.65E-04	1.08E+02	2.10E-05	3.61E+01	7.82E-05	5.28E+01	4.47E-06	1.41E+02	6.29E-05	1.11E+02
8-Nonen-2-one	1.29E-04	5.40E+01	1.46E-04	2.28E+01	3.69E-04	1.15E+02	1.18E-04	2.93E+01	1.56E-02	7.59E+01	9.58E-02	1.19E+02	7.92E-02	1.19E+02	2.32E-02	1.44E+01

	Yeast inoculum (CFU mL-1)															
	Y. lipolytica															
	10^5				10^2				10^5 + spores				10^2 + spores			
	Incubation temperature (°C)															
	5		15		5		15		5		15		5		15	
LRI Suggested Compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
2-Nonanone	1.25E-03	3.11E+01	9.79E-03	1.39E+01	2.13E-03	8.39E+01	4.03E-03	1.71E+01	8.14E-02	7.34E+01	3.85E-01	9.05E+01	2.52E-01	8.70E+01	1.38E-01	5.38E+00
Benzeneethanol	3.14E-04	2.79E+01	2.15E-04	1.97E+01	1.60E-03	1.28E+02	1.56E-03	1.03E+02	1.75E-04	7.47E+01	1.30E-04	2.48E+01	7.73E-05	1.05E+02	1.69E-03	9.37E+01
Hexanoic acid butyl ester	2.16E-06	1.41E+02	1.34E-05	7.10E+01	3.97E-06	1.41E+02	9.36E-05	1.41E+02	5.58E-06	7.81E+01	2.91E-05	9.44E+01	0.00E+00	N/A	1.75E-05	3.36E+01
Octanoic acid	0.00E+00	N/A	4.21E-02	2.45E+00	1.71E-04	1.41E+02	1.07E-02	1.13E+01	4.27E-04	1.41E+02	2.12E-02	3.44E+01	2.52E-04	1.41E+02	8.75E-03	9.84E+01
2-Decanone	9.91E-06	7.38E+01	5.89E-05	2.80E+01	2.10E-05	5.91E+01	4.12E-05	5.18E+01	2.90E-04	7.67E+01	2.72E-03	1.12E+02	1.32E-03	9.78E+01	4.76E-04	9.42E+00
Octanoic acid ethyl ester	2.84E-05	1.27E+02	7.69E-04	4.71E+00	3.49E-05	9.78E+01	3.96E-03	1.37E+02	1.13E-04	1.25E+02	2.83E-04	3.52E+01	1.21E-04	1.70E+01	1.79E-04	7.26E+01
3-methybutyl hexanoate	4.29E-06	1.41E+02	3.83E-05	1.75E+01	4.71E-06	1.41E+02	4.91E-05	1.03E+02	1.05E-05	7.33E+01	4.90E-05	3.78E+01	5.31E-06	7.08E+01	2.10E-05	7.43E+00
Acetic acid 2-phenylethyl ester	1.99E-04	1.25E+02	3.36E-04	2.10E+01	2.39E-04	6.77E+01	1.34E-03	4.84E+01	3.88E-04	5.08E+01	1.05E-03	1.14E+02	1.01E-03	5.89E+01	9.64E-04	7.19E+01
2-Undecanone	1.00E-04	1.15E+01	9.82E-04	1.45E+01	1.38E-04	3.18E+01	4.65E-04	6.51E+00	1.99E-03	7.93E+01	1.37E-02	1.01E+02	7.19E-03	1.03E+02	4.40E-03	1.87E+01
n-Decanoic acid	0.00E+00	N/A	2.00E-03	3.81E+01	0.00E+00	N/A	1.05E-04	1.41E+02	0.00E+00	N/A	1.26E-03	2.59E+01	0.00E+00	N/A	2.46E-04	1.41E+02

	Yeast inoculum (CFU mL-1)															
	K. lactis															
	10^5				10^2				10^5 + spores				10^2 + spores			
	Incubation temperature (°C)															
	5		15		5		15		5		15		5		15	
LRI Suggested Compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Acetaldehyde	2.33E-02	2.03E+01	1.17E-02	6.30E+01	1.60E-02	3.48E+01	5.92E-05	1.41E+02	1.76E-02	2.25E+01	2.65E-02	3.22E+01	8.96E-05	1.41E+02	3.33E-02	2.59E+01
Methanethiol	1.16E-05	7.61E+01	0.00E+00	N/A	1.19E-05	7.08E+01	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	4.69E-06	1.41E+02
Ethanol	3.38E-01	6.71E+00	5.03E-01	6.70E+00	3.29E-01	3.28E+00	1.14E-03	2.59E+01	3.60E-01	9.07E+00	4.02E-01	5.26E+00	2.12E-02	3.25E+01	3.33E-01	4.61E+00
Acetone	1.00E-03	4.33E+00	2.58E-04	1.57E+01	1.42E-03	4.22E+01	1.07E-02	1.26E+01	9.95E-04	3.67E+01	9.21E-04	1.98E+01	2.92E-03	2.23E+01	9.14E-04	1.77E+00

	Yeast inoculum (CFU mL-1)															
	K. lactis															
	10^5				10^2				10^5 + spores				10^2 + spores			
	Incubation temperature (°C)															
	5		15		5		15		5		15		5		15	
LRI Suggested Compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
1-Propanol	4.61E-03	1.33E+01	1.20E-02	3.76E+01	8.06E-03	6.85E+01	1.17E-02	8.39E+00	5.78E-03	5.74E+01	6.40E-03	3.24E+01	1.17E-02	5.53E+00	6.24E-03	1.27E+01
2-Methyl propanal	2.17E-03	8.80E+00	4.48E-04	3.36E+01	2.81E-03	5.16E+01	3.03E-05	7.08E+01	1.62E-03	5.89E+01	1.13E-03	1.77E+01	1.61E-04	2.77E+01	1.57E-03	2.63E+00
2-Butanone	1.01E-03	7.87E+00	4.49E-04	3.62E+01	2.14E-03	7.27E+01	8.49E-03	1.27E+01	1.08E-03	3.87E+01	8.42E-04	1.48E+01	1.00E-03	1.01E+01	4.67E-04	1.76E+01
Ethylacetate	7.79E-01	1.09E+01	5.36E-01	1.43E+01	6.32E-01	2.91E+01	1.74E-04	2.86E+01	6.52E-01	1.39E+01	6.23E-01	3.32E+00	8.83E-03	9.90E+01	6.04E-01	1.89E+01
2-Methyl-1-propanol	1.10E-02	1.61E+01	1.80E-02	2.24E+01	1.40E-02	1.13E+01	2.26E-05	1.41E+02	1.56E-02	6.58E+00	1.61E-02	1.37E+01	7.38E-04	2.65E+01	1.83E-02	1.46E+01
3-Methyl-butanal	5.18E-04	7.66E+00	1.93E-04	6.01E+01	8.22E-04	4.01E+01	1.57E-04	1.27E+02	4.35E-04	5.95E+01	1.36E-03	6.90E+01	5.13E-04	2.99E+01	1.71E-03	3.52E+01
2-Methyl-butanal	1.55E-03	1.32E+01	2.54E-03	1.15E+02	2.35E-03	5.07E+01	1.66E-04	8.56E+01	1.45E-03	4.55E+01	9.18E-03	6.74E+01	2.35E-04	1.68E+01	6.75E-03	3.35E+01
2-Pentanone	2.29E-04	1.43E+01	2.13E-04	1.03E+01	4.43E-04	6.85E+01	2.77E-03	9.35E+01	3.38E-03	1.82E+01	2.43E-03	2.36E+01	3.32E-04	3.06E+01	1.66E-03	2.35E+01
2-Pentanol	1.65E-05	3.85E+01	3.58E-05	1.95E+01	4.98E-06	1.41E+02	1.05E-04	6.45E+01	1.64E-04	3.88E+01	2.14E-04	5.05E+01	8.13E-05	3.14E+01	1.21E-04	2.69E+01
3-Hydroxy-2-butanone	9.84E-03	2.03E+01	6.77E-04	9.09E+01	9.49E-03	4.22E+01	1.60E-04	3.09E+01	6.00E-03	3.01E+01	3.68E-03	4.87E+01	1.01E-04	3.24E+01	7.09E-03	7.31E+00
Ethyl ester propanoic acid	3.69E-02	9.45E+00	2.60E-02	6.79E+00	2.97E-02	2.58E+01	1.15E-05	3.47E+01	2.51E-02	2.99E+01	2.38E-02	1.53E+01	2.73E-05	1.05E+02	2.05E-02	1.22E+01
n-Propyl acetate	6.51E-03	4.99E+01	1.83E-03	6.55E+00	4.77E-03	5.54E+01	3.68E-06	7.44E+01	3.51E-03	5.14E+01	1.53E-03	1.88E+01	2.37E-05	9.14E+01	2.95E-03	1.49E+01
3-Methyl-butanol	1.29E-01	5.47E+00	1.20E-01	2.84E+00	1.42E-01	8.75E+00	1.29E-04	9.53E+01	1.36E-01	1.43E+01	1.43E-01	9.63E+00	2.77E-03	2.72E+01	2.26E-01	3.23E+00
2-Methyl-1-butanol	3.46E-02	1.30E+01	5.54E-02	6.31E+00	4.04E-02	4.93E+00	4.45E-05	1.83E+01	3.95E-02	6.04E+00	7.25E-02	7.07E+00	4.53E-04	1.60E+01	7.18E-02	1.01E+01
Dimethyl-disulfide	3.63E-06	7.16E+01	1.40E-04	6.30E+01	1.11E-06	1.41E+02	4.87E-04	6.55E+01	0.00E+00	N/A	5.64E-05	1.04E+02	2.54E-04	2.53E+01	1.60E-05	5.69E+01
3-Methyl-2-pentanone	0.00E+00	N/A	8.39E-07	1.41E+02	0.00E+00	N/A	1.10E-06	1.41E+02	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
Methy-ethyl ester propanoic acid	3.53E-03	2.17E+00	4.76E-03	7.25E+00	3.27E-03	5.52E+00	8.37E-04	7.29E+00	2.40E-03	2.78E+01	2.88E-03	1.70E+01	1.29E-03	1.90E+01	2.17E-03	1.04E+01
1-Pentanol	3.85E-04	1.45E+01	6.58E-04	1.89E+01	4.06E-04	1.64E+01	4.13E-04	9.21E+00	5.19E-04	2.30E+01	4.63E-04	1.37E+01	1.45E-03	2.68E+01	7.78E-04	9.40E+00
Isobutyl acetate	1.57E-02	2.96E+01	7.95E-03	1.48E+01	1.04E-02	5.50E+01	1.10E-03	4.41E+00	1.16E-02	4.98E+01	8.96E-03	4.44E+00	1.38E-03	2.01E+01	1.68E-02	7.26E+00
2-Hexanone	8.66E-05	1.68E+01	7.86E-05	1.64E+01	1.40E-04	4.70E+01	9.54E-04	1.22E+02	9.95E-04	1.68E+01	5.96E-04	1.04E+01	1.59E-04	4.56E+01	7.03E-04	2.09E+01
Butanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
Octane	8.58E-04	2.15E+01	1.25E-03	3.65E+00	1.18E-03	2.09E+01	1.44E-03	1.14E+01	9.77E-04	8.51E+00	9.66E-04	9.81E+00	2.40E-03	4.93E+00	1.35E-03	5.45E+00

	Yeast inoculum (CFU mL-1)															
	K. lactis															
	10^5				10^2				10^5 + spores				10^2 + spores			
	Incubation temperature (°C)															
	5		15		5		15		5		15		5		15	
LRI Suggested Compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
3-Methyl-butanoic acid	1.33E-05	7.11E+01	0.00E+00	N/A	2.44E-05	7.07E+01	0.00E+00	N/A	1.56E-05	1.41E+02	7.58E-06	1.41E+02	3.73E-06	7.16E+01	1.37E-05	1.41E+02
2-Methyl butanoic acid	1.67E-05	5.68E+01	1.09E-05	7.12E+01	2.55E-05	4.54E+01	0.00E+00	N/A	3.48E-06	7.18E+01	1.61E-05	8.31E+01	3.66E-06	8.48E+01	5.23E-06	9.04E+01
Pentanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	3.26E-06	1.41E+02	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
3-Methyl-1-butanol acetate	1.84E-02	2.30E+01	1.68E-02	4.68E+00	1.23E-02	6.11E+01	0.00E+00	N/A	1.52E-02	6.80E+01	1.70E-02	1.28E+01	7.62E-06	1.41E+02	2.61E-02	1.05E+01
2-Heptanone	6.74E-03	1.23E+01	4.72E-03	1.44E+01	9.23E-03	1.81E+01	1.49E-01	1.35E+02	7.58E-02	1.52E+01	5.19E-02	7.99E+00	1.97E-02	2.81E+01	6.66E-02	2.08E+01
Styrene	5.65E-04	1.02E+02	7.99E-04	7.47E+01	2.30E-04	6.22E+01	1.08E-04	8.56E+01	6.15E-05	9.31E+01	5.77E-04	1.03E+02	9.37E-05	5.16E+01	9.39E-04	4.14E+01
2-Heptanol (solvent GCMS)	1.22E-03	2.87E+01	2.73E-03	4.65E+00	1.02E-03	7.78E+00	6.32E-04	1.41E+02	1.52E-02	3.01E+01	2.86E-02	1.39E+01	1.33E-03	7.80E+00	1.59E-02	2.39E+01
a-Pinene	1.33E-04	5.78E+01	5.23E-05	4.92E+01	1.07E-04	8.08E+01	5.58E-05	2.01E+01	6.59E-05	1.65E+01	4.92E-05	1.69E+01	3.98E-05	1.07E+01	1.20E-04	5.95E+01
2-Octanone	6.09E-05	7.52E+00	5.82E-05	2.85E+01	9.80E-05	3.32E+01	6.12E-03	1.40E+02	1.27E-03	1.49E+01	1.13E-03	7.26E+00	4.06E-04	2.19E+01	1.86E-03	2.53E+01
Hexanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
3-Octanone	1.33E-03	2.46E+01	3.37E-03	1.01E+01	1.14E-03	3.75E+01	1.64E-04	5.63E+01	1.48E-03	5.84E+01	4.05E-03	1.40E+01	5.05E-05	1.87E+01	4.91E-03	1.99E+01
Hexanoic acid ethyl ester	1.85E-03	2.12E+01	4.69E-03	9.53E+00	1.51E-03	4.29E+01	6.95E-05	1.20E+02	2.13E-03	5.83E+01	5.53E-03	1.17E+01	2.24E-05	5.90E+01	6.91E-03	1.85E+01
4-Methylanisole	4.62E-06	8.04E+01	5.21E-06	9.72E+01	3.74E-06	1.41E+02	3.77E-06	7.81E+01	4.02E-06	7.11E+01	1.20E-06	1.41E+02	1.68E-05	4.85E+01	6.75E-05	9.71E+01
Butanoic acid 3-methylbutyl ester	6.08E-05	4.34E+01	7.52E-05	2.07E+01	6.95E-05	5.11E+01	1.10E-05	1.41E+02	3.22E-04	6.44E+01	7.81E-04	7.03E+00	1.73E-05	1.51E+01	3.54E-03	2.57E+01
8-Nonen-2-one	1.82E-04	7.61E+01	2.05E-04	7.98E+01	1.55E-04	7.12E+01	1.45E-02	1.41E+02	3.65E-03	1.58E+01	3.14E-03	1.37E+01	1.08E-03	2.84E+01	3.61E-03	2.79E+01
2-Nonanone	1.98E-03	4.27E+01	3.26E-03	4.38E+01	2.16E-03	6.13E+00	9.72E-02	1.39E+02	4.25E-02	7.80E+00	3.86E-02	6.52E+00	1.78E-02	2.14E+01	4.17E-02	2.32E+01
Benzeneethanol	3.44E-05	3.69E+01	1.55E-04	4.60E+01	4.75E-05	3.34E+01	6.84E-06	7.67E+01	7.77E-05	7.78E+01	5.28E-04	8.49E+01	7.68E-06	7.13E+01	3.86E-04	3.54E+01
Hexanoic acid butyl ester	1.63E-05	2.84E+01	1.68E-05	1.39E+01	4.90E-06	1.41E+02	1.64E-06	1.41E+02	2.30E-05	1.04E+02	3.89E-05	2.15E+01	3.58E-06	9.17E+01	9.19E-05	3.20E+01
Octanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
2-Decanone	3.10E-05	4.91E+01	3.70E-05	1.47E+01	3.14E-05	9.92E+00	5.39E-04	1.38E+02	1.49E-04	5.50E+01	1.70E-04	7.37E+00	3.66E-05	4.89E+01	1.19E-04	2.68E+01
Octanoic acid ethyl ester	2.26E-03	2.40E+01	5.23E-03	5.15E+00	1.78E-03	6.09E+01	5.19E-05	6.41E+01	1.58E-03	8.03E+01	2.31E-03	4.75E+01	1.20E-04	3.49E+01	2.29E-03	2.71E+01
3-methybutyl hexanoate	2.01E-05	3.89E+01	3.63E-06	1.41E+02	6.85E-06	1.41E+02	1.18E-05	7.98E+01	2.68E-05	8.47E+01	2.47E-05	3.31E+00	7.49E-06	9.43E+01	8.96E-05	2.63E+01

	Yeast inoculum (CFU mL-1)															
	K. lactis															
	10^5				10^2				10^5 + spores				10^2 + spores			
	Incubation temperature (°C)															
	5		15		5		15		5		15		5		15	
LRI Suggested Compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Acetic acid 2-phenylethyl ester	2.10E-02	9.19E+00	2.38E-02	6.31E+00	1.76E-02	4.03E+01	2.64E-04	5.14E+01	2.45E-02	5.77E+01	7.96E-02	3.40E+01	3.44E-04	4.26E+01	9.09E-02	2.54E+01
2-Undecanone	1.79E-04	2.57E+01	2.03E-04	4.70E+01	1.91E-04	2.74E+01	3.63E-03	1.37E+02	1.30E-03	1.73E+01	1.22E-03	4.25E+00	3.06E-04	1.71E+01	1.17E-03	2.44E+01
n-Decanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A

	Model inoculum							
	Y. lipolytica & *K. lactis* trials							
	Milk				*P. roqueforti* spores (1x10^3 conidia/mL)			
	Incubation temperature (°C)							
	5		15		5		15	
LRI Suggested Compound	Mean	%CV	Mean	%CV	Mean	%CV	Mean	%CV
Acetaldehyde	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
Methanethiol	0.00E+00	N/A	0.00E+00	N/A	1.43E-05	1.41E+02	0.00E+00	N/A
Ethanol	8.03E-04	5.11E+01	1.88E-03	2.04E+01	8.27E-04	2.95E+01	1.20E-02	1.38E+02
Acetone	1.14E-02	1.37E+01	1.07E-02	4.19E+01	1.91E-03	7.54E-01	3.19E-03	1.90E+01
1-Propanol	1.10E-02	6.26E+00	1.00E-02	3.46E+00	1.20E-02	7.39E+00	8.93E-03	2.42E+01
2-Methyl propanal	3.68E-05	2.32E+01	1.32E-04	8.99E+01	8.09E-05	6.04E+01	2.48E-06	1.41E+02
2-Butanone	7.58E-03	2.57E+01	6.00E-03	4.84E+01	7.82E-04	1.09E+01	6.59E-04	9.51E+01
Ethylacetate	1.41E-04	1.03E+02	2.86E-04	6.98E+01	6.24E-05	7.13E+01	1.85E-04	6.46E+00
2-Methyl-1-propanol	7.50E-05	1.41E+02	2.10E-04	4.11E+01	1.70E-04	2.64E+01	6.61E-04	1.31E+01
3-Methyl-butanal	4.35E-05	2.88E+01	2.46E-04	6.74E+01	4.12E-04	5.74E+01	3.40E-05	6.64E+01
2-Methyl-butanal	1.44E-04	4.57E+01	4.95E-04	1.23E+02	1.49E-04	4.85E+01	4.27E-05	9.95E+01

	Model inoculum							
	Y. lipolytica & K. lactis trials							
	Milk				*P. roqueforti* spores (1x10^5 conidia/mL)			
	Incubation temperature (°C)							
	5		15		5		15	
LRI Suggested Compound	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**
2-Pentanone	1.86E-03	3.83E+01	3.54E-03	8.63E+01	2.06E-04	1.11E+01	2.68E-03	1.23E+02
2-Pentanol	6.09E-05	2.71E+01	1.94E-04	1.36E+02	9.71E-05	6.29E+00	1.36E-04	1.04E+01
3-Hydroxy-2-butanone	1.84E-04	3.40E+01	1.45E-04	7.45E+01	3.16E-04	1.14E+02	2.95E-04	1.22E+02
Ethyl ester propanoic acid	1.07E-05	1.00E+02	6.30E-06	1.41E+02	5.73E-06	1.41E+02	1.08E-05	1.41E+02
n-Propyl acetate	5.48E-06	8.78E+01	8.46E-06	1.41E+02	2.39E-06	1.41E+02	1.74E-05	8.69E+01
3-Methyl-butanol	7.58E-05	4.43E+01	3.08E-04	4.11E+01	6.21E-04	4.13E+01	2.45E-03	4.12E+01
2-Methyl-1-butanol	3.66E-05	3.76E+01	1.00E-04	2.82E+01	1.22E-04	2.49E+01	7.51E-04	3.74E+01
Dimethyl-disulfide	2.92E-04	5.15E+01	3.70E-03	8.27E+01	1.35E-04	7.07E+01	5.23E-05	9.49E+01
3-Methyl-2-pentanone	0.00E+00	N/A	4.58E-06	1.41E+02	4.31E-06	1.41E+02	0.00E+00	N/A
Methy-ethyl ester propanoic acid	5.72E-04	7.94E+00	5.72E-04	1.03E+01	5.23E-04	1.61E+01	3.27E-04	4.91E+00
1-Pentanol	3.88E-04	2.86E+01	8.14E-04	4.16E+01	1.37E-03	4.29E+00	1.42E-03	5.49E+01
Isobutyl acetate	8.63E-04	1.27E+01	1.00E-03	7.58E+00	8.65E-04	5.69E+00	5.82E-04	1.71E+01
2-Hexanone	4.16E-04	5.19E+01	9.45E-04	1.05E+02	1.09E-04	2.74E+01	7.24E-04	1.08E+02
Butanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
Octane	1.28E-03	1.75E+00	1.52E-03	1.12E+00	1.29E-03	8.89E+00	9.77E-04	7.81E+00
3-Methyl-butanoic acid	0.00E+00	N/A	2.73E-05	7.84E+01	4.75E-06	1.41E+02	1.55E-06	1.41E+02
2-Methyl butanoic acid	3.49E-06	3.27E+01	2.31E-06	1.41E+02	9.08E-07	1.41E+02	4.25E-06	7.64E+01
Pentanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
3-Methyl-1-butanol acetate	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	6.83E-06	1.41E+02
2-Heptanone	3.22E-02	5.58E+01	7.56E-02	8.27E+01	1.74E-02	9.78E+00	6.73E-02	1.10E+02
Styrene	1.60E-04	5.08E+01	1.29E-04	7.16E+01	4.13E-05	5.42E+01	6.19E-04	1.00E+02
2-Heptanol (solvent GCMS)	1.25E-04	8.91E+01	7.29E-04	1.26E+02	1.40E-03	2.52E+00	2.88E-03	7.24E+01

	Model inoculum							
	Y. lipolytica & *K. lactis* trials							
	Milk				*P. roqueforti* spores (1x10[5] conidia/mL)			
	Incubation temperature (°C)							
	5		15		5		15	
LRI Suggested Compound	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**	**Mean**	**%CV**
a-Pinene	6.26E-05	2.85E+01	6.76E-05	4.83E+01	3.56E-05	3.05E+00	9.48E-05	5.20E+01
2-Octanone	5.69E-04	6.01E+01	1.64E-03	7.05E+01	4.19E-04	6.59E+00	2.02E-03	1.18E+02
Hexanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
3-Octanone	5.10E-05	5.37E+01	8.44E-05	4.34E+01	5.15E-05	7.21E+01	7.61E-05	3.07E+01
Hexanoic acid ethyl ester	1.97E-05	1.20E+02	2.56E-05	3.20E+01	2.44E-05	7.57E+01	3.68E-05	3.60E+01
4-Methylanisole	2.67E-06	1.41E+02	5.49E-06	1.03E+02	2.55E-05	5.78E+01	1.10E-03	9.35E+01
Butanoic acid 3-methylbutyl ester	1.90E-05	2.12E+01	2.53E-06	1.41E+02	4.72E-06	1.41E+02	4.54E-06	1.41E+02
8-Nonen-2-one	1.15E-03	6.36E+01	3.64E-03	6.93E+01	1.04E-03	1.82E+01	3.31E-03	1.02E+02
2-Nonanone	1.37E-02	5.62E+01	3.89E-02	6.84E+01	1.44E-02	1.25E+01	3.59E-02	9.65E+01
Benzeneethanol	8.44E-06	7.46E+01	5.78E-06	7.72E+01	9.38E-06	2.72E+01	5.57E-05	9.55E+01
Hexanoic acid butyl ester	0.00E+00	N/A	9.81E-06	8.55E+01	4.62E-06	7.07E+01	4.52E-06	1.41E+02
Octanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A
2-Decanone	1.80E-05	3.44E+01	9.10E-05	8.30E+01	3.71E-05	5.12E+00	1.33E-04	9.27E+01
Octanoic acid ethyl ester	1.05E-04	7.69E+01	5.85E-05	6.39E+01	3.54E-05	9.07E+01	5.09E-05	5.78E+01
3-methybutyl hexanoate	0.00E+00	N/A	6.98E-06	9.28E+01	5.72E-06	7.08E+01	0.00E+00	N/A
Acetic acid 2-phenylethyl ester	3.29E-04	1.11E+02	8.50E-04	4.32E+01	2.79E-04	4.57E+01	1.49E-03	5.17E+01
2-Undecanone	2.10E-04	2.61E+01	8.64E-04	8.04E+01	2.95E-04	1.37E+01	1.15E-03	6.01E+01
n-Decanoic acid	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A	0.00E+00	N/A

Appendix 15. Instructions provided to sensory panel for Triangle test.

Before you start the session please provide the following information

First name:

Surname

Number of booth:

Session 1
Breaks are allowed during the session

This study only regards the aroma of the samples. Please bear in mind that you should **not taste** the samples. You only need to smell the samples.

Samples are going to be in opaque bottles and coded with 3 digit numbers. Please do not look in the samples.

Part One

You are goig to be provided with 3 samples simulataneously, each with different 3 digit codes. Two of the samples however will be identical. You need to identify which of the samples is the odd one out. You will also be asked to write down the main attributed which distinguish the odd sample from the others. Please avoid hedonic terms when describing the difference.

You should smell the samples in the order presented, from left to right. You may smell each sample as long as you need and as many times as you like.

Code of Odd sample: ....

Attributes which make this sample different (you may list as many as you like):

Appendix 16. Instructions provided to sensory panel for Paired Comparison test.

Before you start the session please provide the following information

First name:

Surname

Number of booth:

Session 1
Breaks are allowed during the session

This study only regards the aroma of the samples. Please bear in mind that you should **not taste** the samples. You only need to smell the samples.

Samples are going to be in opaque bottles and coded with 3 digit numbers. Please do not look in the samples.

Part Two

You are going to be provided with 2 samples. You need to identify which sample has the most intense aroma.

You may smell the samples in whatever order you like. You may smell each sample as long as you need and as many times as you like.

Code of sample with more intense aroma:

....

Please add any comments below:

Appendix 17. Instructions provided to sensory panel for Constant Reference test.

First name:

Surname

Number of booth:

Session 1
Breaks are allowed during the session

This study only regards the aroma of the samples. Please bear in mind that you should **not taste** the samples. You only need to smell the samples.

Samples are going to be in opaque bottles and coded with 3 digit numbers. Please do not look in the samples.

Part Three

You are going to be provided with 3 samples. One sample will be labelled as 'REF'. Please smell this REF sample first, preferable a few times having a short space between each sniff to allow you to get acquainted with this REF sample odour.
Then sniff each of the three test samples (labelled with 3 digit codes) in turn and determine if they differ from the REF samples and indicate the magnitude of the difference on the sscale below by writing the codes in the appropriate boxes:

No difference

Very slight difference

Slight / moderate difference

Moderate difference

Moderate / large difference

Large difference

Very large difference

Comments:

You may smell each sample as long as you need and as many times as you like. During the session you go back to sampes that you have already smelt and smell them again.

Appendix 18. Anderson-Darling distribution test upon panellists responses from constant reference test (Section 3.4.1.3) comparing the aroma of blue cheese models inoculated to a high or low concentration of *Y. lipolytica* to a real blue cheese aroma.

Anderson-Darling test (High conc.):

A^2	1.421
p-value	0.001
Alpha	0.05

Test interpretation:
H0: The variable from which the sample was extracted follows a Normal distribution.
Ha: The variable from which the sample was extracted does not follow a Normal distribution.
As the computed p-value is lower than the significance level alpha=0.05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0.10%.

Anderson-Darling test (Low conc.):

A^2	2.303
p-value	< 0.0001
Alpha	0.05

Test interpretation:
H0: The variable from which the sample was extracted follows a Normal distribution.
Ha: The variable from which the sample was extracted does not follow a Normal distribution.
As the computed p-value is lower than the significance level alpha=0.05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0.01%.

Anderson-Darling test (Reference (to itself)):

A^2	3.109
p-value	< 0.0001
Alpha	0.05

Test interpretation:
H0: The variable from which the sample was extracted follows a Normal distribution.
Ha: The variable from which the sample was extracted does not follow a Normal distribution.
As the computed p-value is lower than the significance level alpha=0.05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0.01%.

Appendix 19. Friedman's rank test on data responses from contant reference tests (Section 3.4.1.3) comparing the aroma of blue cheese models inoculated with *Y. lipolytica* at a high or low concentration to a real blue cheese aroma.

Friedman's test: **All 60 observation inclusive of 3 replicate model sets**

Q (Observed value)	24.500
Q (Critical value)	5.991
DF	2
p-value (Two-tailed)	< 0.0001
Alpha	0.05

Test interpretation:
H0: The samples come from the same population.
Ha: The samples do not come from the same population.
As the computed p-value is lower than the significance level alpha=0.05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0.01%.
Ties have been detected in the data and the appropriate corrections have been applied.

Friedman's test: 20 Observations, Replicate set 1

Q (Observed value)	4.169
Q (Critical value)	5.991
DF	2
p-value (Two-tailed)	0.124
Alpha	0.05

Test interpretation:
H0: The samples come from the same population.
Ha: The samples do not come from the same population.
As the computed p-value is greater than the significance level alpha=0.05, one cannot reject the null hypothesis H0.
The risk to reject the null hypothesis H0 while it is true is 12.44%.
Ties have been detected in the data and the appropriate corrections have been applied.

Friedman's test: 20 Observations, Replicate set 2

Q (Observed value)	12.182
Q (Critical value)	5.991
DF	2
p-value (Two-tailed)	0.002
Alpha	0.05

Test interpretation:
H0: The samples come from the same population.
Ha: The samples do not come from the same population.
As the computed p-value is lower than the significance level alpha=0.05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0.23%.
Ties have been detected in the data and the appropriate corrections have been applied.

Friedman's test: 20 Observations, Replicate set 3

Q (Observed value)	9.300
Q (Critical value)	5.991
DF	2
p-value (Two-tailed)	0.010
Alpha	0.05

Test interpretation:
H0: The samples come from the same population.
Ha: The samples do not come from the same population.
As the computed p-value is lower than the significance level alpha=0.05, one should reject the null hypothesis H0, and accept the alternative hypothesis Ha.
The risk to reject the null hypothesis H0 while it is true is lower than 0.96%.

Appendix 20. ANOVA on rank data recorded for replicate sample sets of constant reference tests (Section 3.4.1.3) comparing the aroma of blue cheese models inoculated with *Y. lipolytica* at a high or low concentration to a real blue cheese aroma.

Q1 / Fisher (LSD) / Analysis of the differences between the categories with a confidence interval of 95%:

Contrast	Difference	Standardized difference	Critical value	Pr > Diff	Significant
Ref vs High	0.850	1.533	2.002	0.131	No
Ref vs Low	0.200	0.361	2.002	0.720	No
Low vs High	0.650	1.172	2.002	0.246	No

Q1 / Dunnett (two sided) / Analysis of the differences between categories and the control category Q1-3 with a confidence interval of 95%:

Category	Difference	Standardized difference	Critical value	Critical difference	Pr > Diff	Significant
Ref vs High	0.300	0.629	2.268	1.082	0.755	No
Ref vs Low	0.000	0.000	2.268	1.082	1.000	No