Zygomycetes and Serratia marcescens, A Stinky Microbial Bully

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Abstract:

Serratia marcescens lives a lifestyle of diversity and ubiquity. Found nearly everywhere this bacteria is capable of living as a saprobe in soil and water, but also living in community with plants and other rhizobacteria, and in addition as a pathogen to plants, animals and other microbes. Besides being a beautiful example of life's ability to adapt to survive, Serratia also provides insight to one interesting aspect of microbiology. How do bacteria and fungi communicate? We have identified multiple strains of Serratia from unique niches and compared their ability to inhibit the growth of common soil inhabitants known to interact with plants, Mucoromycota.

Importance: Understanding interactions of a member of a larger community gives us insight into how that community functions as whole. In addition, learning about a key player helps us understand how these communities are formed and in turn, allows us to utilize these communities for protection of agriculture and humans. Zygomycetes can cause severe disease and death, discovering inhibition techniques used by bacteria may lead to solutions in the field of medicine.

Introduction:

Interactions between Fungi and Bacteria span mutualistic (Y. Zhang et al. 2018) to antagonistic (Fleming Alexander and Wright Almroth Edward 1922). Improvements in imaging and sequencing approaches have aided in illuminating the niches where fungi and bacteria cooperate from lichen symbioses of cyanobacteria and fungi (Meiser et al. 2017), competition within the soil (Bahram et al. 2018), or coexisting in extreme environments hospitable (Gonzalez et al. 2018). How do microbes sense and communicate with their neighboring microbes? Tools for microbiomics have enabled studies of how fungal and bacterial communities coexist, communicate and cooperate. Fungi live in communities with bacteria (Schroeckh et al. 2009; Partida-Martinez and Hertweck 2005; Scherlach, Graupner, and Hertweck 2013), discoveries from studying these relationships include finding that early lineages of fungi harbor ecto and endohyphal bacteria and their role in asexual reproduction, nitrogen, and carbon utilizations (Uehling et al. 2017; Li et al. 2017; Desirò et al. 2018; Hoffman and Arnold 2010; Partida-Martinez et al. 2007; Shaffer et al. 2017; Pawlowska et al. 2018), mechanisms and applications of bacterial-fungal interactions (Deveau et al. 2018), and microbial volatile bouquets (Misztal et al. 2018) .Bacteria utilize fungal hyphae for high speed travel, they can eat fungi, and they can consume the metabolites. (Nazir et al. 2010, 2017; Warmink et al. 2011/4; Y. Zhang et al. 2018). These relationships have yielded many benefits including furthering our understanding of nutrient cycling in ecosystems, fermented foods and beverages, and antibiotics (Frey-Klett et al. 2011).
Microbial genomes encode genes for many antifungals and antibiotics (Garbeva et al. 2014). Some studies have highlighted antagonism, table 1. Such as work has brought about the approval of Serratia plymuthica as a biocontrol (Rhizostar) that reduces Verticillium wilt by 18.5% and Phytophthora cactorum root rot by 33.4% in strawberry (Kurze et al. 2001). A conserved response to bacteria was demonstrated when antagonistic Lysobacter enzymogenes was shown to repress fungal response genes with effectors. Another repressor produced by Serratia marcescens, inhibits the growth of Candida albicans, (Trunk et al. 2018). Recently, Fusarium fujikuroi and Botrytis cinerea were shown to protect their survival spores after exposure to the bacterial secondary metabolite ralstonin, from Ralstonia solanacearum (Spraker et al. 2018). To add to the complexity, fungal-bacterial interactions occur among communities of organisms where detection and specific response to organisms from plants to animals may be required (Deveau et al. 2018; Frey-Klett et al. 2011).

Although fungi can respond to direct contact with bacterial microbe-associated molecular patterns (Ipcho et al. 2016), strangely, fungi seem to lack common eukaryotic receptors for bacterial recognition (Soanes and Talbot 2010). The lack of receptors may be a result of effective fungal offense such as producing antibiotics, sequestering iron, making their general vicinity inhospitable to bacterial invasion (Ipcho et al. 2016; Gkarmiri et al. 2015). Due to the fact that microbes may be detrimental to each other, perceiving infochemicals from neighboring competitors or acting on each other from a distance is an important and understudied aspect and additionally, what are the volatiles produced by microbes (Wheatley 2002; Schmidt, Cordovez, et al. 2015). Bacteria produce volatiles which can diffuse in the soil, and have been shown to be useful communication signals (Garbeva et al. 2014; Schulz-Bohm, Martín-Sánchez, and Garbeva 2017; Ossowicki, Jafra, and Garbeva 2017; Schmidt, Etalo, et al. 2015). The impact of some volatiles can be harmful to organisms, or may serve as infochemicals which fungi may respond to by avoidance, morphology changes, or arresting growth (Gkarmiri et al. 2015). Some bacteria like Serratia closely interact with plant roots, and form physical barriers barring potential pathogens, in addition, they can provide nutrients and growth hormones like indole-3-acetic acid to the plant (Vespermann, Kai, and Piechulla 2007; Neupane et al. 2015; Kai et al. 2010; Hoffman et al. 2013). Serratia is widely considered a rhizobacteria but how does it interact with the fungal populations nearby? The fungal response to bacterial volatiles has been shown in a few systems such as between Ralstonia and Fusarium and Botrytis (Spraker et al. 2018). Fungal-bacterial communication has been neglected with the lack of tools to analyze the interactions, however with transcriptomics, genomics, and metabolomics increasing in popularity and decreasing in cost more is being done. Rhizoctonia in direct contact with Serratia plymuthicans had transcriptional responses that lead to hyphal morphology changes, defense, and toxin production (Gkarmiri et al. 2015). The interest in indirect contact, volatomes, and their functions and applications are becoming more popular as well. The chemical diversity of volatiles produced by bacteria is broad with some having antifungal properties (Kanchiswamy, Malnoy, and Maffei 2015). Because volatile profiles differ from bacteria to bacteria a resource called mVOC 2.0 was created showing volatome

signatures of many bacteria (Lemfack et al. 2018). A few key volatiles can be a sufficient signature to identity a microbe. In fact, plants have been sensing volatiles from bacteria (Sharifi and Ryu 2018). Volatiles pass through soil through diffusion and advection (Minnich 1993) which makes volatile communication between microbes effective, analogous to quorum sensing. Serratia marcescens is a rhizobacterium and inhabits soils among many environments (Ashelford et al. 2002). Serratia is an effective biocontrol agent due to a number of antimicrobials and enzymes that it secretes. Prodigiosin, a red pigmented tripyrole compound that has been shown to inhibit mycelial growth and it is secreted it into the environment, in fact, traces of prodigiosin have been found in soil of tea plants (Dhar Purkayastha et al. 2018). Serratia can produce and secrete enzymes as well such as chitinases that digest fungal cell walls (De Vleesschauwer and Höfte 2003; Trunk et al. 2018; Gutiérrez-Román et al. 2012; Duzhak et al. 2012). Serratia marcescens has been shown to produce the potent anti-oomycete compound Oocydin which (Srobel et al. 1999). In addition to this arsonal of products, Serratia volatiles have been identified and shown to affect growth, antibiotic production and gene expression of neighboring bacteria (Garbeva et al. 2014; Weise et al. 2014). Due to the metabolic cheapness and high vapor pressure, they easily move around the soil (Schmidt, Cordovez, et al. 2015). Most are thought to be waste products of biosynthetic pathways, but some unique volatiles such as -butyrolactones can inhibit a wide range of bacteria (Schulz et al. 2010). Other bacteria have been shown to produce volatiles that can inhibit spore germination. Streptomyces inhibits Cladosporium (Herrington et al. 1985). Ralstonia produces ralstonins that inhibit germination of Aspergillus flavus (Khalid et al. 2018). Even fungi can produce volatiles to affect other fungi. Yeast volatiles reduced the ability of Aspergillus to resist insect damage (Caballero Ortiz et al. 2018), showing that while volatiles may not be fungicidal they can lead to fungal death indirectly. On of the volatiles produced by Serratia is 2-undecanone, a non-hazardous volatile (Yu et al. 2000; Groenhagen et al. 2013; Plyuta et al. 2016) that has fungistatic properties (Reddy and Al-Rajab 2016; Giorgio et al. 2015), efficacy as a mosquito repellent (Bohbot and Dickens 2010), and is used as a fragrance for its minty properties (Khan and Abourashed 2009). Undecanoic acid elicits a response in the fungus Trichophyton rubrum leading to up regulation of transcripts involved in reduction of fatty acid and metabolize 2-undecanone, oxidative stress, and cell wall integrity loss (Mendes et al. 2018).

***Hypothesis*:**

Strains of *Serratia marcescens* isolated from different environments variably inhibits growth of many zygomycetes. Or Serratia produces volatiles that inhibit Zygomycete growth.

Methods:

Inhibition assay: Ratio of mycelium area with volatiles/mycelium area without volatiles. Spore count was predicted using hemocytometer. Bacteria grown overnight at 28º then approximately 10^6 CFU were plated on outside of 100mm petri dish on LB. Inside is a 60 mm petri dish filled with CMA. After 72 hours the 500 spores/conidia are added to the CMA plates. After 2 days mycelium is collected and resuspended in a 25 ml .01% Tween 20 solution. Spores are quantified using a hemocytometer. To measure pure volatiles DMDS and 2-undecanone we used 100mm plates with 20 ml of Cornmeal Agar. Five 1,000 spore inoculations were placed around the plate with a microscope coverslip placed in the center. 2.5 µl of DMDS and 2-undecanone were place in the middle of the coverslip with stepping dilutions of 10. Growth was measured after 24 hours. Growth rates were measured using Dr. Caroline Roper's Spectrophotometer. Every 60 minutes 8 reading were taken from each well, averaged, and the results were combined and ANOVA was used to measure statistical significance. Fresh strawberries were purchased from a local supermarket, washed with sterile water and weighed. Strawberries with 75% red color and at least 100 gm were carried forward for use in the experiment. Fruit was bruised with cork borer and 100 spores were added to the injury. The fruit was incubated with three day old 60mm petri-dishes containing LB Agar. The fruit, fungi, and serratia were combined together in a sealed quart-sized plastic bag. After 48 hours, the lesion on the fruit was measured then macerated and spores were calculated using a hemocytometer.

Strains used: * ADJS-2C_Red (NCBI Accession number SAMN08373106) * Neurospora crassa OR74A FGSC 4289, * Rhizopus stolonifer (NRRL 66455), * Serratia proteamaculans (BW1) * Bacillus subtilis (E9)

Donut Plates: Luria-Bertani (LB) (10g Peptone, 10g NaCl, 5g Yeast Extract, 7.5g Agar, and 500mL Water) was pipetted into the outer ring of a 100mm petri dish with a 60mm petri dish lid placed inside. Then MEYE or Vogel's Media was added to the 60mm petri dish lid. 1mL of S.m. was inoculated onto the outer LB ring and allowed to grow for 48 hours at 25 C. Then mycelial plugs or 1000 spores/conidia were added to the media in the central 60mm petri dish lid. Measurements were taken 48 hours after fungi were inoculated.

GC-MS: 1mL of S.m. grown overnight was added to a 60mm petri dish, headspace volatile collection was taken at 48 hours for 6 hours at 25ºC at .5L/min with air cleaned by a charcoal purification filter pushed into to sample collection apparati (350 mL Mason Ball jar). Jar lids were fitted with a teflon liner, and two brass bulkhead unions (pipe thread .64 cm Swagelok, San Diego Valve and fitting Co.) with output into a volatile trap. The volatile trap consisted of ¼ inch glass tube filled with 40 mg HayeSepQ beads 80-100 mesh size. Volatiles were eluted with 150 ul Dichloromethane spiked with 4ng/ul nonyl-acetate, 2 ng/ul octane and was stored at -80ºC until GC:MS analysis. For GC coupled Mass spect carrier was helium, over ramp was 32 minute 40ºC to 280ºC. DB Wax column, TG-5MS thermofisher. Spectera were analyzed with Chromeleon 7 software and compounds were identified based on retention times and RSI (Reverse Match Factor) from the NIST library index

Volatile Analysis: Volatile amounts were calculated using area under the curve of a spike control of known mass. The volatiles with a prediction of 85% RSI or higher were kept. Unique volatiles were removed, those only produced by one sample or two samples. The PCA plots and NMDS were produced in R. NMDS was produced with the function metaMDS from the vegan package with the code on github (https://github.com/Derreckadam/NMDS_Volatiles/tree/master). Microscopy: 1000 FGSC 4289 condidia were plated onto 7.5 mL Vogel's media with agar in a 60 mm petri dish and allowed to grow for 12 hours at 25ºC. The hyphae were then examined under an inverted compound microscope at 200x. In 2-undecanone treated samples, 1 mg of 2-undecanone was added near the edge of the hyphae on a piece of filter paper and exposed for 1 hour before imaging.

```
**Pure Volatile Serial Dilutions:** 2-undecanone (SIGMA U1303-5ML) was diluted in ethanol in a series o
```

Results:

We noticed that when Serratia marcescens strain ADJS-2C_Red (ADJS) streaked on the plate across from the fungi, fungal growth was repressed. The growth area could quantitatively be assessed, based on growth with bacteria streaked on either side compared to growth with no bacteria, figure 1. However, this method was not ideal for studying volatiles because it allowed for bacterial products such as metabolites or proteins to diffuse through the media, potentially coming in direct contact with the fungal hyphae. In addition, because the bacteria are mobile they could traverse the distance on the solid media from the bacterial streak to the fungal hyphae. Although ADJS is bright red due to the production of prodigiosin, it is hard to know if a single bacteria or it's products have traveled to the hyphae as it takes several days and a high enough bacterial population for bacteria to be seen. So an assay to limit water diffusion of bacterial products to fungal hyphae was developed. The "Donut" assay, so named for its similarity to a strawberry donut when the ADJS Red strain is at maturity, allows for exchange of gases between the fungi and bacteria, but prevents direct contact. This double plate system also allows for two types of media to be poured. One tailored to the bacteria and the other tailored to the fungi. This is useful for the use of antibiotics in the fungal media or fungi with special growth needs. The exchange of gases was enough to inhibit fungal growth after two days of bacteria growth. LB media was used to grow Serratia and Bacillus and left without a bacteria in the control experiments. The fungal spores and mycelial plugs of N. crassa were introduced to the center plate after 48 hours of bacteria incubation at 25ºC. (Should I include a figure showing the inhibition potential of bacteria over time, a rationale behind why 48 hour of bacteria growth before introducing the fungal spores). The plates were measured after 24 and 48 hours, figure 1. In the presence of S. marcescens, N. crassa had

the most severe growth inhibition. B. subtilis used as a positive control, as it was previously shown to be effective at inhibiting Fusarium (Na 2016). The results show that ADJS-Red was the strongest inhibitor of growth. With the average growth being 1.5 cm at 24 hours and 4 cm at 48 hours. E9 was a weaker inhibitor of growth with the average growth of the fungi being 2.8 and 5.2 cm at 24 and 48 hours, respectively. Control growth of N. crassa with no bacteria inoculated on the LB outer ring was 3.7 cm at 24 hours and had grown to the diameter of the plate (5.7 cm) at 48 hours.

After establishing that fungal growth inhibitors reside in the volatile profiles we used Gas Chromatography coupled with Mass Spectrometry to identify the compounds produced by our strains of bacteria. Based on previous literature we assumed that we would find 2-undecanone and dimethyl disulfide. We grew the bacteria on nutrient rich LB media to enhance the bouquet of volatiles. One colony was picked and grown overnight in liquid LB media, then the culture was inoculated onto three plastic petri dishes and allowed to grow for 48 hours at 28ºC, then volatiles were collected for 6 hours at 25ºC. To serve as positive controls Bacillus subtilis, Strain E9 was used. To serve as negative controls volatiles from blank petri dishes and petri dishes with LB media were collected. On average there were about 50 volatiles produced by each strain. The volatiles identified are listed in supplemental table 1. To analyze the volatome, we restricted the results to only the volatiles with a confident prediction (RSI) of over 85%, figure 2a. Using an internal standard amounts of volatiles were predicted, this left us with an approximate abundance of compounds. We used Principal Component Analysis (PCA) and Non-metric multidimensional scaling (NMDS) plots to analyze the difference between the bacterial volatiles bouquets and found that Serratia and Bacillus were very different. While the PCA only showed 25% of the differences among the volatile profiles, the NMDS indicated a low stress threshold (0.1311). In fact, Serratia marcescens strain ADJS Red and Bacillus subtilis strain E9 had very different profiles, figure 2b,2c. In addition we tested Serratia proteamaculans strain BW1 to see if Serratia species could be differentiated by volatile profiles. There was a small amount of differentiation.

After identifying the volatiles produced by ADJS Red we ordered a few pure volatiles, with consideration for price, abundance in profile as based on GC MS, and variation of chemical structure. We tested 2-undecanone, Dimethyl Trisulfide, Anisole, Lepidine, 2,5-dimethylpyrazine. 2-undecanone was chosen due to that fact that it is a known antifungal, is used in food and fragrance, and is shown to be an effective insect repellent approved for use with humans. To test the volatiles we loaded the volatiles onto a piece of filter paper on a glass microscope slide on the side of a petri dish with vogel's media, spores were inoculated approximately 2 cm away on the media with a layer of cellophane to prevent fungal spores from germinating and growing downwards into the media. The amount of pure volatiles tested was 10mg, about one magnitude of order greater than observed by GCMS. At this amount the differences between non functional volatiles and effective ones are exaggerated. The effective volatiles for preventing growth were 2-undecanone, Anisole, and Dimethyl Trisulfide, figure 3a.

POTENTIALLY FIGURE 1A - Serratia's inhibition relies on a population density. So inhibition capacity increasing as days on plate increases. ## Different Strains Inhibit Differently, potentially as a result of replication rate

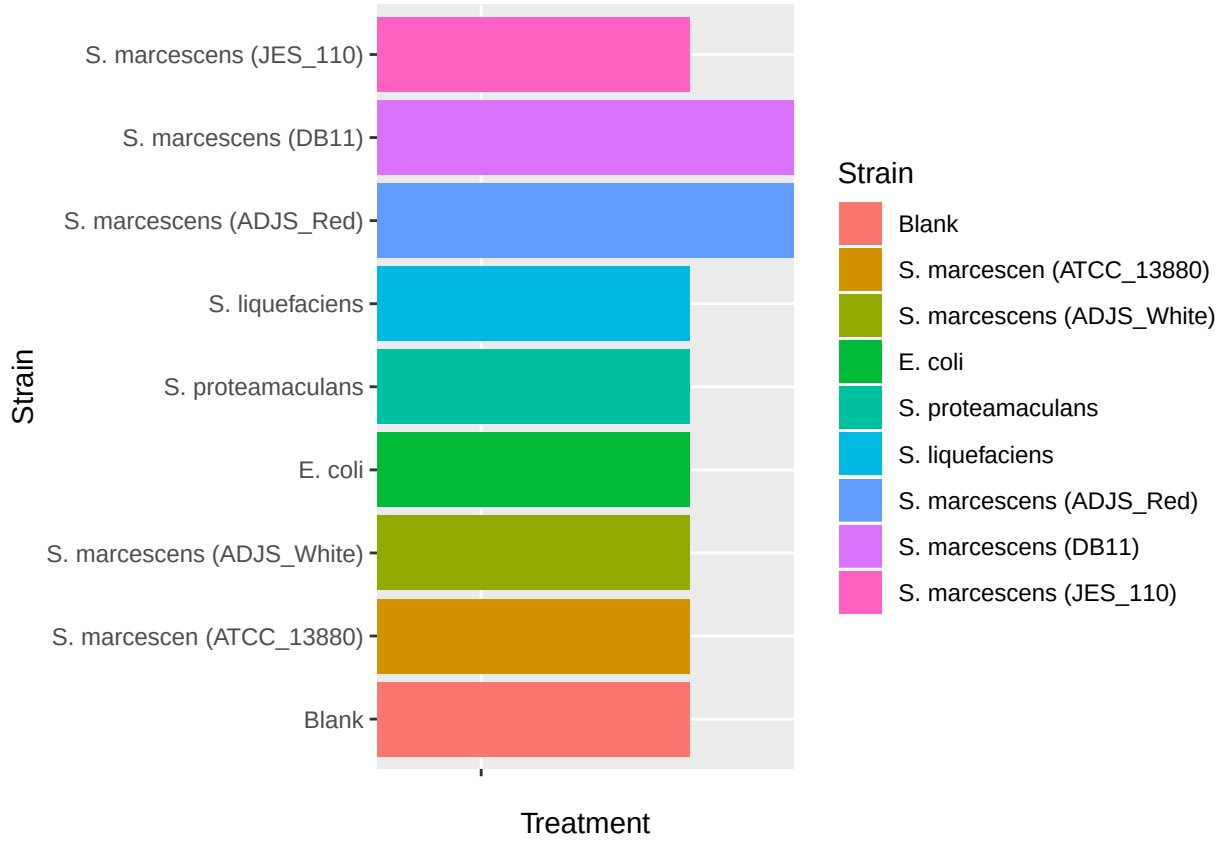
Fig. 1. We tested the ability of various environmental strains of Serratia: ADJS-2C_red, ADJS-2D_white, ADJS-2C_purple, ATCC 13880, and JES_110.

```
# Update figure with S_pro_Exclusive, Serratia Multistrain Analysis,
library(readxl)
library(ggplot2)
# Get Rhizopus data with many strains (48 Hour incubation)
Rhizo <- read_excel("Volatile.xlsx", sheet = "Serratia Multistrain Analysis")
Rhizo.bk <- Rhizo
print(Rhizo)
```

```
## # A tibble: 29 x 4
##    Strain                    `Same Day` `24 Hours Later` `48 Hours Later`
##    <chr>                          <dbl>            <dbl>            <dbl>
##  1 Blank                             34               57               57
```

```
##  2 Blank                          35          57          57
##  3 Blank                          37          57          57
##  4 S. marcescen (ATCC_13880)      45           5           6
##  5 S. marcescen (ATCC_13880)      41           5           5
##  6 S. marcescen (ATCC_13880)      47           5           5
##  7 S. marcescens (ADJS_White)     57           5           4
##  8 S. marcescens (ADJS_White)     57           4           5
##  9 S. marcescens (ADJS_White)     57           4           4
## 10 E. coli                        43           6           5
## # ... with 19 more rows
```

```
data.frame_Rhizo=as.data.frame(Rhizo)
#print(data.frame_Rhizo)

# Rhizopus name ordering
names.data <- unique(Rhizo.bk$Strain)
Rhizo$Strain <- factor(Rhizo$Strain, levels = names.data)
#boxplot(c ~ Strain, Rhizo, las=2)

bp = ggplot(Rhizo, aes(x=Strain, y="", fill=Strain)) + geom_bar(stat="identity") + ylab("Treatment")
bp + coord_flip()
```

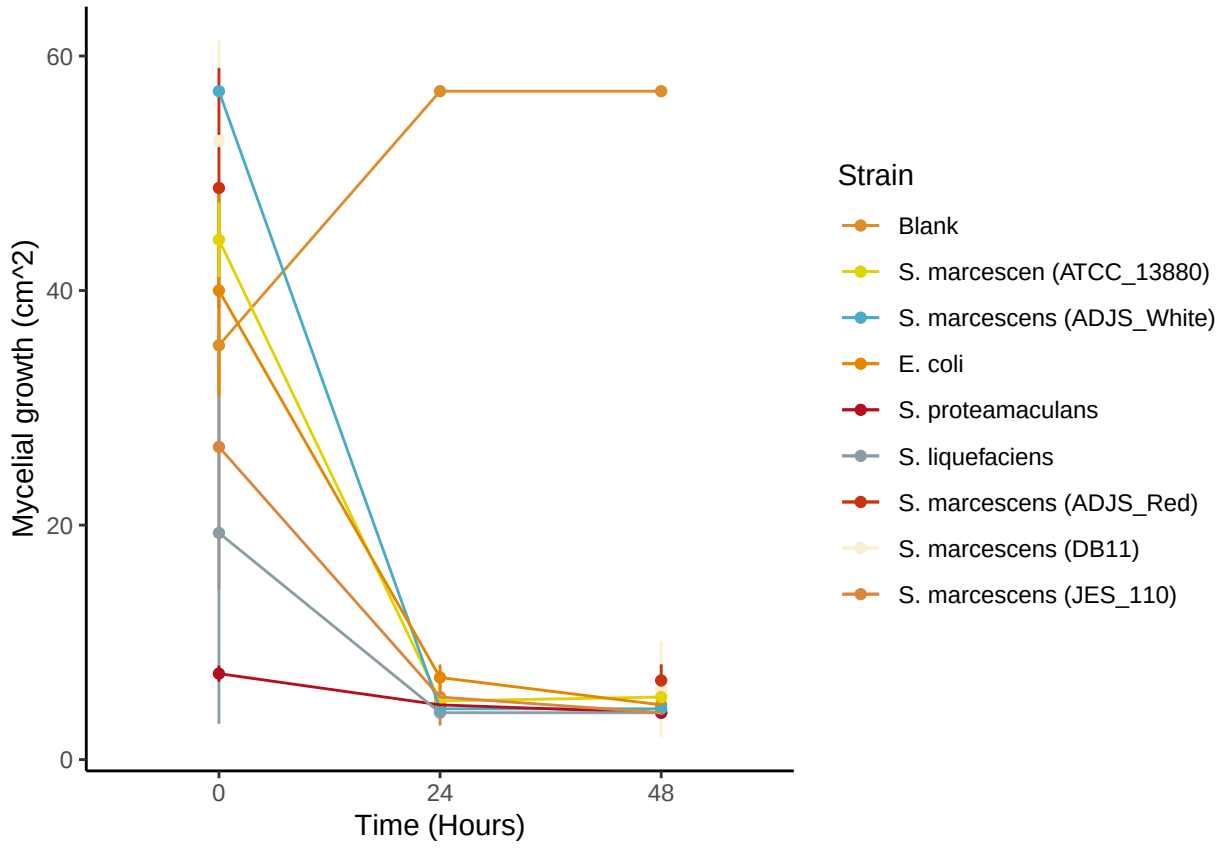



```
## For loop to obtaim averages and stdv
Strain.unique <- unique(Rhizo$Strain)
Strain.list <- list()
```

```
for (i in 1:length(Strain.unique)){
  # Subset the data frame into each strain
  df.test <- Rhizo[Rhizo$Strain %in% Strain.unique[i],]
  # The second element of an apply means: 1 = Rows, 2 = Columns
  # This means we are going to do the mean for all columns in the df
  Strain.list[[i]] <- data.frame(Strain=Strain.unique[i], Time=c("0","24","48"), mean=apply(df.test[,-1
}

final.data <- as.data.frame(do.call(rbind, Strain.list))
rownames(final.data) <- NULL

# Using the Wes Anderson pallette
library(wesanderson)

pd <- position_dodge(0)
ggplot(final.data, aes(x=Time, y=mean, colour=Strain, group = Strain)) +
  geom_errorbar(aes(ymin=mean-sd, ymax=mean+sd), width=.1, position=pd) +
  geom_point(position=pd) + geom_line(position = pd) +
  xlab("Time (Hours)") + ylab("Mycelial growth (cm^2)") +
  scale_color_manual(values = c(wes_palette("FantasticFox1"), wes_palette("Royal1"))) +
  theme_classic()
```

```
## Warning: Removed 2 rows containing missing values (geom_errorbar).
```

```
## Warning: Removed 2 rows containing missing values (geom_point).
```



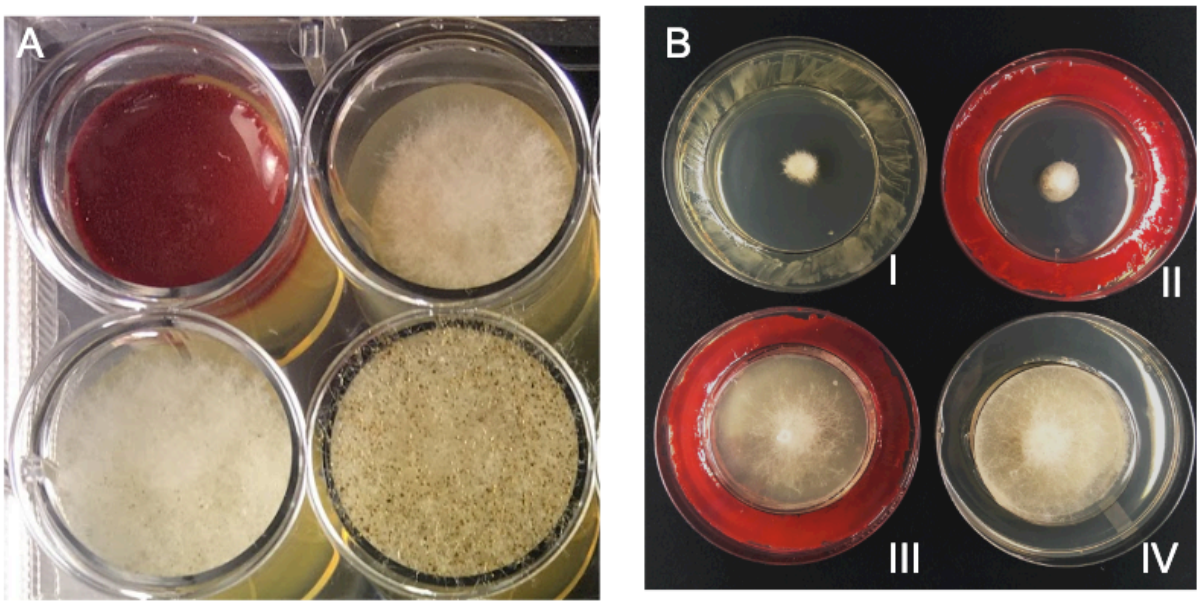


Figure 1: A caption

Figure 1a - Plate-ducken, top to bottom left to right, Rhizopus stolonifer with no bacteria, R. stolonifer covered with a lid with Serratia marcescens ADJS-2C Red, R. stolonifer exposed to volatiles of Serratia marcescens, R. stolonifer with known inhibitor E. coli.

```
#Rhizopus data with on S. pro, S. mar, and B. subtilis

library(readxl)
Rhizo <- read_excel("Volatile.xlsx", sheet = "Serratia Multistrain Analysis")
Rhizo.bk <- Rhizo
#print(Rhizo)

# Transform the table for ggplot2
library(reshape2)
## Melt transforms a wide df into a long df
Rhizo.m <- melt(as.data.frame(Rhizo), id.vars = "Strain")
colnames(Rhizo.m) <- c("Strain","Time","Growth")
## For loop to obtain averages and stdv
Strain.unique <- unique(Rhizo$Strain)
Strain.list <- list()

for (i in 1:length(Strain.unique)){
  # Subset the data frame into each strain
  df.test <- Rhizo[Rhizo$Strain %in% Strain.unique[i],]
  # The second element of an apply means: 1 = Rows, 2 = Columns
  # This means we are going to do the mean for all columns in the df
  Strain.list[[i]] <- data.frame(Strain=Strain.unique[i], Time=c("0","24","48"), mean=apply(df.test[,-1
}

final.data <- as.data.frame(do.call(rbind, Strain.list))
rownames(final.data) <- NULL
```

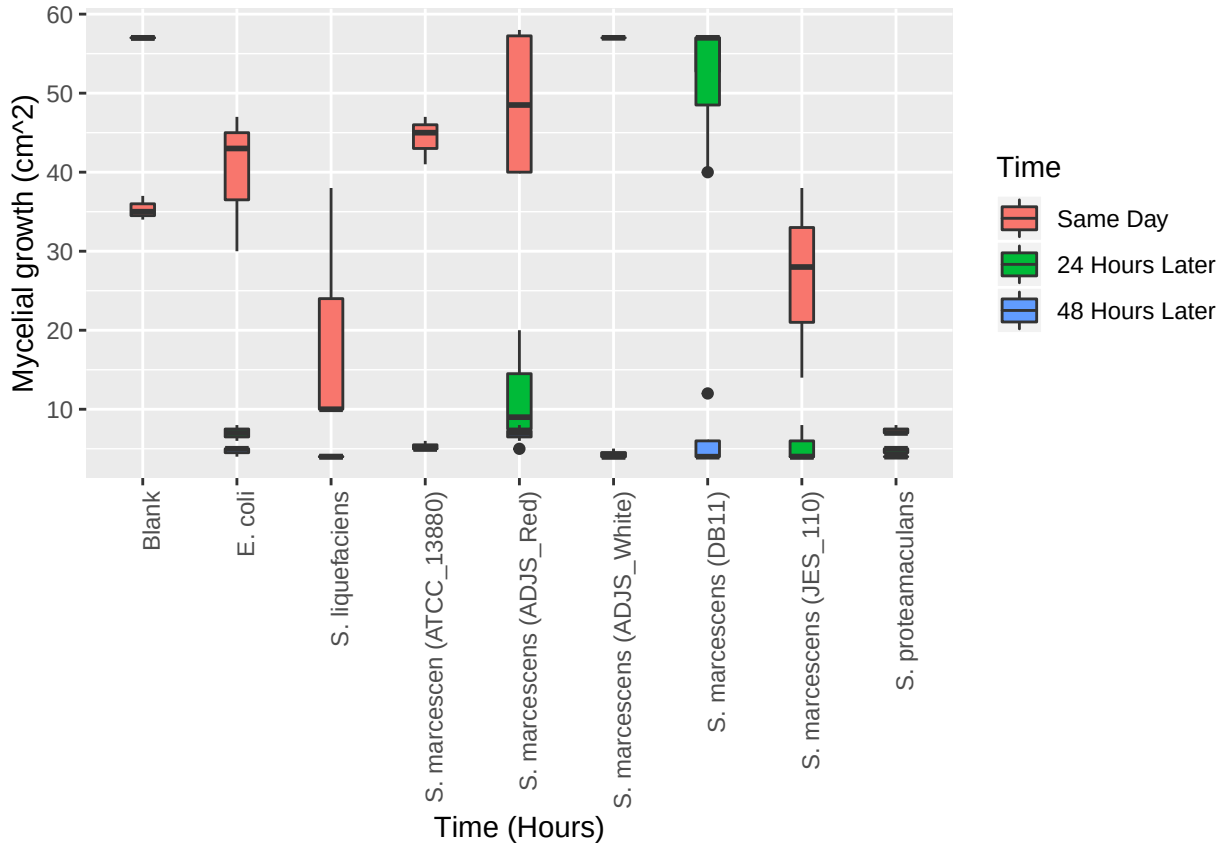
```r
# Using the Wes Anderson pallette
library(wesanderson)
Rhizo.m
```

```
##                        Strain           Time Growth
## 1                       Blank       Same Day     34
## 2                       Blank       Same Day     35
## 3                       Blank       Same Day     37
## 4   S. marcescen (ATCC_13880)       Same Day     45
## 5   S. marcescen (ATCC_13880)       Same Day     41
## 6   S. marcescen (ATCC_13880)       Same Day     47
## 7  S. marcescens (ADJS_White)       Same Day     57
## 8  S. marcescens (ADJS_White)       Same Day     57
## 9  S. marcescens (ADJS_White)       Same Day     57
## 10                     E. coli       Same Day     43
## 11                     E. coli       Same Day     30
## 12                     E. coli       Same Day     47
## 13          S. proteamaculans       Same Day      8
## 14          S. proteamaculans       Same Day      7
## 15          S. proteamaculans       Same Day      7
## 16            S. liquefaciens       Same Day     10
## 17            S. liquefaciens       Same Day     38
## 18            S. liquefaciens       Same Day     10
## 19   S. marcescens (ADJS_Red)       Same Day     58
## 20   S. marcescens (ADJS_Red)       Same Day     40
## 21   S. marcescens (ADJS_Red)       Same Day     40
## 22   S. marcescens (ADJS_Red)       Same Day     57
## 23       S. marcescens (DB11)       Same Day     57
## 24       S. marcescens (DB11)       Same Day     57
## 25       S. marcescens (DB11)       Same Day     40
## 26       S. marcescens (DB11)       Same Day     57
## 27    S. marcescens (JES_110)       Same Day     28
## 28    S. marcescens (JES_110)       Same Day     14
## 29    S. marcescens (JES_110)       Same Day     38
## 30                      Blank 24 Hours Later     57
## 31                      Blank 24 Hours Later     57
## 32                      Blank 24 Hours Later     57
## 33  S. marcescen (ATCC_13880) 24 Hours Later      5
## 34  S. marcescen (ATCC_13880) 24 Hours Later      5
## 35  S. marcescen (ATCC_13880) 24 Hours Later      5
## 36 S. marcescens (ADJS_White) 24 Hours Later      5
## 37 S. marcescens (ADJS_White) 24 Hours Later      4
## 38 S. marcescens (ADJS_White) 24 Hours Later      4
## 39                     E. coli 24 Hours Later      6
## 40                     E. coli 24 Hours Later      8
## 41                     E. coli 24 Hours Later      7
## 42          S. proteamaculans 24 Hours Later      5
## 43          S. proteamaculans 24 Hours Later      4
## 44          S. proteamaculans 24 Hours Later      5
## 45            S. liquefaciens 24 Hours Later      4
## 46            S. liquefaciens 24 Hours Later      4
## 47            S. liquefaciens 24 Hours Later      4
## 48   S. marcescens (ADJS_Red) 24 Hours Later     20
```

```
## 49   S. marcescens (ADJS_Red) 24 Hours Later      9
## 50   S. marcescens (ADJS_Red) 24 Hours Later      6
## 51   S. marcescens (ADJS_Red) 24 Hours Later     NA
## 52       S. marcescens (DB11) 24 Hours Later     NA
## 53       S. marcescens (DB11) 24 Hours Later     57
## 54       S. marcescens (DB11) 24 Hours Later     57
## 55       S. marcescens (DB11) 24 Hours Later     40
## 56    S. marcescens (JES_110) 24 Hours Later      4
## 57    S. marcescens (JES_110) 24 Hours Later      4
## 58    S. marcescens (JES_110) 24 Hours Later      8
## 59                      Blank 48 Hours Later     57
## 60                      Blank 48 Hours Later     57
## 61                      Blank 48 Hours Later     57
## 62  S. marcescen (ATCC_13880) 48 Hours Later      6
## 63  S. marcescen (ATCC_13880) 48 Hours Later      5
## 64  S. marcescen (ATCC_13880) 48 Hours Later      5
## 65 S. marcescens (ADJS_White) 48 Hours Later      4
## 66 S. marcescens (ADJS_White) 48 Hours Later      5
## 67 S. marcescens (ADJS_White) 48 Hours Later      4
## 68                   E. coli 48 Hours Later      5
## 69                   E. coli 48 Hours Later      4
## 70                   E. coli 48 Hours Later      5
## 71          S. proteamaculans 48 Hours Later      4
## 72          S. proteamaculans 48 Hours Later      4
## 73          S. proteamaculans 48 Hours Later      4
## 74            S. liquefaciens 48 Hours Later      4
## 75            S. liquefaciens 48 Hours Later      4
## 76            S. liquefaciens 48 Hours Later      4
## 77   S. marcescens (ADJS_Red) 48 Hours Later      7
## 78   S. marcescens (ADJS_Red) 48 Hours Later      5
## 79   S. marcescens (ADJS_Red) 48 Hours Later      7
## 80   S. marcescens (ADJS_Red) 48 Hours Later      8
## 81       S. marcescens (DB11) 48 Hours Later      4
## 82       S. marcescens (DB11) 48 Hours Later      4
## 83       S. marcescens (DB11) 48 Hours Later      4
## 84       S. marcescens (DB11) 48 Hours Later     12
## 85    S. marcescens (JES_110) 48 Hours Later      4
## 86    S. marcescens (JES_110) 48 Hours Later      4
## 87    S. marcescens (JES_110) 48 Hours Later      4
```

```
ggplot(Rhizo.m, aes(x=Strain, y=Growth, fill=Time)) +
  geom_boxplot(position=position_dodge(0)) +
  xlab("Time (Hours)") + ylab("Mycelial growth (cm^2)") + theme(axis.text.x = element_text(angle = 90, h
```

```
## Warning: Removed 2 rows containing non-finite values (stat_boxplot).
```



Serratia Inhibits a Wide Arrary of Fungi

1b - Serratia inhibit of fungal growth. Using Plate-ducken assay we determined various zygomycetes resistance to the volatiles produced by Serratia marcescens.

```
#Use donut and this data to generate figure with error bars

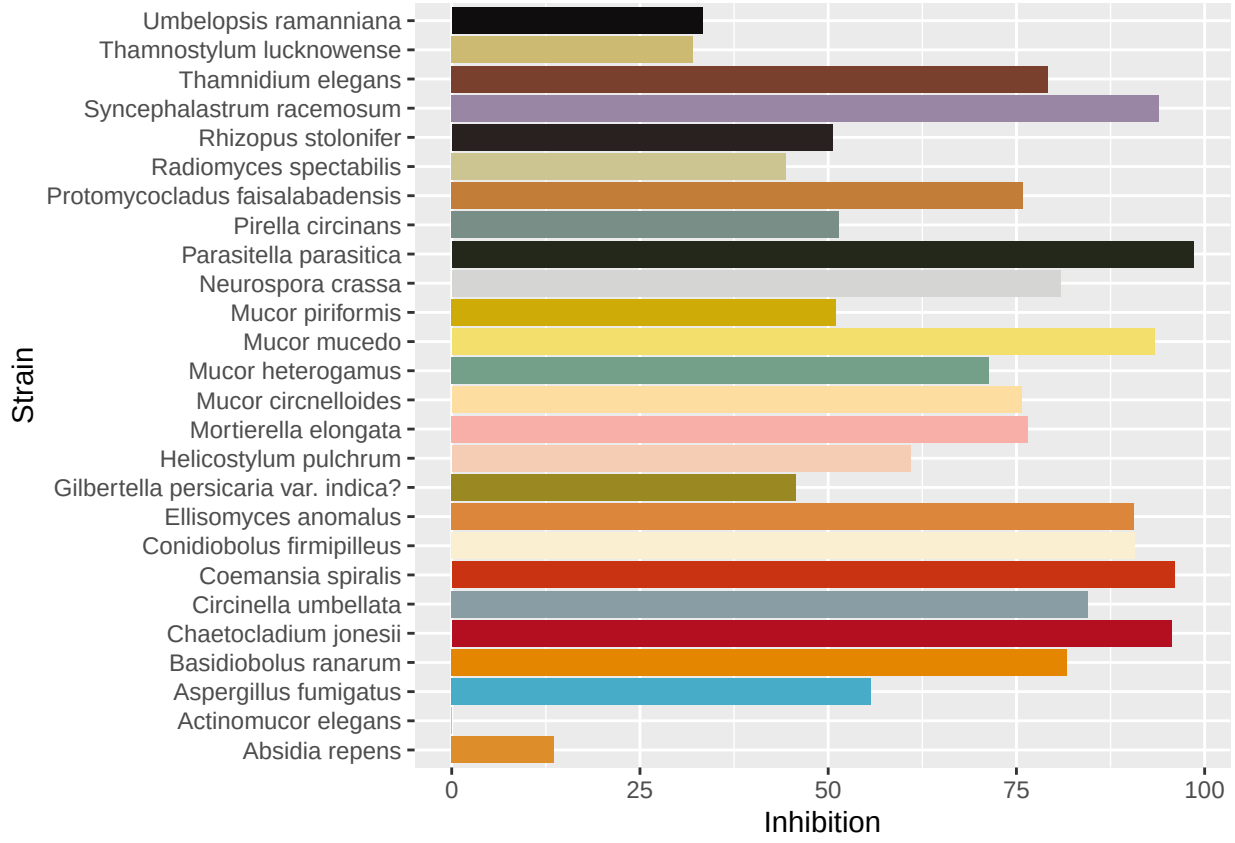
Zygos <- read_excel("Volatile.xlsx", sheet = "Sm Vs Zygos")

library(reshape2)
library(ggplot2)
library(wesanderson)
## Melt transforms a wide df into a long df
Zygo.m <- melt(as.data.frame(Zygos), id = "Species_Name")
print(Zygos)
```

```
## # A tibble: 26 x 2
##    Species_Name              Percent_Inhibition
##    <chr>                                 <dbl>
##  1 Basidiobolus ranarum                   81.7
##  2 Conidiobolus firmipilleus              90.7
##  3 Coemansia spiralis                     96
##  4 Umbelopsis ramanniana                  33.3
##  5 Syncephalastrum racemosum              94.0
```

```
##  6 Circinella umbellata                  84.5
##  7 Absidia repens                        13.6
##  8 Thamnidium elegans                    79.2
##  9 Ellisomyces anomalus                  90.6
## 10 Actinomucor elegans                    0
## # ... with 16 more rows
```

```
colnames(Zygos) <- c("Strain", "Inhibition")
plot=ggplot(Zygos, aes(Strain, Inhibition, fill=Strain)) + geom_col() + scale_fill_manual(values = c(wes
plot
```




```
#pdf("Zygo_inhibiton.pdf",width=6,height=4)
  #plot
#dev.off()
```

```
#Pathogens Inhbition
#Fungal data with S. pro, S. mar, and B. subtilis
library(readxl)
library(reshape2)
library(ggplot2)
#install.packages("gridExtra")
library(gridExtra)
Actino <- read_excel("data.xlsx", sheet = "Actino")
Conidi <- read_excel("data.xlsx", sheet = "Conidi")
Basidi<- read_excel("data.xlsx", sheet = "Basidi")
```

```
Mucor<- read_excel("data.xlsx", sheet = "Mucor")
Alt<- read_excel("data.xlsx", sheet = "Alt")
Rhizo<- read_excel("data.xlsx", sheet = "Rhizo")
Ncra<- read_excel("data.xlsx", sheet = "Ncrassa_donut")

patho <- Actino
patho <- Conidi
patho <- Basidi
patho <- Mucor
patho <- Alt
patho <- Rhizo
patho <- Ncra


#+++++++++++++++++++++++++
# Function to calculate the mean and the standard deviation
  # for each group
#+++++++++++++++++++++++++
# data : a data frame
# varname : the name of a column containing the variable
  #to be summariezed
# groupnames : vector of column names to be used as
  # grouping variables
data_summary <- function(data, varname, groupnames){
  require(plyr)
  summary_func <- function(x, col){
    c(mean = mean(x[[col]], na.rm=TRUE),
      sd = sd(x[[col]], na.rm=TRUE))
  }
  data_sum<-ddply(data, groupnames, .fun=summary_func,
                  varname)
  data_sum <- rename(data_sum, c("mean" = varname))
 return(data_sum)
}


#actino
patho <- Actino
patho.m <- melt(as.data.frame(patho), id.vars = "Bacteria")
colnames(patho.m) <- c("Strain","Time","Growth")

dfm <- data_summary(patho.m, varname="Growth",
                    groupnames=c("Strain", "Time"))
```

```
## Loading required package: plyr
```

```
a <- ggplot(dfm, aes(x=Time, y=Growth, group=Strain, color=Strain)) +
  geom_errorbar(aes(ymin=Growth-sd, ymax=Growth+sd), width=.1) +
    geom_line() + geom_point()+
   scale_color_brewer(palette="Paired")+theme_minimal() + ggtitle("Actinomucor")
#conidiobolus

patho <- Conidi
```

```
patho.m <- melt(as.data.frame(patho), id.vars = "Bacteria")
colnames(patho.m) <- c("Strain","Time","Growth")

dfm <- data_summary(patho.m, varname="Growth",
                    groupnames=c("Strain", "Time"))
b <- ggplot(dfm, aes(x=Time, y=Growth, group=Strain, color=Strain)) +
    geom_errorbar(aes(ymin=Growth-sd, ymax=Growth+sd), width=.1) +
    geom_line() + geom_point()+
   scale_color_brewer(palette="Paired")+theme_minimal()+ theme(legend.position = "none")+ ggtitle("Conio

#basidiobolus
patho <- Basidi
patho.m <- melt(as.data.frame(patho), id.vars = "Bacteria")
colnames(patho.m) <- c("Strain","Time","Growth")

dfm <- data_summary(patho.m, varname="Growth",
                    groupnames=c("Strain", "Time"))
c <- ggplot(dfm, aes(x=Time, y=Growth, group=Strain, color=Strain)) +
    geom_errorbar(aes(ymin=Growth-sd, ymax=Growth+sd), width=.1) +
    geom_line() + geom_point()+
   scale_color_brewer(palette="Paired")+theme_minimal()+ theme(legend.position = "none")+ ggtitle("Basio

#Mucor
patho <- Mucor
patho.m <- melt(as.data.frame(patho), id.vars = "Bacteria")
colnames(patho.m) <- c("Strain","Time","Growth")

dfm <- data_summary(patho.m, varname="Growth",
                    groupnames=c("Strain", "Time"))
d <- ggplot(dfm, aes(x=Time, y=Growth, group=Strain, color=Strain)) +
    geom_errorbar(aes(ymin=Growth-sd, ymax=Growth+sd), width=.1) +
    geom_line() + geom_point()+
   scale_color_brewer(palette="Paired")+theme_minimal()+ theme(legend.position = "none")+ ggtitle("Mucor

#Alternaria
patho <- Alt
patho.m <- melt(as.data.frame(patho), id.vars = "Bacteria")
colnames(patho.m) <- c("Strain","Time","Growth")

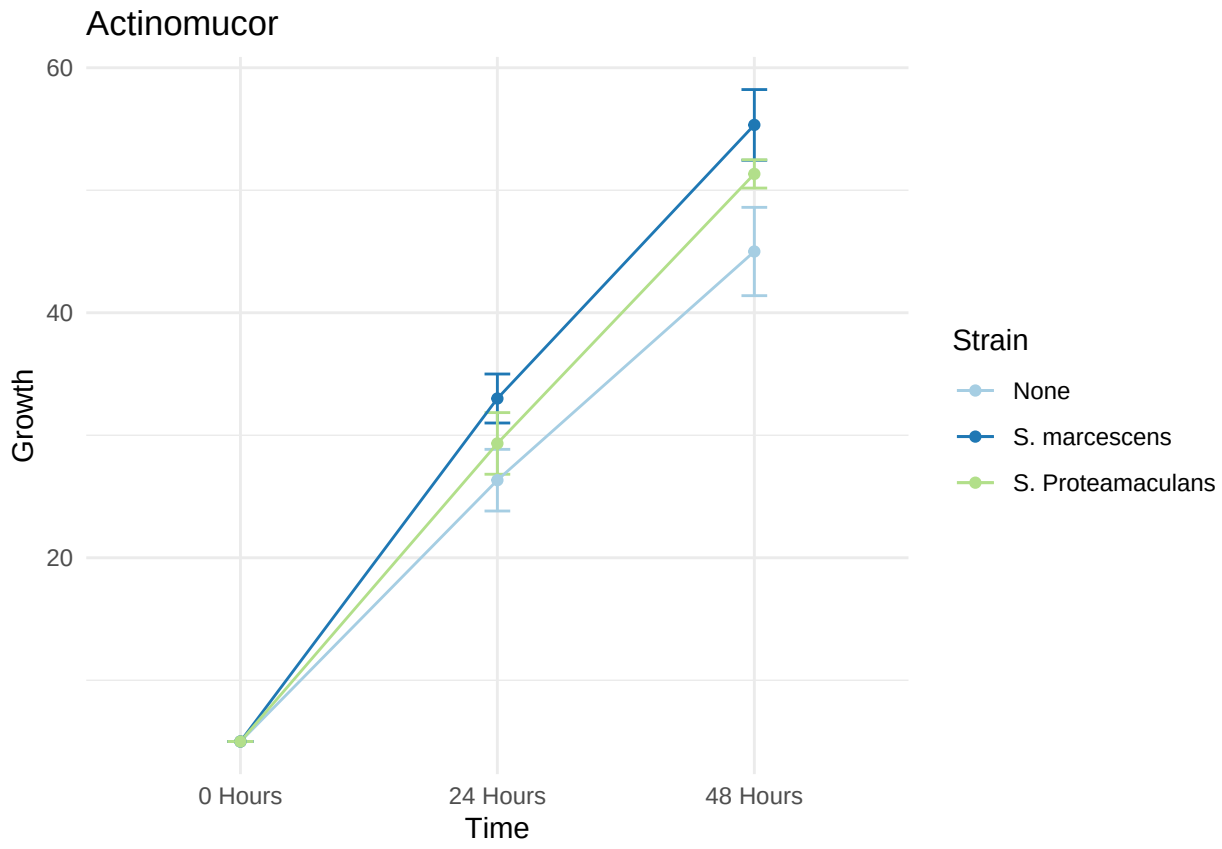
dfm <- data_summary(patho.m, varname="Growth",
                    groupnames=c("Strain", "Time"))
e <- ggplot(dfm, aes(x=Time, y=Growth, group=Strain, color=Strain)) +
    geom_errorbar(aes(ymin=Growth-sd, ymax=Growth+sd), width=.1) +
    geom_line() + geom_point()+
   scale_color_brewer(palette="Paired")+theme_minimal()+ theme(legend.position = "none")+ ggtitle("Alter
#Rhizo
patho <- Rhizo
patho.m <- melt(as.data.frame(patho), id.vars = "Bacteria")
colnames(patho.m) <- c("Strain","Time","Growth")

dfm <- data_summary(patho.m, varname="Growth",
                    groupnames=c("Strain", "Time"))
f <- ggplot(dfm, aes(x=Time, y=Growth, group=Strain, color=Strain)) +
```

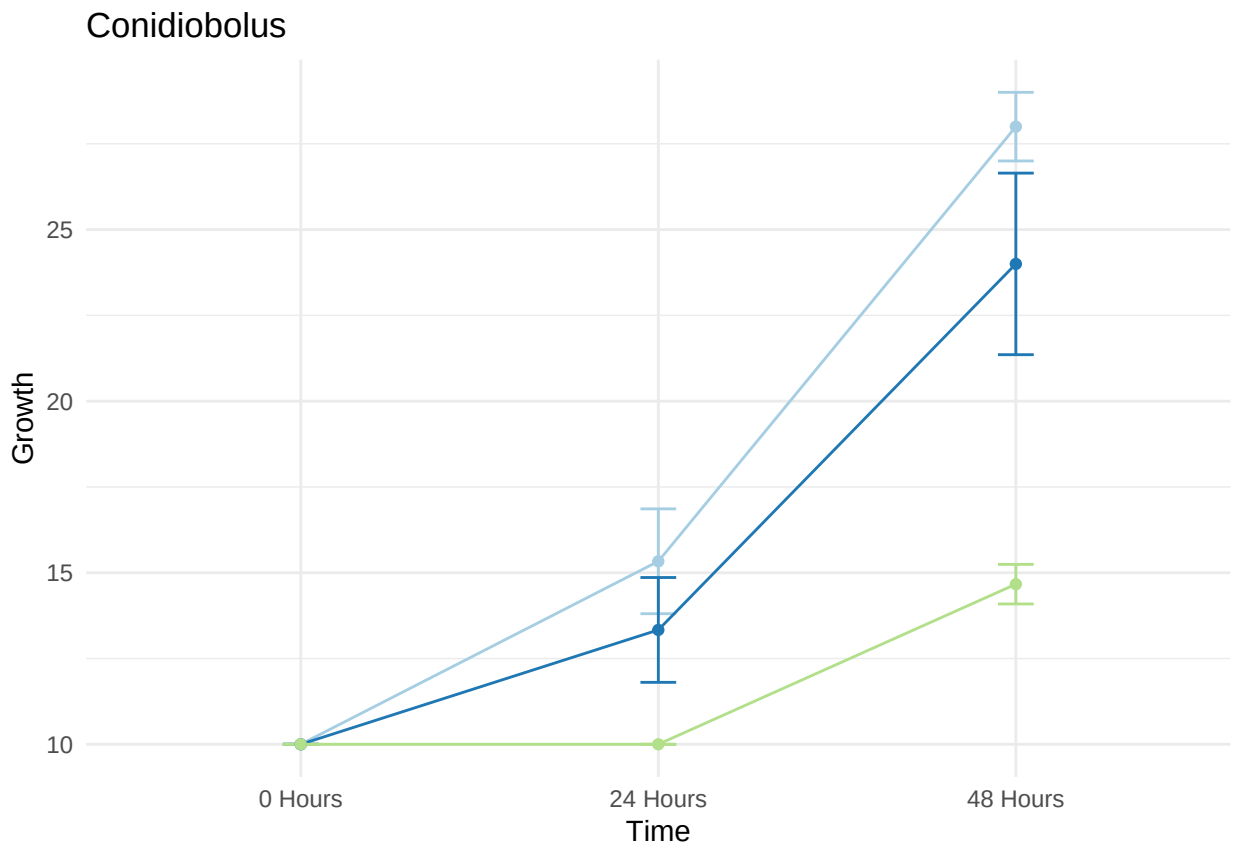
```
    geom_errorbar(aes(ymin=Growth-sd, ymax=Growth+sd), width=.1) +
    geom_line() + geom_point()+
   scale_color_brewer(palette="Paired") + theme_minimal() + theme(legend.position = "none")+ ggtitle("R
#Ncrassa
patho <- Ncra
patho.m <- melt(as.data.frame(patho), id.vars = "Bacteria")
colnames(patho.m) <- c("Strain","Time","Growth")

dfm <- data_summary(patho.m, varname="Growth",
                    groupnames=c("Strain", "Time"))
g <- ggplot(dfm, aes(x=Time, y=Growth, group=Strain, color=Strain)) +
    geom_errorbar(aes(ymin=Growth-sd, ymax=Growth+sd), width=.1) +
    geom_line() + geom_point()+
   scale_color_brewer(palette="Paired")+theme_minimal()+ ggtitle("Neurospora Growth with Bacterial Vola

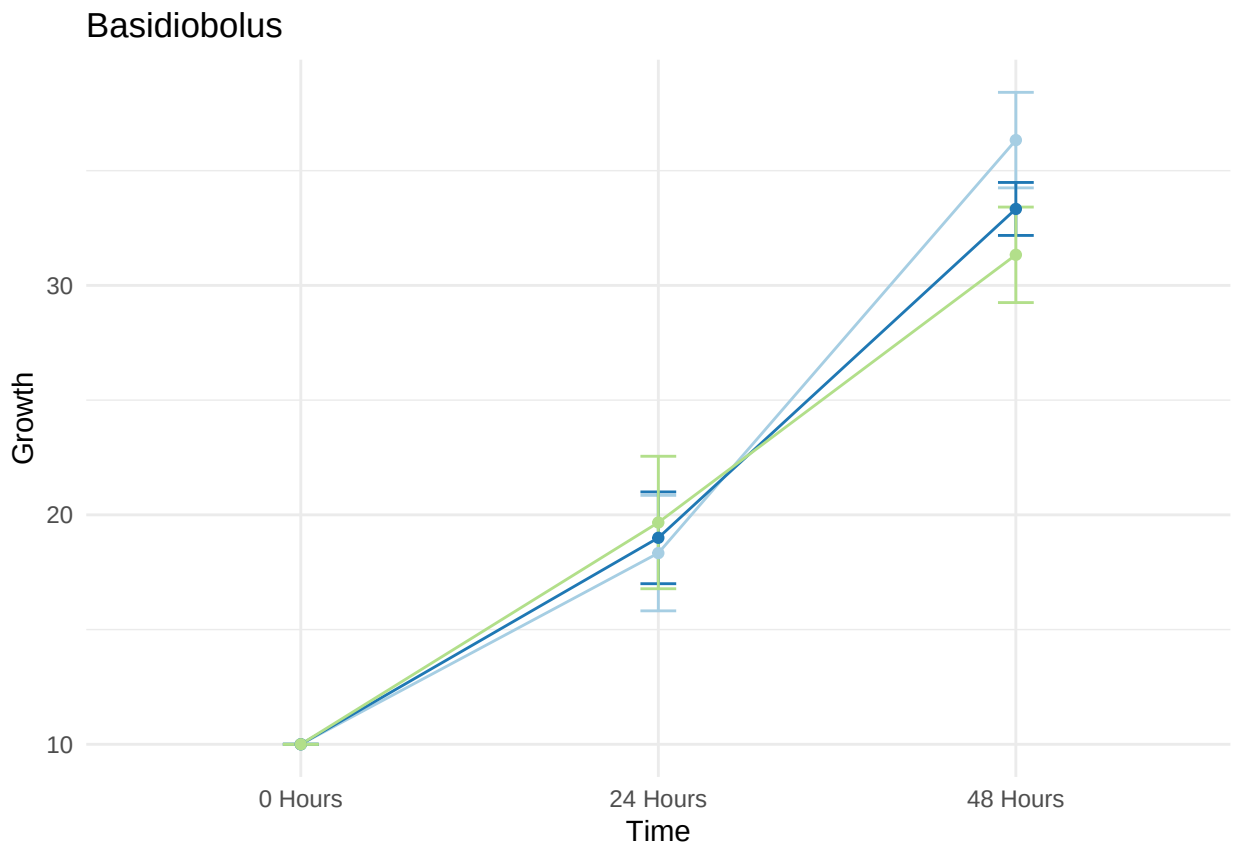
a
```



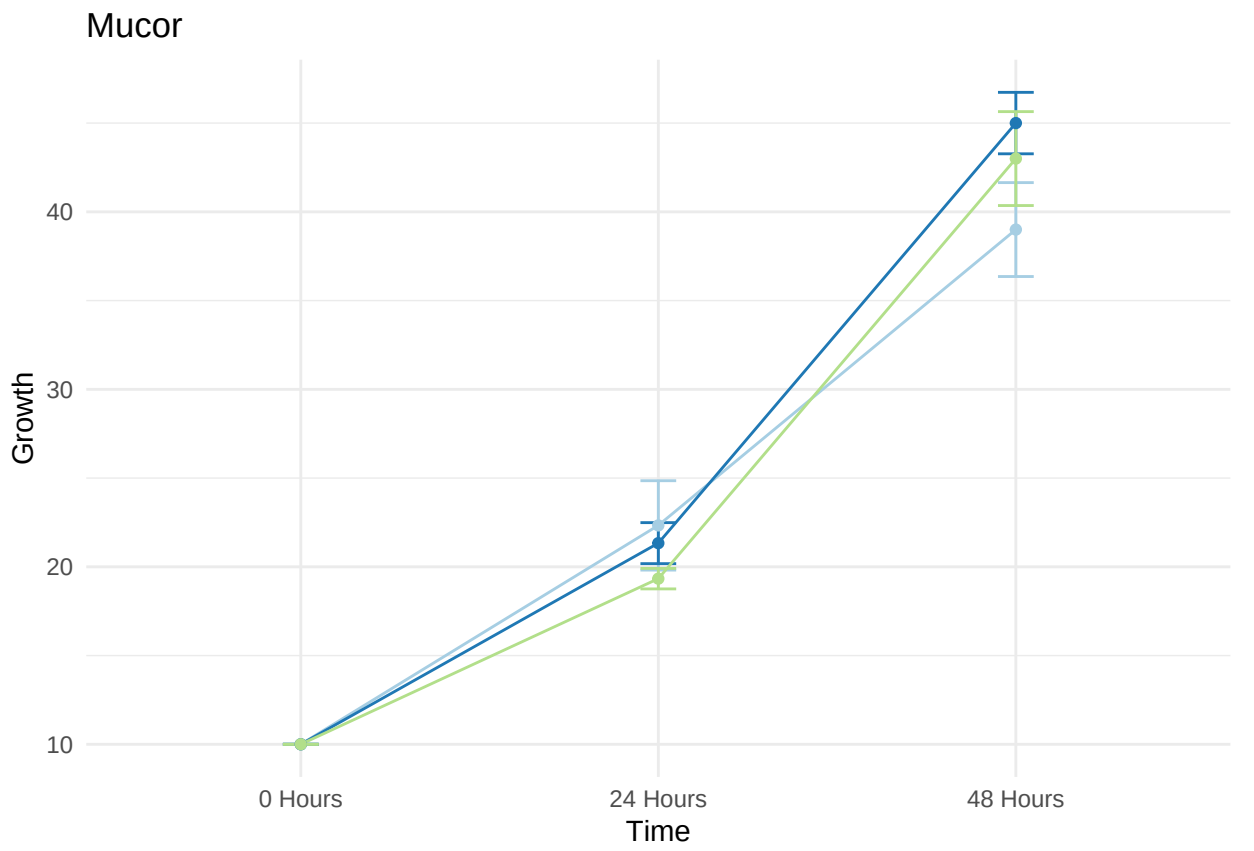

```
b
```


Conidiobolus
Growth
25
20
15
10
0 Hours
24 Hours
48 Hours
Time

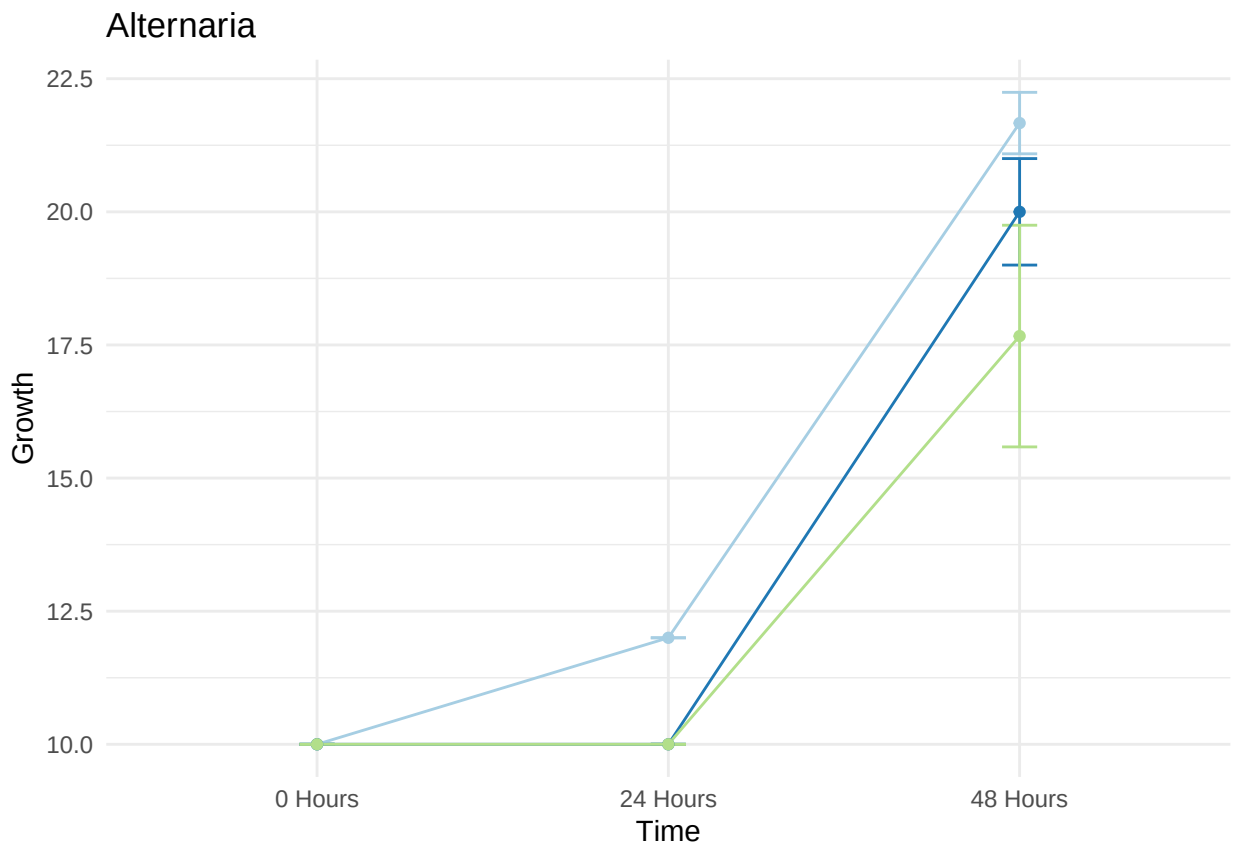
```
c
```



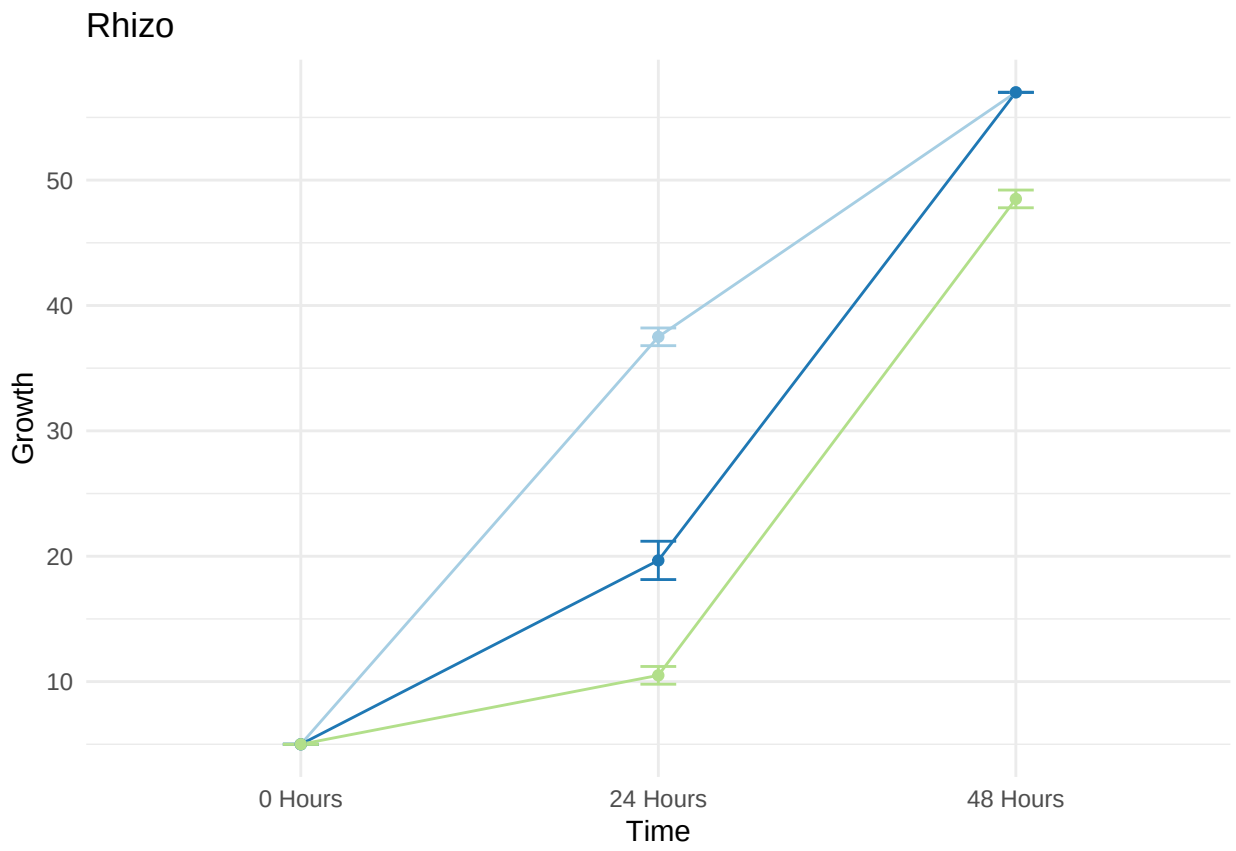

```
d
```



e


Alternaria
22.5
20.0
17.5
15.0
12.5
10.0
Growth
0 Hours
24 Hours
48 Hours
Time

```
f
```

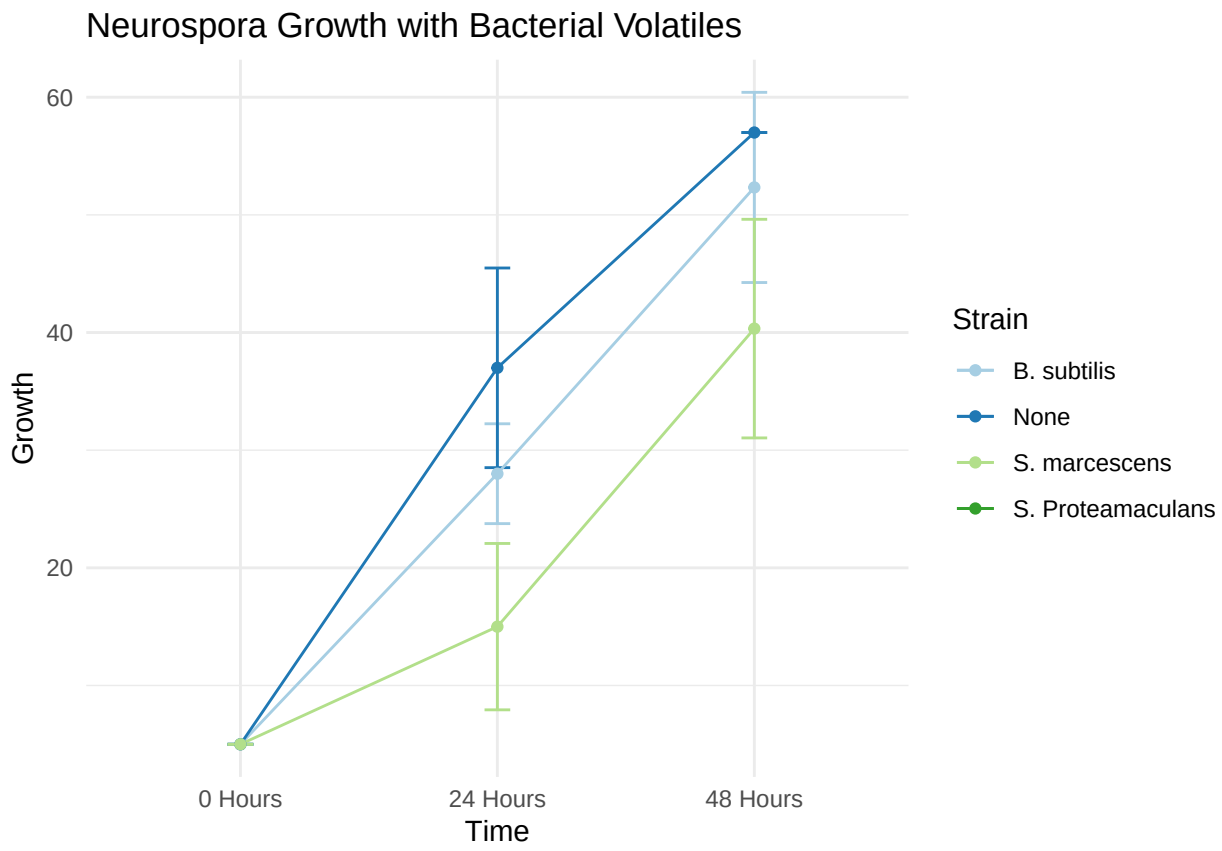



```
g
```

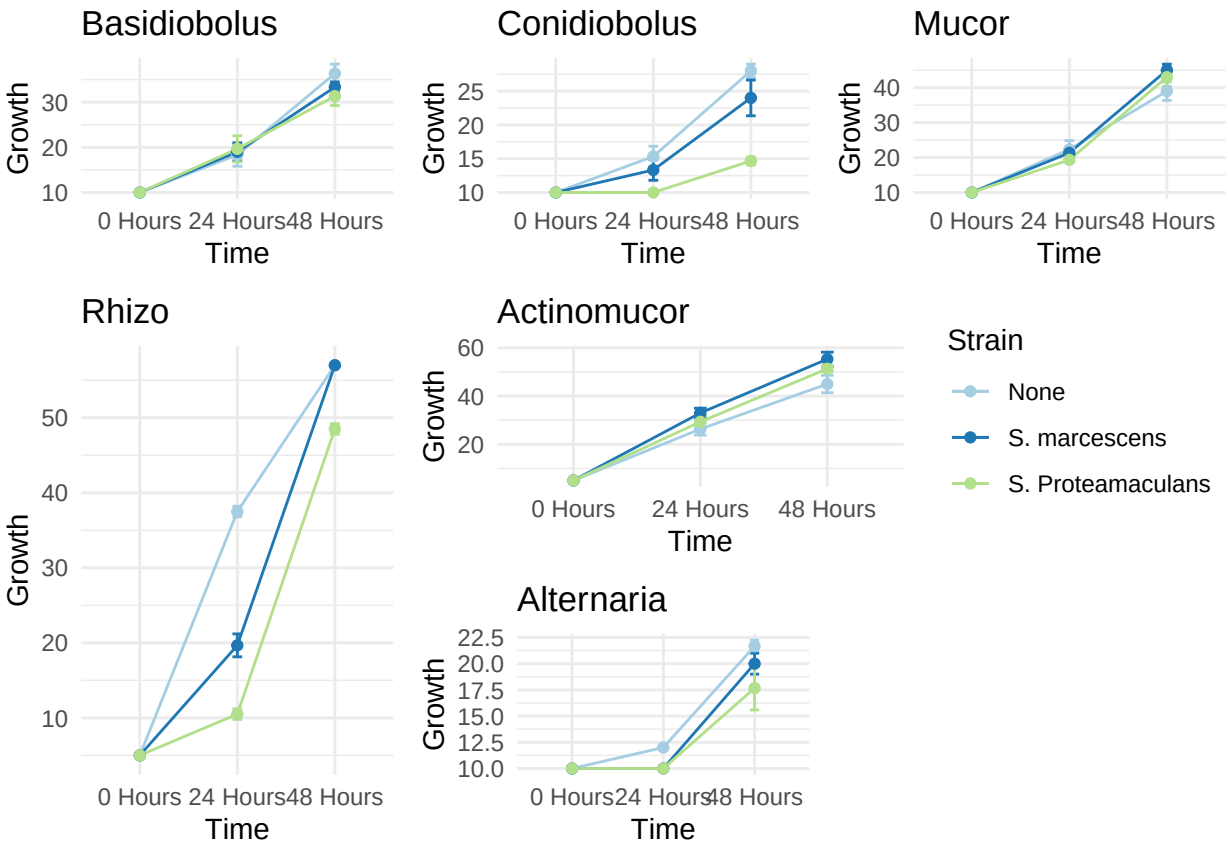
```
## Warning: Removed 3 rows containing missing values (geom_errorbar).
```

```
## Warning: Removed 3 rows containing missing values (geom_path).
```

```
## Warning: Removed 3 rows containing missing values (geom_point).
```




```
grid.arrange(b, c, d, e, f, a, nrow = 3, ncol=3,layout_matrix = rbind(c(2, 1, 3), c(5, 6, 6), c(5, 4, NA
```



Different volatile profiles were detected from different strains of bacteria.

First a look at the samples and their production of volatiles as detected though GC MS

```
library("readxl")
library("ggplot2")

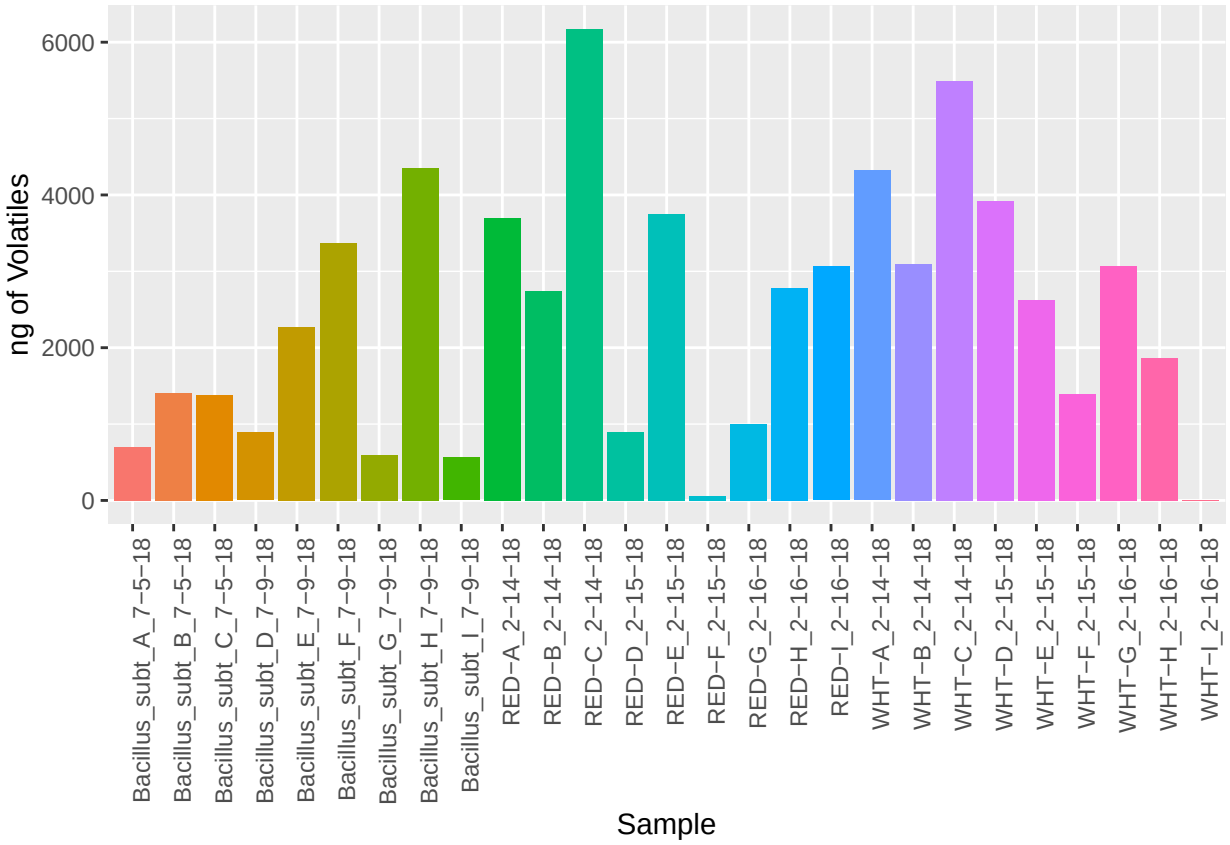
Samples <- read_excel("data.xlsx", sheet = "Heatmap1_total_production")
Samples.df <- as.data.frame(Samples)
rownames(Samples.df) <- Samples$`Sum of amount ng/sample`

Samples.df
```

```
##                       Sum of amount ng/sample Grand Total
## Bacillus_subt_A_7-5-18  Bacillus_subt_A_7-5-18   702.20922
## Bacillus_subt_B_7-5-18  Bacillus_subt_B_7-5-18  1411.50928
## Bacillus_subt_C_7-5-18  Bacillus_subt_C_7-5-18  1385.50263
## Bacillus_subt_D_7-9-18  Bacillus_subt_D_7-9-18   889.45396
## Bacillus_subt_E_7-9-18  Bacillus_subt_E_7-9-18  2270.11088
## Bacillus_subt_F_7-9-18  Bacillus_subt_F_7-9-18  3372.63986
## Bacillus_subt_G_7-9-18  Bacillus_subt_G_7-9-18   592.34646
## Bacillus_subt_H_7-9-18  Bacillus_subt_H_7-9-18  4356.25514
## Bacillus_subt_I_7-9-18  Bacillus_subt_I_7-9-18   561.86917
## RED-A_2-14-18                    RED-A_2-14-18  3694.58639
```

```
## RED-B_2-14-18                    RED-B_2-14-18  2744.95593
## RED-C_2-14-18                    RED-C_2-14-18  6173.69361
## RED-D_2-15-18                    RED-D_2-15-18   896.95131
## RED-E_2-15-18                    RED-E_2-15-18  3745.83987
## RED-F_2-15-18                    RED-F_2-15-18    54.40257
## RED-G_2-16-18                    RED-G_2-16-18  1006.22666
## RED-H_2-16-18                    RED-H_2-16-18  2781.67238
## RED-I_2-16-18                    RED-I_2-16-18  3062.91257
## WHT-A_2-14-18                    WHT-A_2-14-18  4320.60139
## WHT-B_2-14-18                    WHT-B_2-14-18  3096.03274
## WHT-C_2-14-18                    WHT-C_2-14-18  5493.04115
## WHT-D_2-15-18                    WHT-D_2-15-18  3921.78987
## WHT-E_2-15-18                    WHT-E_2-15-18  2618.97103
## WHT-F_2-15-18                    WHT-F_2-15-18  1398.35092
## WHT-G_2-16-18                    WHT-G_2-16-18  3069.32287
## WHT-H_2-16-18                    WHT-H_2-16-18  1861.84356
## WHT-I_2-16-18                    WHT-I_2-16-18     0.00000
```

```
Totes <- ggplot(Samples.df, aes(x=Samples.df$`Sum of amount ng/sample`, y=Samples.df$'Grand Total', fil
Totes
```




```
pdf("AllSample_vol_production", height = 32, width = 12)
Totes
dev.off()
```

```
## pdf
```

```
##   2
```

Examing the overlap between strains

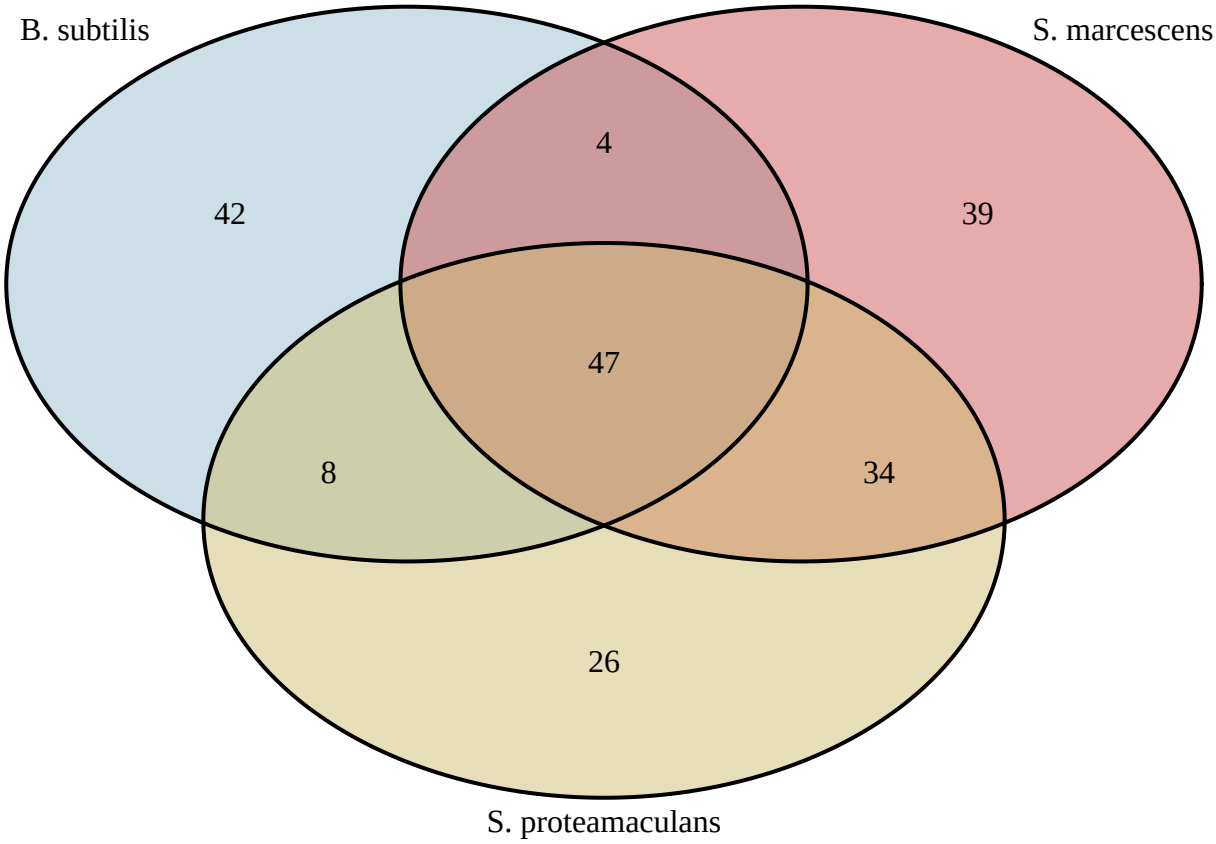
```
#make venn diagram of volatiles
library(readxl)
library(VennDiagram)
```

```
## Loading required package: grid
```

```
## Loading required package: futile.logger
```

```
#Numbers are coming from "data.xlsx", sheet = "VennDia3")

grid.newpage()
Venn <- draw.triple.venn(area1 = 101, area2 = 124, area3 = 115, n12 = 51, n23 = 81, n13 = 55, n123 = 47
```




```
Venn
```

```
## (polygon[GRID.polygon.1285], polygon[GRID.polygon.1286], polygon[GRID.polygon.1287], polygon[GRID.pol
```

```
pdf("Venn_vol_heat.pdf", height = 32, width = 12)
Venn
```

```
## (polygon[GRID.polygon.1285], polygon[GRID.polygon.1286], polygon[GRID.polygon.1287], polygon[GRID.po
```

```
dev.off()
```

```
## pdf
##   2
```

Show how they seperate out with several analyses

```
#NMDS Plot

library(vegan)
```

```
## Loading required package: permute
```

```
## Loading required package: lattice
```

```
## This is vegan 2.5-5
```

```
library(readxl)
set.seed(2)
community_matrix=matrix(
  sample(1:100,300,replace=T),nrow=10,
  dimnames=list(paste("community",1:10,sep=""),paste("sp",1:30,sep="")))

example_NMDS=metaMDS(community_matrix, # Our community-by-species matrix
                     k=2) # The number of reduced dimensions
```

```
## Square root transformation
## Wisconsin double standardization
## Run 0 stress 0.1486476
## Run 1 stress 0.1913739
## Run 2 stress 0.1908305
## Run 3 stress 0.1908317
## Run 4 stress 0.1849162
## Run 5 stress 0.1906937
## Run 6 stress 0.1486489
## ... Procrustes: rmse 0.0007687706  max resid 0.001221702
## ... Similar to previous best
## Run 7 stress 0.1849759
## Run 8 stress 0.1688829
## Run 9 stress 0.1650751
## Run 10 stress 0.1486477
## ... Procrustes: rmse 0.000106901  max resid 0.0001907307
## ... Similar to previous best
## Run 11 stress 0.164544
## Run 12 stress 0.3153591
## Run 13 stress 0.219889
## Run 14 stress 0.2237401
## Run 15 stress 0.1699875
## Run 16 stress 0.1650804
```

```
## Run 17 stress 0.1906937
## Run 18 stress 0.2255724
## Run 19 stress 0.1494912
## Run 20 stress 0.1650751
## *** Solution reached
```

```
volatiles <- read_excel("data.xlsx", sheet = "NMDS_1")
volatiles_names <- read_excel("data.xlsx", sheet = "NMDS_2")

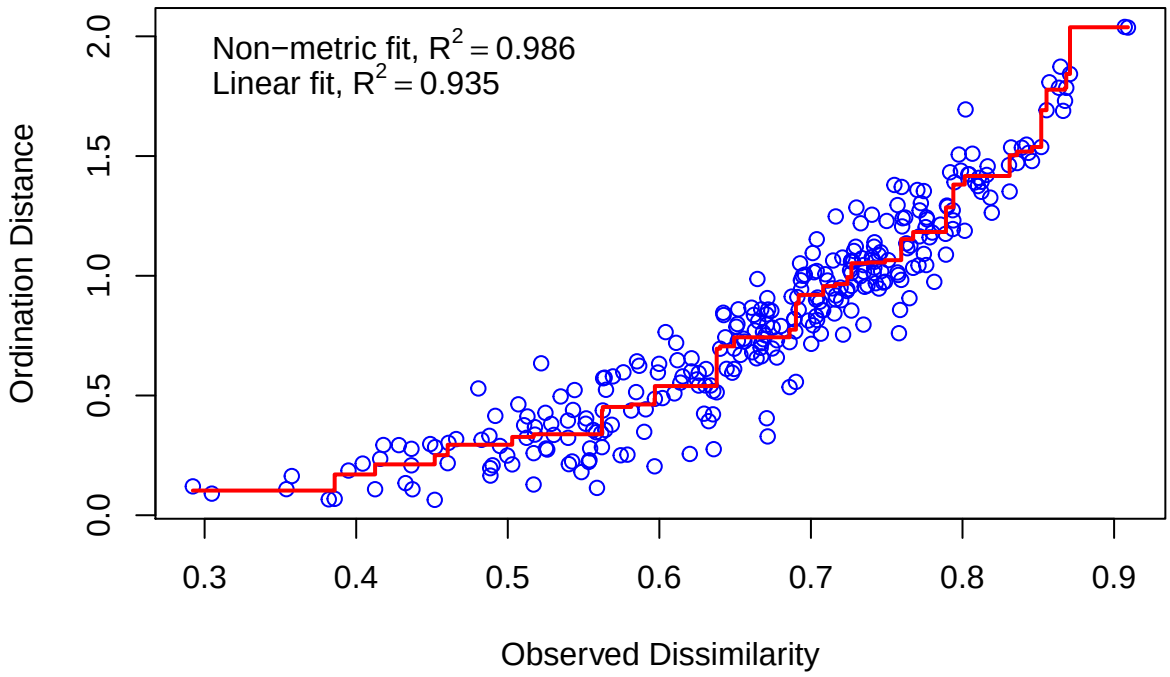
rownames(volatiles) <- volatiles_names$Sample
```

```
## Warning: Setting row names on a tibble is deprecated.
```

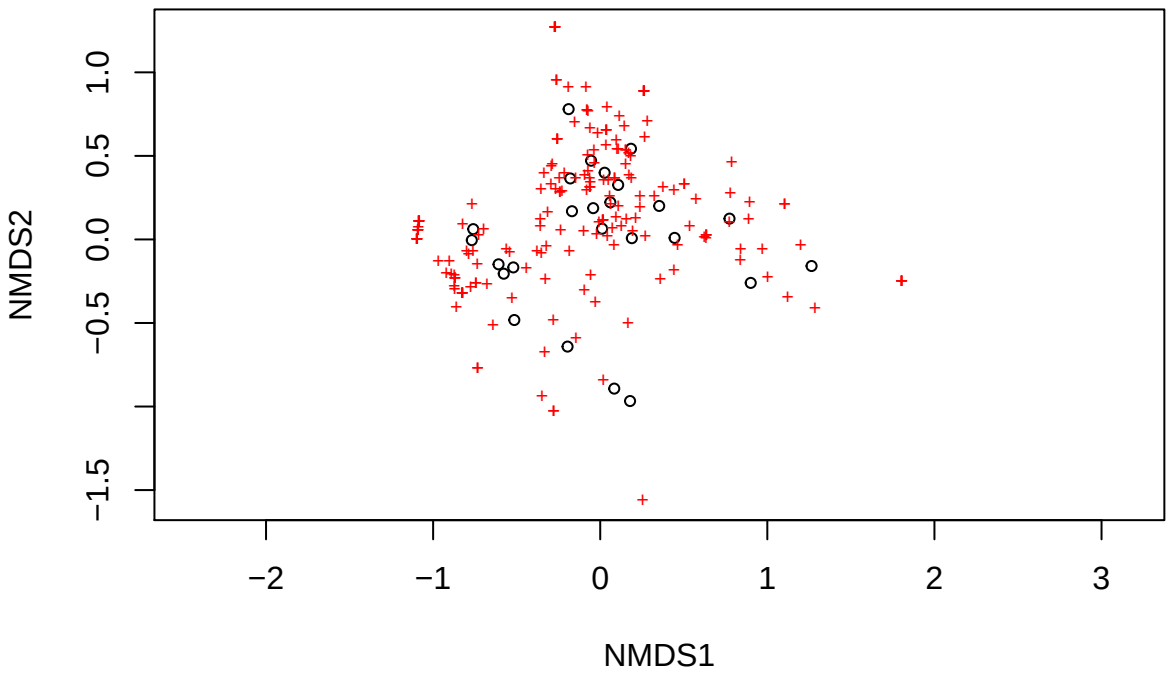
```
volatiles.matrix=as.matrix(volatiles)
NMDS=metaMDS(volatiles.matrix, k=2)
```

```
## Square root transformation
## Wisconsin double standardization
## Run 0 stress 0.1180499
## Run 1 stress 0.1196732
## Run 2 stress 0.1180499
## ... Procrustes: rmse 3.585978e-05  max resid 0.0001350778
## ... Similar to previous best
## Run 3 stress 0.1196732
## Run 4 stress 0.1199098
## Run 5 stress 0.1196732
## Run 6 stress 0.1180499
## ... New best solution
## ... Procrustes: rmse 5.118637e-06  max resid 1.845341e-05
## ... Similar to previous best
## Run 7 stress 0.1180499
## ... New best solution
## ... Procrustes: rmse 6.181096e-06  max resid 2.205723e-05
## ... Similar to previous best
## Run 8 stress 0.1180499
## ... Procrustes: rmse 8.173839e-06  max resid 3.319713e-05
## ... Similar to previous best
## Run 9 stress 0.1180499
## ... Procrustes: rmse 4.402553e-06  max resid 1.305549e-05
## ... Similar to previous best
## Run 10 stress 0.1196732
## Run 11 stress 0.1196732
## Run 12 stress 0.1920025
## Run 13 stress 0.1196732
## Run 14 stress 0.1196732
## Run 15 stress 0.1196732
## Run 16 stress 0.193471
## Run 17 stress 0.1180499
## ... Procrustes: rmse 1.466662e-05  max resid 6.263261e-05
## ... Similar to previous best
## Run 18 stress 0.1196732
## Run 19 stress 0.1199098
## Run 20 stress 0.2041712
## *** Solution reached
```

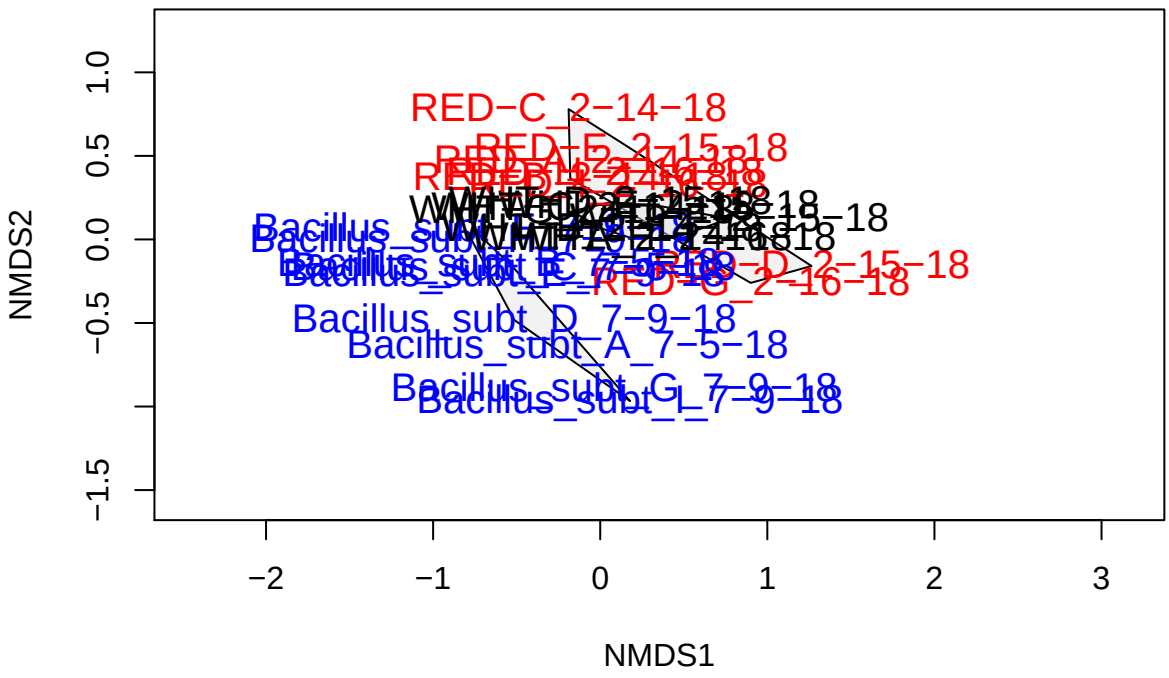
```
stressplot(NMDS)
```




```
plot(NMDS)
```




```
treat=c(rep("Bacillus",9),rep("Red",8),rep("White",8))
ordiplot(NMDS,type="n")
ordihull(NMDS,groups=treat,draw="polygon",col="grey90",label=F)
orditorp(NMDS,display="sites",col=c(rep("blue",9),rep("red",8),rep("black",8)),
         air=0.01,cex=1.25)
```




```
pdf("NMDS.pdf", height = 12, width = 12)
plot(NMDS)
treat=c(rep("Bacillus",9),rep("Red",8),rep("White",8))
ordiplot(NMDS,type="n")
ordihull(NMDS,groups=treat,draw="polygon",col="grey90",label=F)
orditorp(NMDS,display="sites",col=c(rep("blue",9),rep("red",8),rep("black",8)),
         air=0.01,cex=1.25)
dev.off()
```

```
## pdf
##   2
```

```
library("readxl")
library("ggplot2")
library("ggdendro")
library("reshape2")
library("grid")

#Grab and shape data
vol <- read_excel("data.xlsx", sheet = "Heatmap_4_average")
vol.df <- as.data.frame(vol)
vol.df
```

```
##                                                Volatile B. subtilis
## 1                                          2-Undecanone   65.788334
```

```
## 2                           Cyclotetrasiloxane, octamethyl-   24.861569
## 3                                       Diethyl Phthalate    0.000000
## 4                                            Acetophenone   13.443900
## 5                           Cyclopentasiloxane, decamethyl-    3.645482
## 6                                         Benzyl alcohol   12.743759
## 7                           Pyrazine, 3-ethyl-2,5-dimethyl-    9.806626
## 8                                   1-Hexanol, 2-ethyl-   10.881896
## 9                                          2-Undecanol   36.485114
## 10                                            Styrene    7.394190
## 11                        Ethanone, 1-(1H-pyrrol-2-yl)-    7.724929
## 12                                         Caprolactam    9.401807
## 13                              2,4,4-Trimethyl-1-hexene    0.000000
## 14                                         Benzaldehyde    5.889882
## 15                                   Dibutyl phthalate   11.350734
## 16                                    2-Acetylthiazole   11.015745
## 17                                       2-Tridecanone    4.965275
## 18                              2,3,3-Trimethyl-1-hexene    0.000000
## 19                          Pyrazine, 2-ethyl-6-methyl-    2.699596
## 20                                 Benzyl methyl ketone    0.000000
## 21                                          2-Nonanone    5.743211
## 22                                         2-Dodecanone   18.607029
## 23                          2,4,6-Cycloheptatrien-1-one    0.000000
## 24                                           2-Nonanol   11.698919
## 25                                           Undecanal    4.312549
## 26                         Cyclohexasiloxane, dodecamethyl-    7.304148
## 27                                 Butylated Hydroxytoluene    7.314342
## 28                                         Benzyl nitrile    3.652833
## 29                           2,4-Di-tert-butylphenol    2.401032
## 30                                           Nonadecane    5.813875
## 31                                          Benzophenone    4.361363
## 32                            2-Heptanone, 6-methyl-   10.008527
## 33                              Quinoline, 3-methyl-    0.000000
## 34                                           Dodecanal    4.828842
## 35                                           1-Nonanol    0.000000
## 36 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester    6.059075
## 37                            2-Heptanone, 5-methyl-    8.242499
## 38                                       Benzothiazole    3.413640
## 39                          Benzene, 3-cyclohexen-1-yl-    0.000000
## 40                                 Quinoline, 4-methyl-    2.725803
## 41                                          2-Decanol    5.331696
## 42                           Benzene, 1-chloro-2-methoxy-    0.000000
##    S. marcescens S. proteamaculans       sum
## 1       8.103901          7.610332 81.502567
## 2      37.807927          0.000000 62.669495
## 3      16.351702         27.265811 43.617513
## 4      13.548946         15.249631 42.242477
## 5      38.389940          0.000000 42.035422
## 6       3.739744         25.373854 41.857357
## 7      13.550469         18.062958 41.420052
## 8      21.279233          8.883402 41.044530
## 9       0.000000          0.000000 36.485114
## 10      6.827112         18.979317 33.200618
## 11     16.389580          8.157120 32.271629
## 12     15.127583          6.640843 31.170232
```

```
## 13     14.948664         13.960901 28.909565
## 14      8.540497         11.501003 25.931381
## 15      6.381384          5.569892 23.302011
## 16      2.963814          8.381929 22.361488
## 17     10.503033          6.719692 22.188000
## 18     11.546623         10.320259 21.866882
## 19      2.963037         14.790536 20.453168
## 20      7.759105         12.255717 20.014822
## 21      3.779451         10.357248 19.879910
## 22      0.000000          0.000000 18.607029
## 23      7.508897         10.566061 18.074959
## 24      1.586398          4.243541 17.528859
## 25      7.689498          5.453554 17.455600
## 26      9.618909          0.000000 16.923057
## 27      6.266743          2.878902 16.459986
## 28      4.989917          5.286645 13.929395
## 29      6.625763          4.717473 13.744268
## 30      3.483712          3.215243 12.512829
## 31      4.192673          3.857433 12.411470
## 32      0.000000          0.000000 10.008527
## 33      7.164959          2.725815  9.890774
## 34      0.000000          4.830726  9.659568
## 35      3.756624          5.176402  8.933027
## 36      1.599047          1.017218  8.675340
## 37      0.000000          0.000000  8.242499
## 38      2.066972          2.451162  7.931774
## 39      3.036559          2.713634  5.750193
## 40      0.000000          2.670478  5.396281
## 41      0.000000          0.000000  5.331696
## 42      4.393618          0.000000  4.393618
```

```
rownames(vol.df) <- vol$Volatile
vol.df
```

```
##
## 2-Undecanone                                                                2
## Cyclotetrasiloxane, octamethyl-                                  Cyclotetrasiloxane, 
## Diethyl Phthalate                                                          Diethyl
## Acetophenone                                                                   A
## Cyclopentasiloxane, decamethyl-                                  Cyclopentasiloxane, 
## Benzyl alcohol                                                              Benz
## Pyrazine, 3-ethyl-2,5-dimethyl-                                  Pyrazine, 3-ethyl-2,5
## 1-Hexanol, 2-ethyl-                                                    1-Hexanol
## 2-Undecanol                                                                 1
## Styrene
## Ethanone, 1-(1H-pyrrol-2-yl)-                                      Ethanone, 1-(1H-pyr
## Caprolactam                                                                 C
## 2,4,4-Trimethyl-1-hexene                                          2,4,4-Trimethy
## Benzaldehyde                                                                Be
## Dibutyl phthalate                                                          Dibutyl
## 2-Acetylthiazole                                                         2-Acet
## 2-Tridecanone                                                               2-T
## 2,3,3-Trimethyl-1-hexene                                          2,3,3-Trimethy
## Pyrazine, 2-ethyl-6-methyl-                                       Pyrazine, 2-ethyl
```

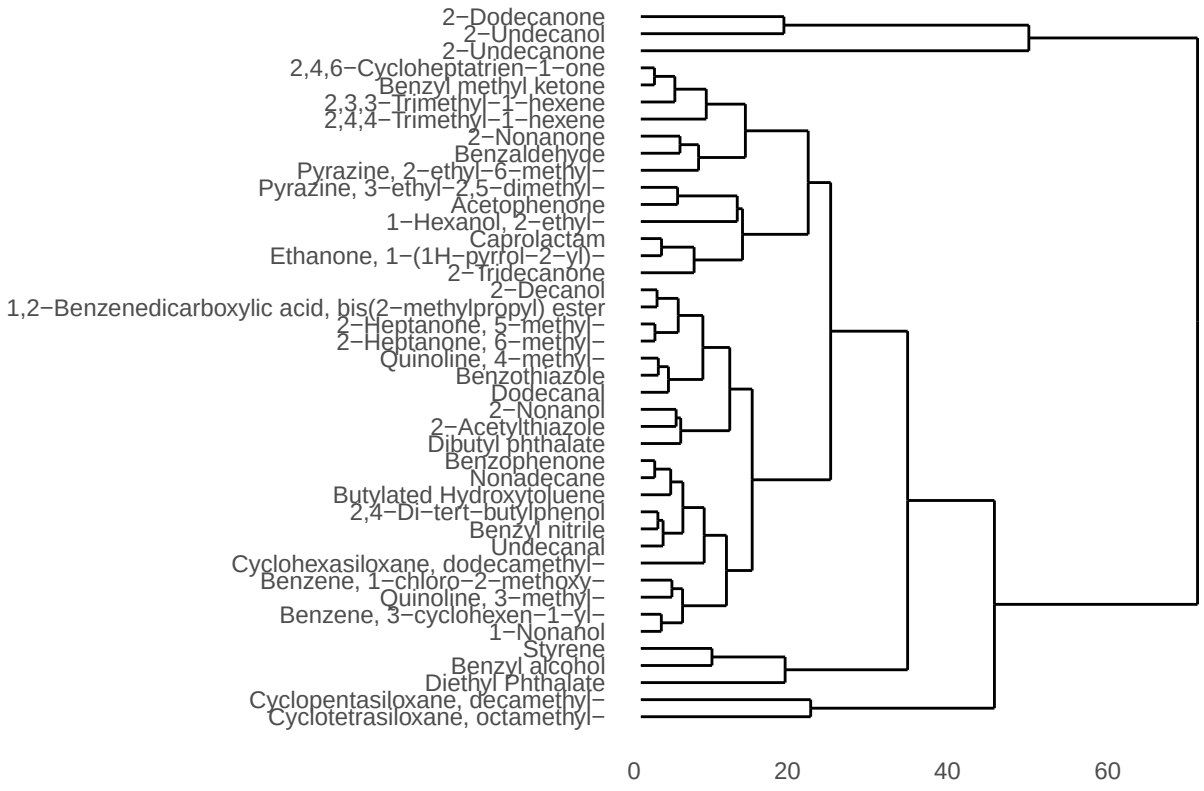
```
## Benzyl methyl ketone                                                                         Benzyl met
## 2-Nonanone
## 2-Dodecanone                                                                                         2-
## 2,4,6-Cycloheptatrien-1-one                                                            2,4,6-Cyclohepta
## 2-Nonanol
## Undecanal
## Cyclohexasiloxane, dodecamethyl-                                                  Cyclohexasiloxane, doc
## Butylated Hydroxytoluene                                                                 Butylated Hydr
## Benzyl nitrile                                                                                     Benz
## 2,4-Di-tert-butylphenol                                                                   2,4-Di-tert-b
## Nonadecane
## Benzophenone                                                                                         Be
## 2-Heptanone, 6-methyl-                                                                      2-Heptanone
## Quinoline, 3-methyl-                                                                          Quinoline
## Dodecanal
## 1-Nonanol
## 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester 1,2-Benzenedicarboxylic acid, bis(2-methylpro
## 2-Heptanone, 5-methyl-                                                                      2-Heptanone
## Benzothiazole                                                                                       Ben
## Benzene, 3-cyclohexen-1-yl-                                                            Benzene, 3-cyclo
## Quinoline, 4-methyl-                                                                          Quinoline
## 2-Decanol
## Benzene, 1-chloro-2-methoxy-                                                          Benzene, 1-chloro-
##                                                          B. subtilis
## 2-Undecanone                                               65.788334
## Cyclotetrasiloxane, octamethyl-                            24.861569
## Diethyl Phthalate                                           0.000000
## Acetophenone                                               13.443900
## Cyclopentasiloxane, decamethyl-                             3.645482
## Benzyl alcohol                                             12.743759
## Pyrazine, 3-ethyl-2,5-dimethyl-                             9.806626
## 1-Hexanol, 2-ethyl-                                        10.881896
## 2-Undecanol                                                36.485114
## Styrene                                                     7.394190
## Ethanone, 1-(1H-pyrrol-2-yl)-                               7.724929
## Caprolactam                                                 9.401807
## 2,4,4-Trimethyl-1-hexene                                    0.000000
## Benzaldehyde                                                5.889882
## Dibutyl phthalate                                          11.350734
## 2-Acetylthiazole                                           11.015745
## 2-Tridecanone                                               4.965275
## 2,3,3-Trimethyl-1-hexene                                    0.000000
## Pyrazine, 2-ethyl-6-methyl-                                 2.699596
## Benzyl methyl ketone                                        0.000000
## 2-Nonanone                                                  5.743211
## 2-Dodecanone                                               18.607029
## 2,4,6-Cycloheptatrien-1-one                                 0.000000
## 2-Nonanol                                                  11.698919
## Undecanal                                                   4.312549
## Cyclohexasiloxane, dodecamethyl-                            7.304148
## Butylated Hydroxytoluene                                    7.314342
## Benzyl nitrile                                              3.652833
## 2,4-Di-tert-butylphenol                                     2.401032
## Nonadecane                                                  5.813875
```

```
## Benzophenone                                                4.361363
## 2-Heptanone, 6-methyl-                                     10.008527
## Quinoline, 3-methyl-                                        0.000000
## Dodecanal                                                   4.828842
## 1-Nonanol                                                   0.000000
## 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester     6.059075
## 2-Heptanone, 5-methyl-                                      8.242499
## Benzothiazole                                               3.413640
## Benzene, 3-cyclohexen-1-yl-                                 0.000000
## Quinoline, 4-methyl-                                        2.725803
## 2-Decanol                                                   5.331696
## Benzene, 1-chloro-2-methoxy-                                0.000000
##                                                          S. marcescens
## 2-Undecanone                                                8.103901
## Cyclotetrasiloxane, octamethyl-                            37.807927
## Diethyl Phthalate                                          16.351702
## Acetophenone                                               13.548946
## Cyclopentasiloxane, decamethyl-                            38.389940
## Benzyl alcohol                                              3.739744
## Pyrazine, 3-ethyl-2,5-dimethyl-                            13.550469
## 1-Hexanol, 2-ethyl-                                        21.279233
## 2-Undecanol                                                 0.000000
## Styrene                                                     6.827112
## Ethanone, 1-(1H-pyrrol-2-yl)-                              16.389580
## Caprolactam                                                15.127583
## 2,4,4-Trimethyl-1-hexene                                   14.948664
## Benzaldehyde                                                8.540497
## Dibutyl phthalate                                           6.381384
## 2-Acetylthiazole                                            2.963814
## 2-Tridecanone                                              10.503033
## 2,3,3-Trimethyl-1-hexene                                   11.546623
## Pyrazine, 2-ethyl-6-methyl-                                 2.963037
## Benzyl methyl ketone                                        7.759105
## 2-Nonanone                                                  3.779451
## 2-Dodecanone                                                0.000000
## 2,4,6-Cycloheptatrien-1-one                                 7.508897
## 2-Nonanol                                                   1.586398
## Undecanal                                                   7.689498
## Cyclohexasiloxane, dodecamethyl-                            9.618909
## Butylated Hydroxytoluene                                    6.266743
## Benzyl nitrile                                              4.989917
## 2,4-Di-tert-butylphenol                                     6.625763
## Nonadecane                                                  3.483712
## Benzophenone                                                4.192673
## 2-Heptanone, 6-methyl-                                      0.000000
## Quinoline, 3-methyl-                                        7.164959
## Dodecanal                                                   0.000000
## 1-Nonanol                                                   3.756624
## 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester     1.599047
## 2-Heptanone, 5-methyl-                                      0.000000
## Benzothiazole                                               2.066972
## Benzene, 3-cyclohexen-1-yl-                                 3.036559
## Quinoline, 4-methyl-                                        0.000000
## 2-Decanol                                                   0.000000
```

```
## Benzene, 1-chloro-2-methoxy-                                  4.393618
##                                                          S. proteamaculans
## 2-Undecanone                                                      7.610332
## Cyclotetrasiloxane, octamethyl-                                   0.000000
## Diethyl Phthalate                                                27.265811
## Acetophenone                                                     15.249631
## Cyclopentasiloxane, decamethyl-                                   0.000000
## Benzyl alcohol                                                   25.373854
## Pyrazine, 3-ethyl-2,5-dimethyl-                                  18.062958
## 1-Hexanol, 2-ethyl-                                               8.883402
## 2-Undecanol                                                       0.000000
## Styrene                                                          18.979317
## Ethanone, 1-(1H-pyrrol-2-yl)-                                     8.157120
## Caprolactam                                                       6.640843
## 2,4,4-Trimethyl-1-hexene                                         13.960901
## Benzaldehyde                                                     11.501003
## Dibutyl phthalate                                                 5.569892
## 2-Acetylthiazole                                                  8.381929
## 2-Tridecanone                                                     6.719692
## 2,3,3-Trimethyl-1-hexene                                         10.320259
## Pyrazine, 2-ethyl-6-methyl-                                      14.790536
## Benzyl methyl ketone                                             12.255717
## 2-Nonanone                                                       10.357248
## 2-Dodecanone                                                      0.000000
## 2,4,6-Cycloheptatrien-1-one                                      10.566061
## 2-Nonanol                                                         4.243541
## Undecanal                                                         5.453554
## Cyclohexasiloxane, dodecamethyl-                                  0.000000
## Butylated Hydroxytoluene                                          2.878902
## Benzyl nitrile                                                    5.286645
## 2,4-Di-tert-butylphenol                                           4.717473
## Nonadecane                                                        3.215243
## Benzophenone                                                      3.857433
## 2-Heptanone, 6-methyl-                                            0.000000
## Quinoline, 3-methyl-                                              2.725815
## Dodecanal                                                         4.830726
## 1-Nonanol                                                         5.176402
## 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester           1.017218
## 2-Heptanone, 5-methyl-                                            0.000000
## Benzothiazole                                                     2.451162
## Benzene, 3-cyclohexen-1-yl-                                       2.713634
## Quinoline, 4-methyl-                                              2.670478
## 2-Decanol                                                         0.000000
## Benzene, 1-chloro-2-methoxy-                                      0.000000
##                                                                      sum
## 2-Undecanone                                                   81.502567
## Cyclotetrasiloxane, octamethyl-                                62.669495
## Diethyl Phthalate                                              43.617513
## Acetophenone                                                   42.242477
## Cyclopentasiloxane, decamethyl-                                42.035422
## Benzyl alcohol                                                 41.857357
## Pyrazine, 3-ethyl-2,5-dimethyl-                                41.420052
## 1-Hexanol, 2-ethyl-                                            41.044530
## 2-Undecanol                                                    36.485114
```

```
## Styrene                                                    33.200618
## Ethanone, 1-(1H-pyrrol-2-yl)-                              32.271629
## Caprolactam                                                31.170232
## 2,4,4-Trimethyl-1-hexene                                   28.909565
## Benzaldehyde                                               25.931381
## Dibutyl phthalate                                          23.302011
## 2-Acetylthiazole                                           22.361488
## 2-Tridecanone                                              22.188000
## 2,3,3-Trimethyl-1-hexene                                   21.866882
## Pyrazine, 2-ethyl-6-methyl-                                20.453168
## Benzyl methyl ketone                                       20.014822
## 2-Nonanone                                                 19.879910
## 2-Dodecanone                                               18.607029
## 2,4,6-Cycloheptatrien-1-one                                18.074959
## 2-Nonanol                                                  17.528859
## Undecanal                                                  17.455600
## Cyclohexasiloxane, dodecamethyl-                           16.923057
## Butylated Hydroxytoluene                                   16.459986
## Benzyl nitrile                                             13.929395
## 2,4-Di-tert-butylphenol                                    13.744268
## Nonadecane                                                 12.512829
## Benzophenone                                               12.411470
## 2-Heptanone, 6-methyl-                                     10.008527
## Quinoline, 3-methyl-                                        9.890774
## Dodecanal                                                   9.659568
## 1-Nonanol                                                   8.933027
## 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester     8.675340
## 2-Heptanone, 5-methyl-                                      8.242499
## Benzothiazole                                               7.931774
## Benzene, 3-cyclohexen-1-yl-                                 5.750193
## Quinoline, 4-methyl-                                        5.396281
## 2-Decanol                                                   5.331696
## Benzene, 1-chloro-2-methoxy-                                4.393618
```

```
#Cluster
vol.df <- vol.df[,2:4]
vol.m <- as.matrix(vol.df)
vol.dendro <- as.dendrogram(hclust(d = dist(x=vol.m)))
dendro.plot <- ggdendrogram(data=vol.dendro, rotate = TRUE)
dendro.plot
```




```
pdf("RSI_over85_average_vol_dendro.pdf")
dendro.plot
dev.off()
```

```
## pdf
##   2
```

```
#Heatmap
vol.long <- melt(vol.m)
vol.long
```

```
##                                                  Var1
## 1                                      2-Undecanone
## 2                  Cyclotetrasiloxane, octamethyl-
## 3                             Diethyl Phthalate
## 4                                  Acetophenone
## 5                  Cyclopentasiloxane, decamethyl-
## 6                                  Benzyl alcohol
## 7                  Pyrazine, 3-ethyl-2,5-dimethyl-
## 8                            1-Hexanol, 2-ethyl-
## 9                                    2-Undecanol
## 10                                       Styrene
## 11                 Ethanone, 1-(1H-pyrrol-2-yl)-
## 12                                   Caprolactam
## 13                        2,4,4-Trimethyl-1-hexene
```

```
## 14                                          Benzaldehyde
## 15                                       Dibutyl phthalate
## 16                                        2-Acetylthiazole
## 17                                           2-Tridecanone
## 18                                  2,3,3-Trimethyl-1-hexene
## 19                                Pyrazine, 2-ethyl-6-methyl-
## 20                                       Benzyl methyl ketone
## 21                                            2-Nonanone
## 22                                           2-Dodecanone
## 23                                2,4,6-Cycloheptatrien-1-one
## 24                                            2-Nonanol
## 25                                            Undecanal
## 26                              Cyclohexasiloxane, dodecamethyl-
## 27                                      Butylated Hydroxytoluene
## 28                                          Benzyl nitrile
## 29                                 2,4-Di-tert-butylphenol
## 30                                           Nonadecane
## 31                                          Benzophenone
## 32                                  2-Heptanone, 6-methyl-
## 33                                    Quinoline, 3-methyl-
## 34                                            Dodecanal
## 35                                            1-Nonanol
## 36  1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester
## 37                                       2-Heptanone, 5-methyl-
## 38                                           Benzothiazole
## 39                                Benzene, 3-cyclohexen-1-yl-
## 40                                       Quinoline, 4-methyl-
## 41                                            2-Decanol
## 42                                Benzene, 1-chloro-2-methoxy-
## 43                                           2-Undecanone
## 44                               Cyclotetrasiloxane, octamethyl-
## 45                                        Diethyl Phthalate
## 46                                           Acetophenone
## 47                               Cyclopentasiloxane, decamethyl-
## 48                                         Benzyl alcohol
## 49                               Pyrazine, 3-ethyl-2,5-dimethyl-
## 50                                    1-Hexanol, 2-ethyl-
## 51                                           2-Undecanol
## 52                                               Styrene
## 53                                 Ethanone, 1-(1H-pyrrol-2-yl)-
## 54                                           Caprolactam
## 55                                2,4,4-Trimethyl-1-hexene
## 56                                          Benzaldehyde
## 57                                       Dibutyl phthalate
## 58                                        2-Acetylthiazole
## 59                                           2-Tridecanone
## 60                                  2,3,3-Trimethyl-1-hexene
## 61                                Pyrazine, 2-ethyl-6-methyl-
## 62                                       Benzyl methyl ketone
## 63                                            2-Nonanone
## 64                                           2-Dodecanone
## 65                                2,4,6-Cycloheptatrien-1-one
## 66                                            2-Nonanol
## 67                                            Undecanal
```

```
## 68                           Cyclohexasiloxane, dodecamethyl-
## 69                                   Butylated Hydroxytoluene
## 70                                            Benzyl nitrile
## 71                                    2,4-Di-tert-butylphenol
## 72                                                Nonadecane
## 73                                               Benzophenone
## 74                                    2-Heptanone, 6-methyl-
## 75                                      Quinoline, 3-methyl-
## 76                                                Dodecanal
## 77                                                1-Nonanol
## 78  1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester
## 79                                    2-Heptanone, 5-methyl-
## 80                                               Benzothiazole
## 81                               Benzene, 3-cyclohexen-1-yl-
## 82                                      Quinoline, 4-methyl-
## 83                                                2-Decanol
## 84                               Benzene, 1-chloro-2-methoxy-
## 85                                               2-Undecanone
## 86                            Cyclotetrasiloxane, octamethyl-
## 87                                         Diethyl Phthalate
## 88                                               Acetophenone
## 89                            Cyclopentasiloxane, decamethyl-
## 90                                            Benzyl alcohol
## 91                            Pyrazine, 3-ethyl-2,5-dimethyl-
## 92                                  1-Hexanol, 2-ethyl-
## 93                                               2-Undecanol
## 94                                                   Styrene
## 95                             Ethanone, 1-(1H-pyrrol-2-yl)-
## 96                                                Caprolactam
## 97                                 2,4,4-Trimethyl-1-hexene
## 98                                            Benzaldehyde
## 99                                         Dibutyl phthalate
## 100                                         2-Acetylthiazole
## 101                                            2-Tridecanone
## 102                                2,3,3-Trimethyl-1-hexene
## 103                              Pyrazine, 2-ethyl-6-methyl-
## 104                                    Benzyl methyl ketone
## 105                                              2-Nonanone
## 106                                             2-Dodecanone
## 107                               2,4,6-Cycloheptatrien-1-one
## 108                                               2-Nonanol
## 109                                               Undecanal
## 110                          Cyclohexasiloxane, dodecamethyl-
## 111                                  Butylated Hydroxytoluene
## 112                                           Benzyl nitrile
## 113                                   2,4-Di-tert-butylphenol
## 114                                               Nonadecane
## 115                                              Benzophenone
## 116                                   2-Heptanone, 6-methyl-
## 117                                     Quinoline, 3-methyl-
## 118                                               Dodecanal
## 119                                               1-Nonanol
## 120 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester
## 121                                   2-Heptanone, 5-methyl-
```

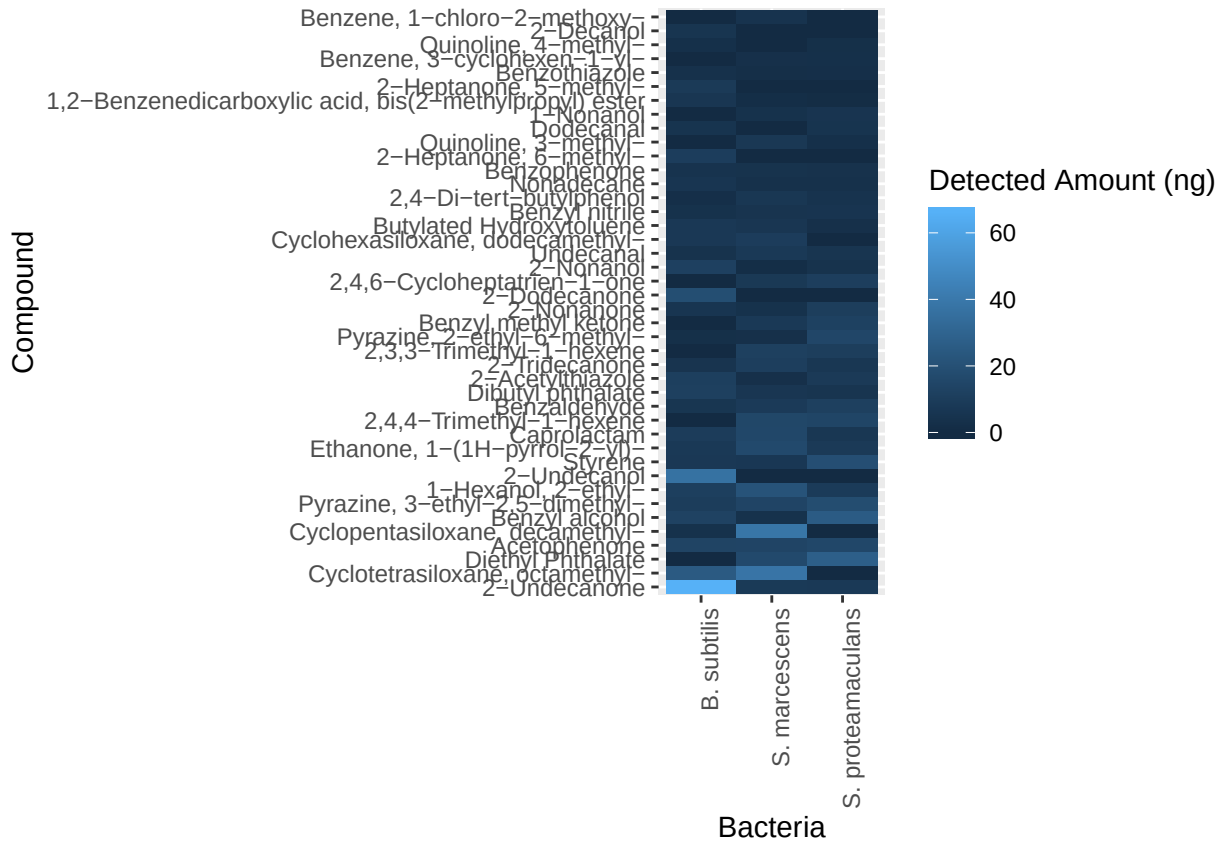
```
## 122                                        Benzothiazole
## 123                              Benzene, 3-cyclohexen-1-yl-
## 124                                    Quinoline, 4-methyl-
## 125                                               2-Decanol
## 126                              Benzene, 1-chloro-2-methoxy-
##                  Var2     value
## 1         B. subtilis 65.788334
## 2         B. subtilis 24.861569
## 3         B. subtilis  0.000000
## 4         B. subtilis 13.443900
## 5         B. subtilis  3.645482
## 6         B. subtilis 12.743759
## 7         B. subtilis  9.806626
## 8         B. subtilis 10.881896
## 9         B. subtilis 36.485114
## 10        B. subtilis  7.394190
## 11        B. subtilis  7.724929
## 12        B. subtilis  9.401807
## 13        B. subtilis  0.000000
## 14        B. subtilis  5.889882
## 15        B. subtilis 11.350734
## 16        B. subtilis 11.015745
## 17        B. subtilis  4.965275
## 18        B. subtilis  0.000000
## 19        B. subtilis  2.699596
## 20        B. subtilis  0.000000
## 21        B. subtilis  5.743211
## 22        B. subtilis 18.607029
## 23        B. subtilis  0.000000
## 24        B. subtilis 11.698919
## 25        B. subtilis  4.312549
## 26        B. subtilis  7.304148
## 27        B. subtilis  7.314342
## 28        B. subtilis  3.652833
## 29        B. subtilis  2.401032
## 30        B. subtilis  5.813875
## 31        B. subtilis  4.361363
## 32        B. subtilis 10.008527
## 33        B. subtilis  0.000000
## 34        B. subtilis  4.828842
## 35        B. subtilis  0.000000
## 36        B. subtilis  6.059075
## 37        B. subtilis  8.242499
## 38        B. subtilis  3.413640
## 39        B. subtilis  0.000000
## 40        B. subtilis  2.725803
## 41        B. subtilis  5.331696
## 42        B. subtilis  0.000000
## 43      S. marcescens  8.103901
## 44      S. marcescens 37.807927
## 45      S. marcescens 16.351702
## 46      S. marcescens 13.548946
## 47      S. marcescens 38.389940
## 48      S. marcescens  3.739744
```

```
## 49      S. marcescens 13.550469
## 50      S. marcescens 21.279233
## 51      S. marcescens  0.000000
## 52      S. marcescens  6.827112
## 53      S. marcescens 16.389580
## 54      S. marcescens 15.127583
## 55      S. marcescens 14.948664
## 56      S. marcescens  8.540497
## 57      S. marcescens  6.381384
## 58      S. marcescens  2.963814
## 59      S. marcescens 10.503033
## 60      S. marcescens 11.546623
## 61      S. marcescens  2.963037
## 62      S. marcescens  7.759105
## 63      S. marcescens  3.779451
## 64      S. marcescens  0.000000
## 65      S. marcescens  7.508897
## 66      S. marcescens  1.586398
## 67      S. marcescens  7.689498
## 68      S. marcescens  9.618909
## 69      S. marcescens  6.266743
## 70      S. marcescens  4.989917
## 71      S. marcescens  6.625763
## 72      S. marcescens  3.483712
## 73      S. marcescens  4.192673
## 74      S. marcescens  0.000000
## 75      S. marcescens  7.164959
## 76      S. marcescens  0.000000
## 77      S. marcescens  3.756624
## 78      S. marcescens  1.599047
## 79      S. marcescens  0.000000
## 80      S. marcescens  2.066972
## 81      S. marcescens  3.036559
## 82      S. marcescens  0.000000
## 83      S. marcescens  0.000000
## 84      S. marcescens  4.393618
## 85  S. proteamaculans  7.610332
## 86  S. proteamaculans  0.000000
## 87  S. proteamaculans 27.265811
## 88  S. proteamaculans 15.249631
## 89  S. proteamaculans  0.000000
## 90  S. proteamaculans 25.373854
## 91  S. proteamaculans 18.062958
## 92  S. proteamaculans  8.883402
## 93  S. proteamaculans  0.000000
## 94  S. proteamaculans 18.979317
## 95  S. proteamaculans  8.157120
## 96  S. proteamaculans  6.640843
## 97  S. proteamaculans 13.960901
## 98  S. proteamaculans 11.501003
## 99  S. proteamaculans  5.569892
## 100 S. proteamaculans  8.381929
## 101 S. proteamaculans  6.719692
## 102 S. proteamaculans 10.320259
```

```
## 103 S. proteamaculans 14.790536
## 104 S. proteamaculans 12.255717
## 105 S. proteamaculans 10.357248
## 106 S. proteamaculans  0.000000
## 107 S. proteamaculans 10.566061
## 108 S. proteamaculans  4.243541
## 109 S. proteamaculans  5.453554
## 110 S. proteamaculans  0.000000
## 111 S. proteamaculans  2.878902
## 112 S. proteamaculans  5.286645
## 113 S. proteamaculans  4.717473
## 114 S. proteamaculans  3.215243
## 115 S. proteamaculans  3.857433
## 116 S. proteamaculans  0.000000
## 117 S. proteamaculans  2.725815
## 118 S. proteamaculans  4.830726
## 119 S. proteamaculans  5.176402
## 120 S. proteamaculans  1.017218
## 121 S. proteamaculans  0.000000
## 122 S. proteamaculans  2.451162
## 123 S. proteamaculans  2.713634
## 124 S. proteamaculans  2.670478
## 125 S. proteamaculans  0.000000
## 126 S. proteamaculans  0.000000
```

```
vol.heatmap <- ggplot(data = vol.long, mapping = aes(x = Var2, y = Var1, fill = value)) +
  geom_tile() + xlab(label = "Bacteria") +  ylab("Compound") +
  labs(fill = "Detected Amount (ng)") + theme(axis.text.x = element_text(angle = 90, hjust = 1))

vol.heatmap
```




```
pdf("RSI_over85_average_vol_heat.pdf", height = 32, width = 12)
vol.heatmap
dev.off()
```

```
## pdf
##   2
```

```
#HIGH Heat

#Grab and shape data
vol <- read_excel("data.xlsx", sheet = "Heatmap_4_high")
vol.df <- as.data.frame(vol)
vol.df
```

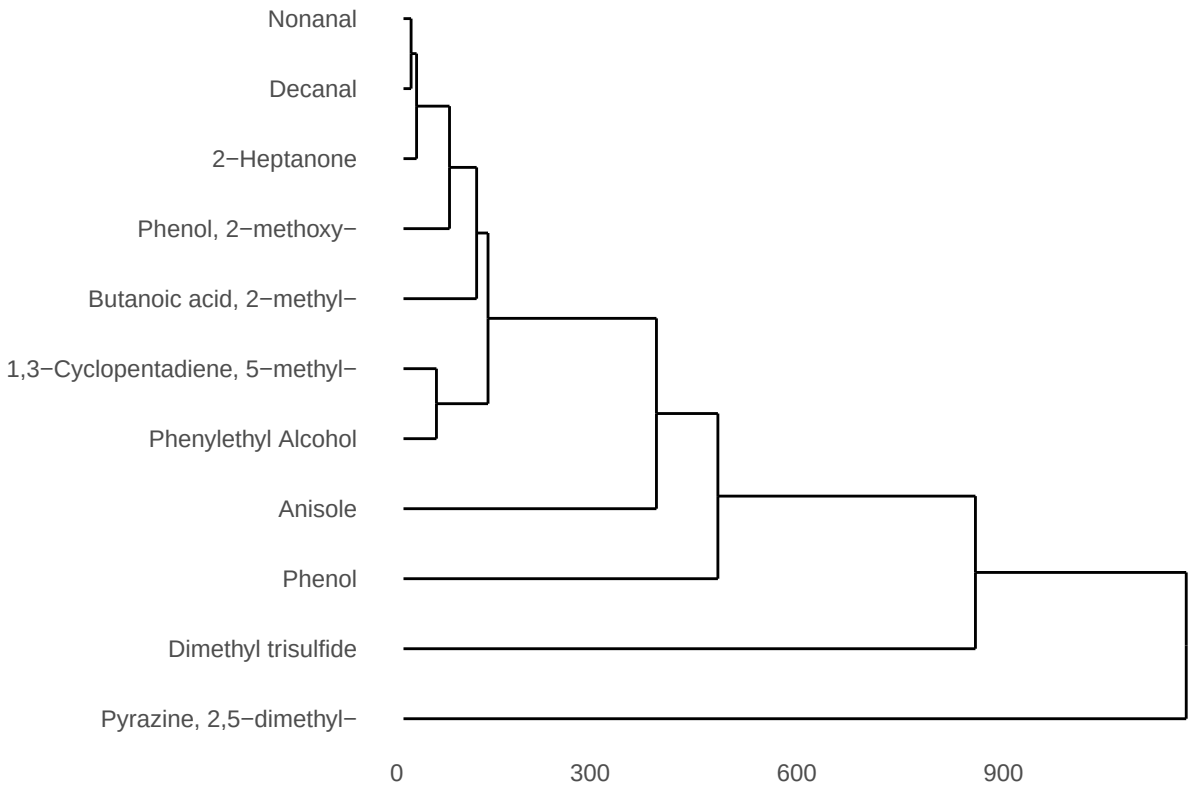
```
##                          Volatile B. subtilis S. marcescens
## 1         Pyrazine, 2,5-dimethyl-   134.71293     881.27653
## 2                          Phenol    67.72702     359.74353
## 3             Dimethyl trisulfide     0.00000      31.52681
## 4                          Anisole     0.00000     416.56834
## 5             Phenylethyl Alcohol    18.85410     107.26457
## 6        Butanoic acid, 2-methyl-   100.60116      85.51390
## 7  1,3-Cyclopentadiene, 5-methyl-     0.00000      64.03001
## 8                          Decanal    18.49873      69.58014
## 9                          Nonanal    10.34142      65.42259
## 10                    2-Heptanone    21.60136      52.61435
```

```
## 11             Phenol, 2-methoxy-     0.00000      97.85141
##    S. proteamaculans        sum
## 1          812.13326 1828.12272
## 2          367.65654  795.12709
## 3          735.69743  767.22424
## 4            0.00000  416.56834
## 5          106.39582  232.51449
## 6           31.61349  217.72855
## 7           98.48953  162.51953
## 8           52.11414  140.19301
## 9           46.00378  121.76779
## 10          44.14306  118.35877
## 11           0.00000   97.85141
```

```
rownames(vol.df) <- vol$Volatile
vol.df
```

```
##                                                 Volatile B. subtilis
## Pyrazine, 2,5-dimethyl-               Pyrazine, 2,5-dimethyl-   134.71293
## Phenol                                              Phenol    67.72702
## Dimethyl trisulfide                    Dimethyl trisulfide     0.00000
## Anisole                                             Anisole     0.00000
## Phenylethyl Alcohol                   Phenylethyl Alcohol    18.85410
## Butanoic acid, 2-methyl-             Butanoic acid, 2-methyl-   100.60116
## 1,3-Cyclopentadiene, 5-methyl- 1,3-Cyclopentadiene, 5-methyl-     0.00000
## Decanal                                             Decanal    18.49873
## Nonanal                                             Nonanal    10.34142
## 2-Heptanone                                      2-Heptanone    21.60136
## Phenol, 2-methoxy-                    Phenol, 2-methoxy-     0.00000
##                                 S. marcescens S. proteamaculans        sum
## Pyrazine, 2,5-dimethyl-             881.27653         812.13326 1828.12272
## Phenol                              359.74353         367.65654  795.12709
## Dimethyl trisulfide                  31.52681         735.69743  767.22424
## Anisole                             416.56834           0.00000  416.56834
## Phenylethyl Alcohol                 107.26457         106.39582  232.51449
## Butanoic acid, 2-methyl-             85.51390          31.61349  217.72855
## 1,3-Cyclopentadiene, 5-methyl-       64.03001          98.48953  162.51953
## Decanal                              69.58014          52.11414  140.19301
## Nonanal                              65.42259          46.00378  121.76779
## 2-Heptanone                          52.61435          44.14306  118.35877
## Phenol, 2-methoxy-                   97.85141           0.00000   97.85141
```

```
#Cluster
vol.df <- vol.df[,2:4]
vol.m <- as.matrix(vol.df)
vol.dendro <- as.dendrogram(hclust(d = dist(x=vol.m)))
dendro.plot <- ggdendrogram(data=vol.dendro, rotate = TRUE)
dendro.plot
```




```
pdf("RSI_over85_high_vol_dendro.pdf")
dendro.plot
dev.off()
```

```
## pdf
##   2
```

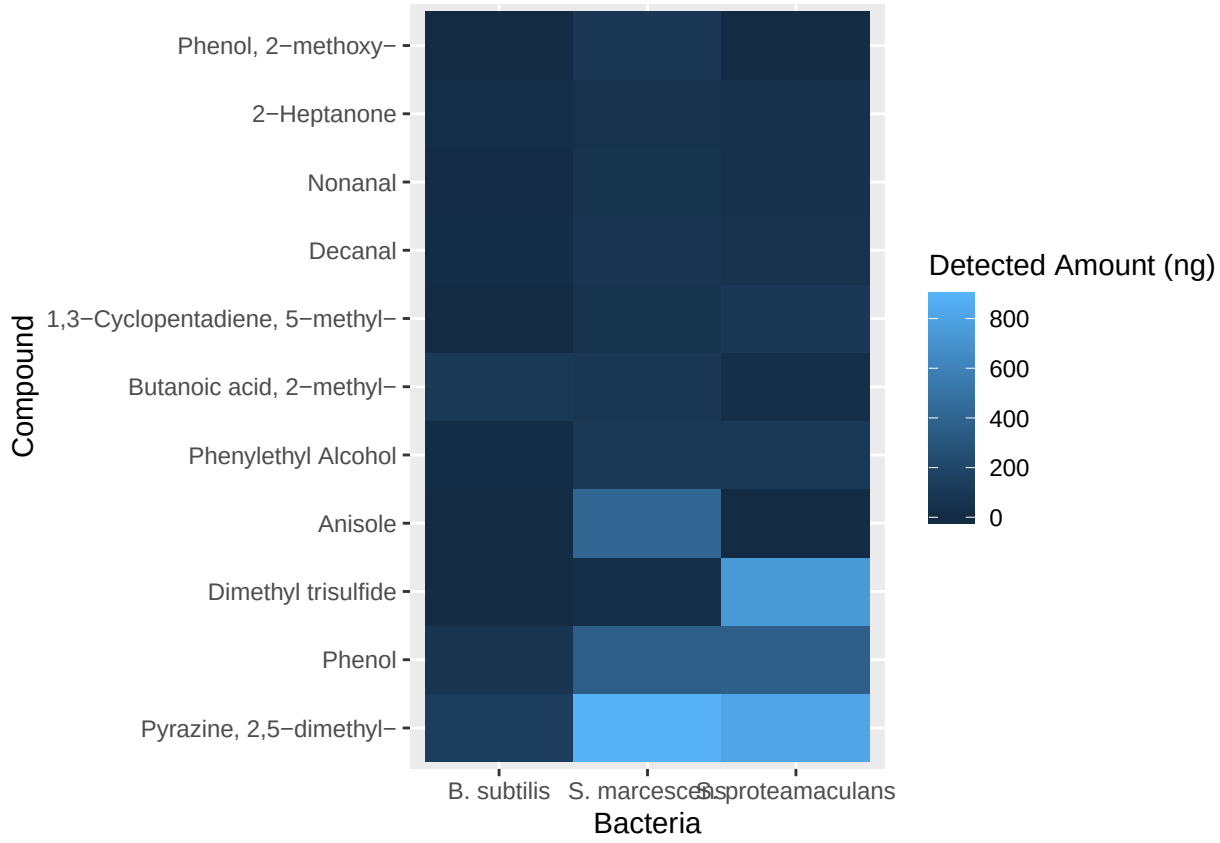
```
#Heatmap
vol.long <- melt(vol.m)
vol.long
```

```
##                              Var1             Var2     value
## 1         Pyrazine, 2,5-dimethyl-      B. subtilis 134.71293
## 2                          Phenol      B. subtilis  67.72702
## 3             Dimethyl trisulfide      B. subtilis   0.00000
## 4                         Anisole      B. subtilis   0.00000
## 5             Phenylethyl Alcohol      B. subtilis  18.85410
## 6        Butanoic acid, 2-methyl-      B. subtilis 100.60116
## 7  1,3-Cyclopentadiene, 5-methyl-      B. subtilis   0.00000
## 8                          Decanal      B. subtilis  18.49873
## 9                          Nonanal      B. subtilis  10.34142
## 10                    2-Heptanone      B. subtilis  21.60136
## 11             Phenol, 2-methoxy-      B. subtilis   0.00000
## 12        Pyrazine, 2,5-dimethyl-    S. marcescens 881.27653
## 13                         Phenol    S. marcescens 359.74353
```

```
## 14            Dimethyl trisulfide     S. marcescens  31.52681
## 15                        Anisole     S. marcescens 416.56834
## 16            Phenylethyl Alcohol     S. marcescens 107.26457
## 17       Butanoic acid, 2-methyl-     S. marcescens  85.51390
## 18 1,3-Cyclopentadiene, 5-methyl-     S. marcescens  64.03001
## 19                        Decanal     S. marcescens  69.58014
## 20                        Nonanal     S. marcescens  65.42259
## 21                     2-Heptanone     S. marcescens  52.61435
## 22             Phenol, 2-methoxy-     S. marcescens  97.85141
## 23        Pyrazine, 2,5-dimethyl- S. proteamaculans 812.13326
## 24                         Phenol S. proteamaculans 367.65654
## 25            Dimethyl trisulfide S. proteamaculans 735.69743
## 26                        Anisole S. proteamaculans   0.00000
## 27            Phenylethyl Alcohol S. proteamaculans 106.39582
## 28       Butanoic acid, 2-methyl- S. proteamaculans  31.61349
## 29 1,3-Cyclopentadiene, 5-methyl- S. proteamaculans  98.48953
## 30                        Decanal S. proteamaculans  52.11414
## 31                        Nonanal S. proteamaculans  46.00378
## 32                     2-Heptanone S. proteamaculans  44.14306
## 33             Phenol, 2-methoxy- S. proteamaculans   0.00000
```

```
vol.heatmap <- ggplot(data = vol.long, mapping = aes(x = Var2, y = Var1, fill = value)) +
  geom_tile() + xlab(label = "Bacteria") +  ylab("Compound") +
  labs(fill = "Detected Amount (ng)")

vol.heatmap
```



```
pdf("RSI_over85_high_vol_heat.pdf", height = 12, width = 10)
vol.heatmap
dev.off()
```

```
## pdf
##   2
```

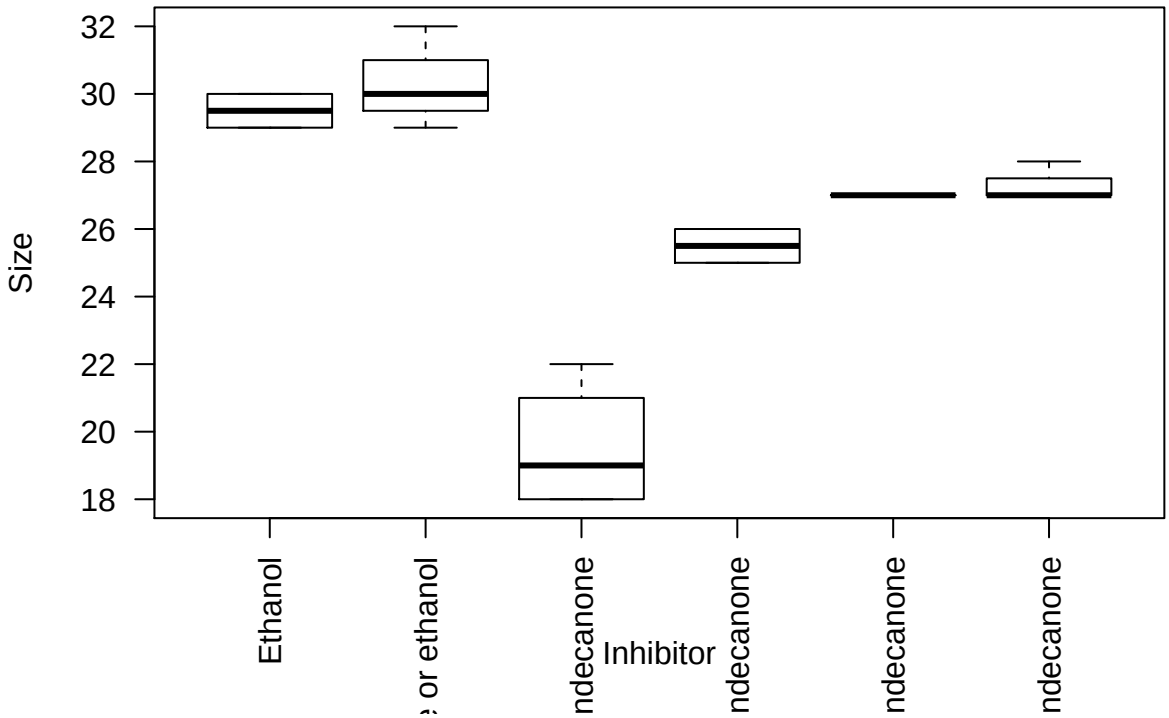
Pure volatiles from *Serratia marcescens* affect Zygomycetous fungi growth

```
# Pure volatile inhibition
#Get pure volatile assay data
Volatile <- read_excel("Volatile.xlsx", sheet = "Pure Volatiles Trial 2")
```

```
## New names:
## * `` -> ...3
## * `` -> ...4
## * `` -> ...5
## * `` -> ...6
```

```
Volatile.bk <- Volatile
#print(Volatile)
data.frame_volatile=as.data.frame(Volatile)
#print(data.frame_volatile)

# Pure Volatile, Ordering the names
names.data <- unique(Volatile.bk$Inhibitor)
Volatile$Inhibitor <- factor(Volatile.bk$Inhibitor, levels = names.data)
boxplot(Size ~ Inhibitor, Volatile, las=2)
```




```
bp = ggplot(Volatile, aes(x=Inhibitor, y=Size, fill=Inhibitor)) + geom_boxplot()
bp + coord_flip()
```

```
## Warning: Removed 16 rows containing non-finite values (stat_boxplot).
```

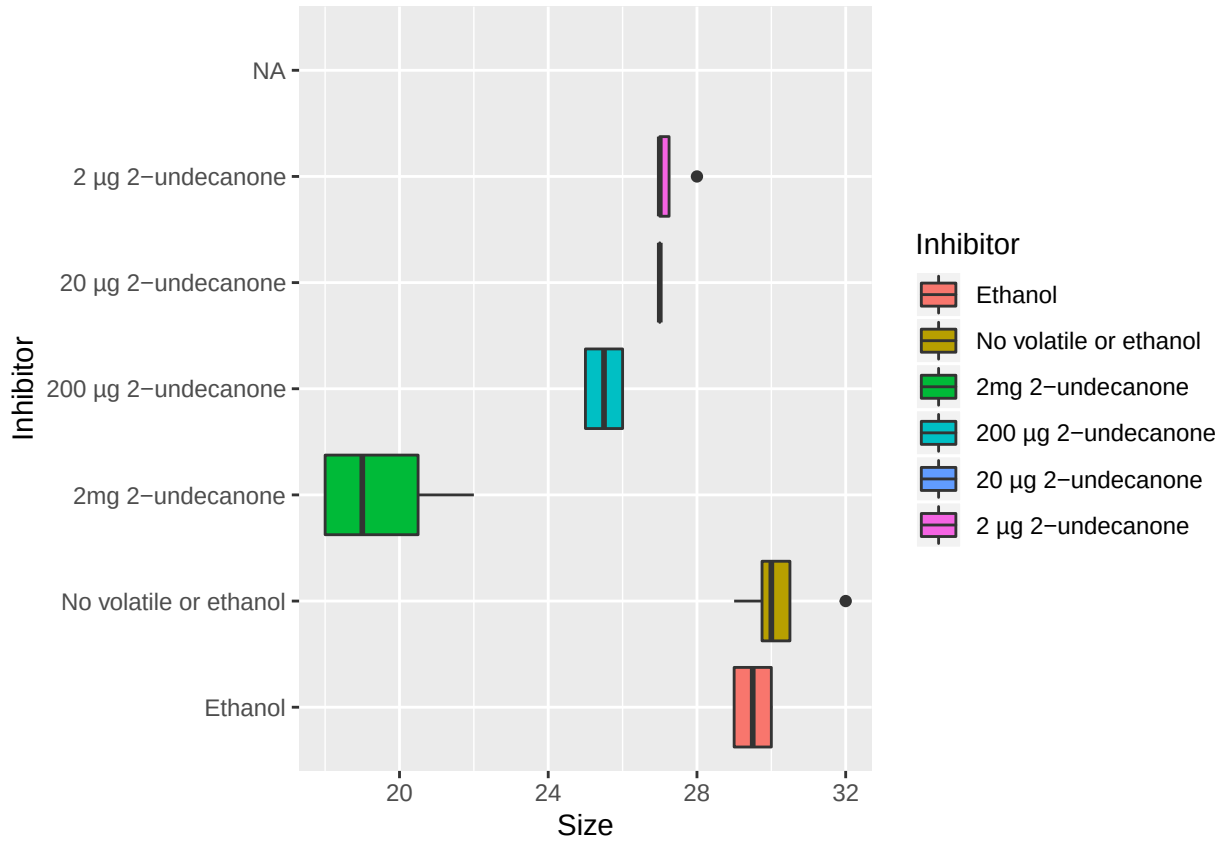


Figure 1c - Pure volatile inhibition R. stolonifer cultures exposed to pure volatiles 2-undecanone and Dimethyl Disulfide exhibited growth retardation

To test if volatiles could inhibit zygomycete growth we used 2-undecanone and dimethyl disulfide. Using 1000 R. stolonifer spores as initial inoculum, we added 2.5 µl of both 2-undecanone and dimethyl disulfide in serial dilutions. We found that blank was the EC50. Figure 2 - Inhibition assay.

```
library("ggplot2")
library("ggdendro")
library("reshape2")
library("grid")
library("readxl")
rm(list = ls())

#import tables and combine

#RSI is the number Kerry uses
Over85 <- read_excel("Volatile.xlsx", sheet = "RSI_Over85")
```

```
## New names:
## * `` -> ...5
## * `` -> ...6
```

```
volatiles <- Over85
#volatiles <- total
volatiles.bk <- volatiles
```

```
#RSI without unique individuals
NUOver85 <- read_excel("Volatile.xlsx", sheet = "RSI_Over85_nounique")
volatiles <- NUOver85
#volatiles <- total
volatiles.bk <- volatiles


# Run clustering
volatiles.matrix <- as.matrix(volatiles)
#head(volatiles.matrix)
rownames(volatiles.matrix) <- volatiles$Sample

#table optional (doesn't consider amounts)
volatiles.table <- dcast(volatiles, Sample ~ variable)
```

```
## Aggregation function missing: defaulting to length
```

```
volatiles.table
```

```
##                    Sample 1-Decanol 1-Hexanol 1-Hexanol, 2-ethyl-
## 1   Bacillus_subt_A_7-5-18         0         0                    1
## 2   Bacillus_subt_B_7-5-18         0         0                    1
## 3   Bacillus_subt_C_7-5-18         0         0                    1
## 4   Bacillus_subt_D_7-9-18         0         0                    1
## 5   Bacillus_subt_E_7-9-18         0         0                    0
## 6   Bacillus_subt_F_7-9-18         0         0                    0
## 7   Bacillus_subt_G_7-9-18         0         0                    1
## 8   Bacillus_subt_H_7-9-18         0         0                    0
## 9   Bacillus_subt_I_7-9-18         0         0                    1
## 10          RED-A_2-14-18         0         0                    1
## 11          RED-B_2-14-18         0         0                    1
## 12          RED-C_2-14-18         0         0                    0
## 13          RED-D_2-15-18         0         0                    0
## 14          RED-E_2-15-18         0         0                    0
## 15          RED-F_2-15-18         0         0                    0
## 16          RED-G_2-16-18         0         0                    0
## 17          RED-H_2-16-18         0         0                    0
## 18          RED-I_2-16-18         0         0                    1
## 19          WHT-A_2-14-18         0         0                    1
## 20          WHT-B_2-14-18         0         1                    1
## 21          WHT-C_2-14-18         0         0                    1
## 22          WHT-D_2-15-18         1         1                    0
## 23          WHT-E_2-15-18         1         0                    0
## 24          WHT-F_2-15-18         1         0                    0
## 25          WHT-G_2-16-18         1         0                    0
## 26          WHT-H_2-16-18         0         0                    0
##    1-Isoquinolinecarbonitrile 1-Nonanol 1-Phenyl-2-propanone 1-Undecanol
## 1                           0         0                    0           0
## 2                           0         0                    0           0
## 3                           0         0                    0           0
## 4                           0         0                    0           0
## 5                           0         0                    0           0
```

```
## 6                          1         0                    0           0
## 7                          0         0                    0           0
## 8                          1         0                    0           0
## 9                          0         0                    0           0
## 10                         0         1                    1           0
## 11                         0         1                    1           0
## 12                         0         1                    1           0
## 13                         0         0                    0           0
## 14                         0         0                    0           0
## 15                         0         0                    0           0
## 16                         0         1                    0           0
## 17                         0         1                    1           0
## 18                         0         0                    0           0
## 19                         0         0                    1           0
## 20                         0         1                    0           0
## 21                         0         1                    1           1
## 22                         0         1                    0           0
## 23                         0         1                    0           0
## 24                         0         0                    0           0
## 25                         0         1                    0           0
## 26                         0         0                    0           0
##    1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester
## 1                                                        0
## 2                                                        1
## 3                                                        1
## 4                                                        0
## 5                                                        1
## 6                                                        1
## 7                                                        0
## 8                                                        1
## 9                                                        0
## 10                                                       0
## 11                                                       1
## 12                                                       0
## 13                                                       0
## 14                                                       0
## 15                                                       0
## 16                                                       0
## 17                                                       0
## 18                                                       0
## 19                                                       0
## 20                                                       0
## 21                                                       0
## 22                                                       0
## 23                                                       0
## 24                                                       0
## 25                                                       1
## 26                                                       0
##    1,2-Benzisothiazole 1,3-Cyclopentadiene, 5-methyl-
## 1                    0                              0
## 2                    0                              0
## 3                    0                              0
## 4                    1                              0
## 5                    0                              0
```

```
## 6                    1                           0
## 7                    0                           0
## 8                    0                           0
## 9                    0                           0
## 10                   0                           1
## 11                   0                           1
## 12                   1                           1
## 13                   0                           0
## 14                   0                           1
## 15                   0                           0
## 16                   0                           0
## 17                   0                           1
## 18                   1                           2
## 19                   0                           0
## 20                   0                           0
## 21                   0                           0
## 22                   1                           0
## 23                   0                           0
## 24                   0                           0
## 25                   0                           2
## 26                   1                           0
##    1,3,5-Cycloheptatriene, 1-methoxy- 1,3,5,7-Cyclooctatetraene
## 1                                   0                         0
## 2                                   0                         1
## 3                                   0                         0
## 4                                   0                         0
## 5                                   0                         1
## 6                                   0                         0
## 7                                   0                         0
## 8                                   0                         0
## 9                                   0                         0
## 10                                  0                         0
## 11                                  0                         0
## 12                                  0                         1
## 13                                  0                         1
## 14                                  0                         0
## 15                                  0                         0
## 16                                  0                         0
## 17                                  1                         1
## 18                                  1                         1
## 19                                  0                         1
## 20                                  0                         1
## 21                                  0                         0
## 22                                  0                         0
## 23                                  0                         0
## 24                                  0                         1
## 25                                  0                         0
## 26                                  0                         0
##    2-(3-Methylbutyl)-3,5-dimethylpyrazine 2-Acetylthiazole
## 1                                       0                1
## 2                                       0                1
## 3                                       0                1
## 4                                       0                1
## 5                                       0                1
```

```
## 6                                       1               1
## 7                                       0               1
## 8                                       0               1
## 9                                       0               1
## 10                                      0               0
## 11                                      0               0
## 12                                      0               0
## 13                                      0               0
## 14                                      0               0
## 15                                      0               0
## 16                                      0               0
## 17                                      0               0
## 18                                      0               1
## 19                                      0               0
## 20                                      0               1
## 21                                      0               1
## 22                                      0               0
## 23                                      0               0
## 24                                      0               0
## 25                                      0               1
## 26                                      0               0
##    2-Butenoic acid, 2-methyl-, (Z)- 2-Decanol 2-Decanone 2-Dodecanol
## 1                                 0         0          0           0
## 2                                 0         2          1           1
## 3                                 0         2          1           2
## 4                                 0         1          0           0
## 5                                 0         0          1           0
## 6                                 1         3          0           1
## 7                                 0         0          0           0
## 8                                 1         3          1           1
## 9                                 0         0          0           0
## 10                                0         0          0           0
## 11                                0         0          0           0
## 12                                0         0          0           0
## 13                                0         0          0           0
## 14                                0         0          0           0
## 15                                0         0          0           0
## 16                                0         0          0           0
## 17                                0         0          0           0
## 18                                0         0          0           0
## 19                                0         0          0           0
## 20                                0         0          0           0
## 21                                0         0          0           0
## 22                                0         0          1           0
## 23                                0         0          0           0
## 24                                0         0          0           0
## 25                                0         0          0           0
## 26                                0         0          0           0
##    2-Dodecanone 2-Ethyl-1-hexanol 2-Heptanone 2-Heptanone, 4-methyl-
## 1             2                 0           0                      0
## 2             3                 0           1                      1
## 3             4                 0           1                      1
## 4             1                 0           1                      0
## 5             3                 1           0                      1
```

```
## 6             3                 1           1                     0
## 7             0                 0           0                     0
## 8             5                 1           0                     1
## 9             1                 0           0                     0
## 10            0                 0           1                     0
## 11            0                 0           1                     0
## 12            0                 1           0                     0
## 13            0                 0           0                     0
## 14            0                 0           1                     0
## 15            0                 0           0                     0
## 16            0                 0           0                     0
## 17            0                 0           1                     0
## 18            0                 0           1                     0
## 19            0                 0           0                     0
## 20            0                 0           1                     0
## 21            0                 0           1                     0
## 22            0                 0           1                     0
## 23            0                 0           0                     0
## 24            0                 0           0                     0
## 25            0                 0           1                     0
## 26            0                 0           0                     0
##    2-Heptanone, 5-methyl- 2-Heptanone, 6-methyl-
## 1                       0                     0
## 2                       1                     1
## 3                       1                     1
## 4                       1                     1
## 5                       0                     1
## 6                       1                     1
## 7                       0                     0
## 8                       1                     1
## 9                       0                     0
## 10                      0                     0
## 11                      0                     0
## 12                      0                     0
## 13                      0                     0
## 14                      0                     0
## 15                      0                     0
## 16                      0                     0
## 17                      0                     0
## 18                      0                     0
## 19                      0                     0
## 20                      0                     0
## 21                      0                     0
## 22                      0                     0
## 23                      0                     0
## 24                      0                     0
## 25                      0                     0
## 26                      0                     0
##    2-Methyl-3-isopropylpyrazine 2-Nonanol 2-Nonanone
## 1                             0         1          1
## 2                             0         1          1
## 3                             0         1          1
## 4                             0         1          1
## 5                             0         1          1
```

```
## 6                              1         1          1
## 7                              0         0          0
## 8                              0         1          1
## 9                              0         0          0
## 10                             0         0          0
## 11                             0         1          1
## 12                             0         0          0
## 13                             0         0          0
## 14                             1         0          0
## 15                             0         0          0
## 16                             0         0          0
## 17                             0         0          0
## 18                             0         0          0
## 19                             0         0          0
## 20                             0         0          1
## 21                             0         0          0
## 22                             0         1          0
## 23                             1         0          0
## 24                             0         0          0
## 25                             0         1          1
## 26                             0         0          0
##    2-Pentadecanone, 6,10,14-trimethyl- 2-Pyrrolidinone, 1-methyl-
## 1                                    0                          0
## 2                                    1                          0
## 3                                    1                          0
## 4                                    0                          0
## 5                                    1                          0
## 6                                    0                          0
## 7                                    0                          0
## 8                                    1                          0
## 9                                    0                          0
## 10                                   0                          0
## 11                                   0                          1
## 12                                   0                          0
## 13                                   0                          0
## 14                                   0                          0
## 15                                   0                          0
## 16                                   0                          0
## 17                                   0                          0
## 18                                   0                          0
## 19                                   0                          1
## 20                                   0                          0
## 21                                   0                          0
## 22                                   0                          0
## 23                                   0                          0
## 24                                   0                          0
## 25                                   0                          0
## 26                                   0                          0
##    2-Tetradecanol 2-Tridecanone 2-Undecanol 2-Undecanone
## 1               0             1           1            1
## 2               0             1           1            1
## 3               0             1           1            1
## 4               0             0           1            1
## 5               0             1           2            1
```

```
## 6               1             2           2            1
## 7               0             1           1            1
## 8               1             1           2            1
## 9               0             0           1            1
## 10              0             1           0            1
## 11              0             1           0            1
## 12              0             1           0            0
## 13              0             0           0            0
## 14              0             1           0            1
## 15              0             0           0            0
## 16              0             0           0            0
## 17              0             1           0            1
## 18              0             1           0            1
## 19              0             0           0            1
## 20              0             1           0            1
## 21              0             1           0            0
## 22              0             1           0            1
## 23              0             0           0            1
## 24              0             0           0            1
## 25              0             1           0            1
## 26              0             1           0            1
##    2,3,3-Trimethyl-1-hexene 2,4-Di-tert-butylphenol
## 1                         0                       1
## 2                         0                       1
## 3                         0                       1
## 4                         0                       0
## 5                         0                       0
## 6                         0                       0
## 7                         0                       0
## 8                         0                       0
## 9                         0                       0
## 10                        0                       0
## 11                        0                       0
## 12                        0                       0
## 13                        1                       0
## 14                        0                       1
## 15                        0                       0
## 16                        1                       0
## 17                        0                       1
## 18                        0                       0
## 19                        1                       1
## 20                        1                       1
## 21                        1                       1
## 22                        0                       1
## 23                        0                       1
## 24                        1                       0
## 25                        0                       1
## 26                        1                       1
##    2,4,4-Trimethyl-1-hexene 2,4,6-Cycloheptatrien-1-one
## 1                         0                           0
## 2                         0                           0
## 3                         0                           0
## 4                         0                           0
## 5                         0                           0
```

```
## 6                        0                          0
## 7                        0                          0
## 8                        0                          0
## 9                        0                          0
## 10                       1                          1
## 11                       0                          1
## 12                       0                          1
## 13                       2                          0
## 14                       1                          1
## 15                       0                          0
## 16                       2                          0
## 17                       0                          1
## 18                       2                          1
## 19                       1                          1
## 20                       1                          1
## 21                       2                          1
## 22                       1                          1
## 23                       2                          1
## 24                       2                          1
## 25                       1                          1
## 26                       2                          1
##    3-Aminoacetophenone 3-Penten-1-ol, 2,2,4-trimethyl-
## 1                    0                                0
## 2                    0                                0
## 3                    0                                0
## 4                    0                                0
## 5                    0                                0
## 6                    0                                0
## 7                    0                                0
## 8                    0                                0
## 9                    0                                0
## 10                   0                                0
## 11                   0                                0
## 12                   1                                0
## 13                   0                                0
## 14                   1                                1
## 15                   0                                0
## 16                   0                                0
## 17                   0                                0
## 18                   0                                0
## 19                   0                                0
## 20                   0                                0
## 21                   0                                0
## 22                   1                                0
## 23                   1                                0
## 24                   0                                0
## 25                   1                                0
## 26                   1                                0
##    4,8,12,16-tetraoxaeicosan-1-ol 5-Decen-1-ol, acetate, (E)-
## 1                               0                           0
## 2                               0                           0
## 3                               0                           0
## 4                               0                           0
## 5                               0                           0
```

```
## 6                                0                                0
## 7                                0                                0
## 8                                0                                0
## 9                                0                                0
## 10                               0                                0
## 11                               0                                0
## 12                               0                                0
## 13                               0                                0
## 14                               0                                1
## 15                               0                                0
## 16                               1                                0
## 17                               0                                1
## 18                               1                                0
## 19                               0                                0
## 20                               0                                0
## 21                               0                                0
## 22                               0                                0
## 23                               0                                1
## 24                               0                                0
## 25                               1                                0
## 26                               1                                0
##    5-Hepten-2-one, 6-methyl- 5-Isoquinolinecarbonitrile
## 1                          0                          0
## 2                          1                          0
## 3                          1                          0
## 4                          0                          0
## 5                          0                          1
## 6                          1                          0
## 7                          0                          0
## 8                          1                          0
## 9                          0                          0
## 10                         0                          0
## 11                         0                          0
## 12                         0                          0
## 13                         1                          0
## 14                         1                          0
## 15                         0                          0
## 16                         1                          0
## 17                         0                          0
## 18                         0                          0
## 19                         0                          0
## 20                         0                          0
## 21                         0                          0
## 22                         0                          0
## 23                         1                          0
## 24                         0                          0
## 25                         0                          0
## 26                         0                          0
##    5,9-Undecadien-2-one, 6,10-dimethyl-
## 1                                     0
## 2                                     1
## 3                                     0
## 4                                     0
## 5                                     0
```

```
## 6                                      1
## 7                                      0
## 8                                      1
## 9                                      0
## 10                                     0
## 11                                     1
## 12                                     0
## 13                                     0
## 14                                     0
## 15                                     0
## 16                                     0
## 17                                     1
## 18                                     1
## 19                                     0
## 20                                     0
## 21                                     1
## 22                                     1
## 23                                     0
## 24                                     0
## 25                                     1
## 26                                     0
##    5,9-Undecadien-2-one, 6,10-dimethyl-, (E)- 9H-Fluorene, 9-methylene-
## 1                                           0                         0
## 2                                           0                         0
## 3                                           0                         0
## 4                                           1                         0
## 5                                           0                         0
## 6                                           0                         0
## 7                                           0                         0
## 8                                           0                         1
## 9                                           0                         0
## 10                                          0                         0
## 11                                          0                         0
## 12                                          0                         0
## 13                                          0                         0
## 14                                          1                         0
## 15                                          0                         0
## 16                                          0                         0
## 17                                          0                         0
## 18                                          0                         0
## 19                                          0                         0
## 20                                          0                         0
## 21                                          0                         0
## 22                                          0                         0
## 23                                          0                         0
## 24                                          0                         0
## 25                                          0                         1
## 26                                          0                         0
##    Acetophenone Anisole Benzaldehyde Benzaldehyde, 3-ethyl-
## 1             1       0            0                      0
## 2             1       0            0                      0
## 3             1       0            1                      0
## 4             1       0            1                      0
## 5             1       0            1                      0
```

```
## 6             1       0           0                     0
## 7             1       0           0                     0
## 8             1       0           1                     0
## 9             1       0           0                     0
## 10            1       1           1                     0
## 11            1       1           0                     0
## 12            0       1           0                     0
## 13            0       0           1                     0
## 14            1       1           0                     0
## 15            0       0           0                     0
## 16            1       1           0                     1
## 17            1       1           1                     0
## 18            1       1           1                     0
## 19            1       0           1                     0
## 20            1       0           1                     0
## 21            1       0           1                     0
## 22            1       0           1                     0
## 23            1       0           1                     0
## 24            1       0           1                     0
## 25            1       0           1                     0
## 26            1       0           1                     1
##    Benzene, (1-methyldecyl)- Benzene, (1-methylnonyl)-
## 1                          0                         0
## 2                          0                         0
## 3                          0                         0
## 4                          0                         0
## 5                          0                         0
## 6                          1                         1
## 7                          0                         0
## 8                          0                         0
## 9                          0                         0
## 10                         0                         0
## 11                         0                         0
## 12                         0                         0
## 13                         0                         0
## 14                         0                         0
## 15                         0                         0
## 16                         0                         0
## 17                         0                         0
## 18                         0                         0
## 19                         0                         0
## 20                         0                         0
## 21                         0                         0
## 22                         0                         0
## 23                         0                         0
## 24                         0                         0
## 25                         0                         0
## 26                         0                         0
##    Benzene, 1-chloro-2-methoxy- Benzene, 1-isocyano-2-methyl-
## 1                             0                             0
## 2                             0                             0
## 3                             0                             0
## 4                             0                             0
## 5                             0                             0
```

```
## 6                              0                              0
## 7                              0                              0
## 8                              0                              0
## 9                              0                              0
## 10                             1                              1
## 11                             1                              0
## 12                             1                              0
## 13                             0                              0
## 14                             0                              1
## 15                             0                              0
## 16                             0                              0
## 17                             1                              0
## 18                             1                              1
## 19                             0                              0
## 20                             0                              0
## 21                             0                              0
## 22                             0                              0
## 23                             0                              0
## 24                             0                              0
## 25                             0                              0
## 26                             0                              0
##    Benzene, 1-methoxy-4-methyl- Benzene, 1,3-dimethyl-
## 1                              0                      1
## 2                              0                      0
## 3                              0                      0
## 4                              0                      0
## 5                              0                      0
## 6                              0                      0
## 7                              0                      0
## 8                              0                      0
## 9                              0                      0
## 10                             1                      1
## 11                             1                      0
## 12                             1                      0
## 13                             0                      0
## 14                             1                      0
## 15                             0                      0
## 16                             0                      0
## 17                             0                      1
## 18                             0                      0
## 19                             0                      0
## 20                             0                      0
## 21                             0                      0
## 22                             0                      0
## 23                             0                      1
## 24                             0                      0
## 25                             0                      0
## 26                             0                      1
##    Benzene, 3-cyclohexen-1-yl- Benzeneacetaldehyde Benzophenone
## 1                            0                   0            0
## 2                            0                   0            1
## 3                            0                   0            1
## 4                            0                   0            0
## 5                            0                   1            1
```

```
## 6                          0                  0           1
## 7                          0                  0           0
## 8                          0                  0           1
## 9                          0                  0           0
## 10                         0                  0           1
## 11                         0                  0           1
## 12                         0                  0           1
## 13                         1                  0           0
## 14                         1                  0           1
## 15                         0                  0           0
## 16                         1                  0           0
## 17                         1                  1           1
## 18                         1                  1           1
## 19                         0                  0           1
## 20                         0                  0           1
## 21                         0                  0           1
## 22                         1                  0           1
## 23                         1                  0           1
## 24                         1                  0           1
## 25                         1                  2           1
## 26                         1                  0           1
##    Benzothiazole Benzyl alcohol Benzyl methyl ketone Benzyl nitrile
## 1              1              1                    0              1
## 2              1              1                    0              0
## 3              1              1                    0              1
## 4              0              1                    0              1
## 5              1              1                    0              1
## 6              0              1                    0              1
## 7              0              1                    0              0
## 8              1              1                    0              1
## 9              0              1                    0              0
## 10             1              0                    0              0
## 11             1              0                    0              1
## 12             0              0                    0              1
## 13             0              0                    0              0
## 14             0              0                    1              0
## 15             0              0                    0              0
## 16             0              0                    0              1
## 17             1              0                    0              1
## 18             0              1                    1              0
## 19             1              1                    0              1
## 20             1              1                    1              1
## 21             1              1                    0              1
## 22             0              1                    1              1
## 23             0              1                    1              1
## 24             0              1                    1              0
## 25             1              1                    1              1
## 26             0              1                    1              1
##    Bicyclo[4.2.0]octa-1,3,5-triene Butanoic acid, 2-methyl-
## 1                                0                       0
## 2                                0                       2
## 3                                0                       2
## 4                                0                       2
## 5                                0                       4
```

```
## 6                                  0                          9
## 7                                  0                          0
## 8                                  0                          8
## 9                                  0                          0
## 10                                 1                          0
## 11                                 0                          0
## 12                                 0                          6
## 13                                 0                          0
## 14                                 1                          0
## 15                                 0                          0
## 16                                 0                          0
## 17                                 0                          0
## 18                                 0                          0
## 19                                 0                          2
## 20                                 0                          0
## 21                                 1                          1
## 22                                 1                          0
## 23                                 1                          0
## 24                                 0                          0
## 25                                 0                          2
## 26                                 0                          0
##    Butanoic acid, 3-bromo-3-methyl- Butanoic acid, 3-methyl-
## 1                                  0                         0
## 2                                  0                         0
## 3                                  0                         0
## 4                                  0                         0
## 5                                  0                         0
## 6                                  1                         3
## 7                                  0                         0
## 8                                  1                         5
## 9                                  0                         0
## 10                                 0                         0
## 11                                 0                         0
## 12                                 0                         0
## 13                                 0                         0
## 14                                 0                         0
## 15                                 0                         0
## 16                                 0                         0
## 17                                 0                         0
## 18                                 0                         0
## 19                                 0                         0
## 20                                 0                         0
## 21                                 0                         0
## 22                                 0                         0
## 23                                 0                         0
## 24                                 0                         0
## 25                                 0                         0
## 26                                 0                         0
##    Butylated Hydroxytoluene Caprolactam
## 1                         1           0
## 2                         1           0
## 3                         1           0
## 4                         1           0
## 5                         1           1
```

```
## 6                          1           1
## 7                          0           0
## 8                          1           1
## 9                          0           0
## 10                         1           1
## 11                         1           1
## 12                         1           0
## 13                         0           0
## 14                         1           1
## 15                         0           0
## 16                         0           0
## 17                         1           1
## 18                         1           1
## 19                         0           1
## 20                         1           1
## 21                         0           1
## 22                         1           1
## 23                         0           1
## 24                         0           0
## 25                         1           1
## 26                         1           0
##    Carbamodithioic acid, diethyl-, methyl ester Cyclohept-4-enone
## 1                                             0                 0
## 2                                             0                 0
## 3                                             0                 0
## 4                                             0                 0
## 5                                             0                 0
## 6                                             0                 0
## 7                                             0                 0
## 8                                             0                 0
## 9                                             0                 0
## 10                                            0                 0
## 11                                            0                 1
## 12                                            0                 1
## 13                                            0                 0
## 14                                            0                 0
## 15                                            0                 0
## 16                                            0                 0
## 17                                            1                 0
## 18                                            0                 0
## 19                                            0                 0
## 20                                            0                 0
## 21                                            0                 0
## 22                                            0                 0
## 23                                            0                 0
## 24                                            0                 0
## 25                                            1                 0
## 26                                            0                 0
##    Cyclohexane, 2-propyl-1,1,3-trimethyl- Cyclohexanone
## 1                                       0             0
## 2                                       0             0
## 3                                       0             0
## 4                                       0             0
## 5                                       0             0
```

```
## 6                                        0             0
## 7                                        0             0
## 8                                        0             0
## 9                                        0             0
## 10                                       0             0
## 11                                       0             0
## 12                                       0             0
## 13                                       0             0
## 14                                       0             0
## 15                                       0             0
## 16                                       0             0
## 17                                       0             0
## 18                                       0             0
## 19                                       0             1
## 20                                       0             1
## 21                                       0             1
## 22                                       0             0
## 23                                       1             0
## 24                                       1             0
## 25                                       0             0
## 26                                       0             0
##    Cyclohexasiloxane, dodecamethyl-
## 1                                  0
## 2                                  1
## 3                                  1
## 4                                  0
## 5                                  1
## 6                                  0
## 7                                  0
## 8                                  1
## 9                                  0
## 10                                 1
## 11                                 1
## 12                                 1
## 13                                 1
## 14                                 1
## 15                                 1
## 16                                 1
## 17                                 1
## 18                                 1
## 19                                 0
## 20                                 1
## 21                                 0
## 22                                 0
## 23                                 0
## 24                                 0
## 25                                 1
## 26                                 1
##    Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-
## 1                                                 0
## 2                                                 0
## 3                                                 0
## 4                                                 0
## 5                                                 0
```

```
## 6                                                0
## 7                                                0
## 8                                                0
## 9                                                0
## 10                                               0
## 11                                               0
## 12                                               0
## 13                                               1
## 14                                               0
## 15                                               0
## 16                                               0
## 17                                               0
## 18                                               0
## 19                                               0
## 20                                               0
## 21                                               0
## 22                                               0
## 23                                               1
## 24                                               0
## 25                                               0
## 26                                               1
##    Cyclooctasiloxane, hexadecamethyl- Cyclooctene, (Z)-
## 1                                   0                 0
## 2                                   0                 0
## 3                                   0                 0
## 4                                   1                 0
## 5                                   1                 0
## 6                                   0                 0
## 7                                   0                 0
## 8                                   0                 0
## 9                                   0                 0
## 10                                  0                 0
## 11                                  0                 1
## 12                                  0                 1
## 13                                  0                 0
## 14                                  0                 1
## 15                                  0                 0
## 16                                  0                 0
## 17                                  0                 0
## 18                                  0                 0
## 19                                  0                 0
## 20                                  0                 0
## 21                                  1                 0
## 22                                  0                 0
## 23                                  1                 0
## 24                                  0                 1
## 25                                  0                 0
## 26                                  0                 0
##    Cyclopentasiloxane, decamethyl- Cyclopropane, pentyl-
## 1                                1                     0
## 2                                0                     0
## 3                                0                     0
## 4                                0                     0
## 5                                0                     0
```

```
## 6                                0                   0
## 7                                1                   0
## 8                                0                   0
## 9                                1                   0
## 10                               1                   0
## 11                               1                   1
## 12                               0                   0
## 13                               1                   0
## 14                               1                   0
## 15                               1                   0
## 16                               1                   0
## 17                               1                   0
## 18                               1                   0
## 19                               1                   0
## 20                               1                   0
## 21                               1                   0
## 22                               1                   0
## 23                               1                   0
## 24                               1                   0
## 25                               1                   1
## 26                               1                   0
##    Cyclotetrasiloxane, octamethyl- D-Limonene Decanal Dibutyl phthalate
## 1                                0          0       1                  1
## 2                                0          0       1                  1
## 3                                1          0       1                  1
## 4                                1          0       1                  1
## 5                                1          0       1                  1
## 6                                0          0       1                  1
## 7                                0          0       1                  1
## 8                                0          0       1                  1
## 9                                1          0       1                  1
## 10                               0          0       1                  1
## 11                               1          0       1                  1
## 12                               0          0       1                  1
## 13                               2          0       1                  0
## 14                               1          1       1                  1
## 15                               1          0       0                  0
## 16                               1          0       1                  1
## 17                               1          0       1                  1
## 18                               1          0       1                  1
## 19                               0          0       1                  1
## 20                               0          0       1                  1
## 21                               0          0       1                  1
## 22                               0          0       1                  1
## 23                               1          0       1                  1
## 24                               0          1       1                  1
## 25                               0          0       1                  1
## 26                               1          0       1                  1
##    Diethyl Phthalate Dimethyl trisulfide Diphenylamine
## 1                  0                   0             0
## 2                  0                   0             0
## 3                  0                   0             0
## 4                  0                   0             0
## 5                  0                   0             1
```

```
## 6                  0                  0             1
## 7                  0                  0             0
## 8                  0                  0             1
## 9                  0                  0             0
## 10                 1                  1             0
## 11                 1                  1             0
## 12                 1                  1             0
## 13                 0                  0             0
## 14                 1                  1             0
## 15                 0                  0             0
## 16                 0                  0             0
## 17                 1                  1             0
## 18                 0                  1             1
## 19                 1                  1             0
## 20                 1                  1             0
## 21                 1                  1             0
## 22                 1                  1             0
## 23                 0                  1             0
## 24                 0                  2             0
## 25                 1                  1             0
## 26                 0                  1             0
##    Disulfide, isopentyl methyl Dodecanal Ethanone, 1-(1H-pyrrol-2-yl)-
## 1                            0         1                             0
## 2                            0         1                             1
## 3                            0         1                             1
## 4                            0         1                             0
## 5                            0         1                             1
## 6                            0         1                             1
## 7                            0         0                             0
## 8                            0         1                             1
## 9                            0         0                             0
## 10                           0         0                             1
## 11                           0         0                             1
## 12                           0         0                             1
## 13                           0         0                             0
## 14                           0         0                             1
## 15                           0         0                             0
## 16                           0         0                             0
## 17                           0         0                             1
## 18                           0         0                             1
## 19                           1         0                             1
## 20                           0         1                             1
## 21                           1         1                             0
## 22                           0         1                             1
## 23                           0         1                             1
## 24                           0         0                             1
## 25                           0         2                             1
## 26                           0         0                             1
##    Ethanone, 1-(2-aminophenyl)- Ethanone, 1-(2-furanyl)-
## 1                             0                        0
## 2                             0                        0
## 3                             0                        1
## 4                             0                        0
## 5                             0                        0
```

```
## 6                                0                                0
## 7                                0                                0
## 8                                0                                0
## 9                                0                                0
## 10                               1                                1
## 11                               0                                0
## 12                               0                                0
## 13                               0                                0
## 14                               0                                0
## 15                               0                                0
## 16                               0                                0
## 17                               0                                1
## 18                               0                                1
## 19                               1                                0
## 20                               0                                1
## 21                               1                                1
## 22                               0                                0
## 23                               0                                0
## 24                               0                                0
## 25                               0                                1
## 26                               0                                0
##    Ethanone, 1-(3,4-dimethylphenyl)- Ethanone, 1-(4-ethylphenyl)-
## 1                                  0                              0
## 2                                  0                              0
## 3                                  0                              0
## 4                                  0                              0
## 5                                  0                              0
## 6                                  0                              0
## 7                                  0                              0
## 8                                  0                              0
## 9                                  0                              0
## 10                                 0                              0
## 11                                 0                              0
## 12                                 0                              0
## 13                                 0                              0
## 14                                 0                              0
## 15                                 0                              0
## 16                                 1                              1
## 17                                 0                              0
## 18                                 0                              2
## 19                                 1                              0
## 20                                 0                              0
## 21                                 0                              0
## 22                                 0                              0
## 23                                 0                              0
## 24                                 0                              0
## 25                                 0                              2
## 26                                 0                              2
##    Eucalyptol Formamide, N,N-dibutyl- Furan, 2-ethyl-5-methyl-
## 1           0                       0                       0
## 2           0                       0                       0
## 3           0                       0                       0
## 4           0                       0                       0
## 5           0                       0                       0
```

```
## 6           0                       0                       0
## 7           0                       0                       0
## 8           0                       0                       0
## 9           0                       0                       0
## 10          0                       0                       0
## 11          0                       0                       1
## 12          0                       1                       0
## 13          0                       0                       0
## 14          0                       0                       0
## 15          0                       0                       0
## 16          1                       0                       0
## 17          1                       0                       0
## 18          0                       0                       0
## 19          0                       0                       1
## 20          0                       0                       0
## 21          0                       0                       0
## 22          0                       0                       1
## 23          0                       0                       0
## 24          0                       0                       0
## 25          0                       1                       0
## 26          1                       0                       0
##    Glutaric acid, di(isobutyl) ester Heneicosane Heptadecane
## 1                                  0           0           0
## 2                                  0           0           0
## 3                                  0           1           0
## 4                                  0           0           1
## 5                                  0           1           0
## 6                                  0           0           1
## 7                                  0           0           0
## 8                                  0           0           0
## 9                                  0           0           0
## 10                                 0           0           1
## 11                                 0           0           0
## 12                                 0           0           0
## 13                                 0           0           0
## 14                                 0           0           0
## 15                                 0           0           0
## 16                                 0           0           0
## 17                                 0           0           0
## 18                                 0           0           0
## 19                                 1           0           0
## 20                                 0           0           0
## 21                                 0           0           0
## 22                                 1           0           0
## 23                                 0           0           0
## 24                                 0           0           0
## 25                                 1           0           1
## 26                                 0           0           0
##    Heptadecane, 2,6-dimethyl- Heptadecane, 2,6,10,15-tetramethyl-
## 1                           0                                    0
## 2                           0                                    0
## 3                           0                                    0
## 4                           0                                    1
## 5                           0                                    0
```

```
## 6                           0                                     0
## 7                           0                                     0
## 8                           0                                     0
## 9                           0                                     0
## 10                          0                                     0
## 11                          0                                     0
## 12                          1                                     0
## 13                          0                                     0
## 14                          0                                     0
## 15                          0                                     0
## 16                          0                                     0
## 17                          0                                     0
## 18                          0                                     0
## 19                          0                                     0
## 20                          0                                     0
## 21                          0                                     0
## 22                          0                                     0
## 23                          0                                     0
## 24                          0                                     0
## 25                          0                                     0
## 26                          0                                     0
##    Hexadecane Hexanoic acid Homosalate Limonene Mequinol
## 1           0             0          0        0        0
## 2           1             0          1        0        0
## 3           0             1          1        0        1
## 4           0             0          0        0        0
## 5           0             0          1        0        1
## 6           0             0          0        0        1
## 7           0             0          0        0        0
## 8           1             0          1        0        0
## 9           0             0          0        0        0
## 10          0             0          0        0        0
## 11          0             0          1        0        0
## 12          0             0          0        0        0
## 13          0             0          0        0        0
## 14          0             0          0        0        0
## 15          0             0          0        0        0
## 16          0             0          0        1        0
## 17          0             0          0        0        0
## 18          0             0          0        0        0
## 19          0             0          0        0        1
## 20          0             0          0        0        1
## 21          0             0          0        0        0
## 22          0             0          0        1        0
## 23          0             0          0        0        0
## 24          0             0          0        0        0
## 25          0             0          0        0        0
## 26          0             0          0        0        0
##    Methane, oxybis[dichloro- Nonadecane Nonanal Octadecane
## 1                          0          0       1          0
## 2                          0          4       1          0
## 3                          0          4       1          0
## 4                          0          1       1          0
## 5                          0          4       1          0
```

```
## 6                          0          2       1          0
## 7                          0          1       1          0
## 8                          0          3       1          1
## 9                          0          0       1          0
## 10                         1          2       1          0
## 11                         0          2       1          0
## 12                         0          2       1          0
## 13                         0          0       0          0
## 14                         0          2       1          0
## 15                         0          1       0          0
## 16                         0          0       1          0
## 17                         0          2       1          0
## 18                         0          2       1          0
## 19                         1          0       1          0
## 20                         0          0       1          0
## 21                         1          3       1          0
## 22                         0          0       1          0
## 23                         0          1       1          0
## 24                         1          0       0          0
## 25                         0          1       1          0
## 26                         1          0       1          0
##    Octadecane, 2-methyl- Octanal Octane, 1-chloro- Phenol Phenol, 2-iodo-
## 1                      0       0                 0      1               0
## 2                      1       0                 0      1               0
## 3                      0       0                 0      1               0
## 4                      1       1                 0      1               0
## 5                      0       0                 0      1               0
## 6                      0       1                 0      1               0
## 7                      0       0                 0      1               0
## 8                      1       1                 0      1               0
## 9                      0       0                 0      1               0
## 10                     0       1                 0      1               1
## 11                     0       1                 0      1               1
## 12                     0       1                 1      1               0
## 13                     0       0                 0      1               0
## 14                     0       0                 0      1               0
## 15                     0       0                 0      0               0
## 16                     0       0                 0      1               0
## 17                     0       1                 0      1               1
## 18                     0       0                 0      1               1
## 19                     0       0                 0      1               0
## 20                     0       0                 0      1               0
## 21                     0       1                 1      1               0
## 22                     0       1                 0      1               0
## 23                     0       0                 0      1               0
## 24                     0       0                 0      1               0
## 25                     0       1                 0      1               0
## 26                     0       0                 0      1               0
##    Phenol, 2-methoxy- Phenol, 3-ethyl- Phenylethyl Alcohol
## 1                   0                0                   1
## 2                   0                0                   1
## 3                   0                0                   1
## 4                   0                0                   1
## 5                   0                0                   1
```

```
## 6                   0                0                   1
## 7                   0                0                   1
## 8                   0                0                   1
## 9                   0                0                   1
## 10                  1                1                   1
## 11                  1                1                   1
## 12                  1                0                   1
## 13                  0                0                   1
## 14                  1                0                   1
## 15                  0                0                   0
## 16                  1                0                   1
## 17                  1                0                   1
## 18                  1                0                   1
## 19                  0                0                   1
## 20                  0                0                   1
## 21                  0                0                   1
## 22                  0                0                   1
## 23                  0                0                   1
## 24                  0                0                   1
## 25                  0                0                   1
## 26                  0                0                   1
##    Propanol, [(butoxymethylethoxy)methylethoxy]-
## 1                                              0
## 2                                              0
## 3                                              0
## 4                                              0
## 5                                              0
## 6                                              0
## 7                                              0
## 8                                              0
## 9                                              0
## 10                                             0
## 11                                             0
## 12                                             0
## 13                                             0
## 14                                             0
## 15                                             0
## 16                                             2
## 17                                             0
## 18                                             2
## 19                                             0
## 20                                             0
## 21                                             0
## 22                                             0
## 23                                             0
## 24                                             0
## 25                                             2
## 26                                             2
##    Pyrazine, 2-ethyl-5-methyl- Pyrazine, 2-ethyl-6-methyl-
## 1                            1                           0
## 2                            1                           1
## 3                            0                           1
## 4                            0                           0
## 5                            0                           1
```

```
## 6                            0                            1
## 7                            0                            0
## 8                            1                            1
## 9                            0                            0
## 10                           1                            1
## 11                           0                            1
## 12                           1                            1
## 13                           0                            0
## 14                           1                            1
## 15                           0                            0
## 16                           0                            0
## 17                           2                            0
## 18                           0                            0
## 19                           2                            0
## 20                           2                            0
## 21                           0                            2
## 22                           0                            2
## 23                           1                            0
## 24                           0                            0
## 25                           1                            1
## 26                           0                            0
##    Pyrazine, 2,5-dimethyl- Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-
## 1                         1                                         0
## 2                         1                                         0
## 3                         1                                         0
## 4                         1                                         0
## 5                         1                                         0
## 6                         2                                         0
## 7                         1                                         0
## 8                         1                                         1
## 9                         1                                         0
## 10                        1                                         1
## 11                        1                                         1
## 12                        1                                         0
## 13                        2                                         0
## 14                        1                                         0
## 15                        0                                         0
## 16                        2                                         0
## 17                        1                                         0
## 18                        1                                         0
## 19                        1                                         0
## 20                        2                                         0
## 21                        1                                         0
## 22                        1                                         1
## 23                        2                                         0
## 24                        1                                         0
## 25                        1                                         1
## 26                        2                                         0
##    Pyrazine, 3-ethyl-2,5-dimethyl- Pyrazine, trimethyl-
## 1                                0                    0
## 2                                0                    0
## 3                                1                    0
## 4                                1                    0
## 5                                1                    0
```

```
## 6                                1                   1
## 7                                0                   0
## 8                                1                   1
## 9                                0                   0
## 10                               1                   0
## 11                               1                   0
## 12                               1                   0
## 13                               0                   0
## 14                               1                   0
## 15                               0                   0
## 16                               0                   0
## 17                               1                   0
## 18                               1                   0
## 19                               1                   1
## 20                               1                   0
## 21                               1                   1
## 22                               0                   0
## 23                               0                   0
## 24                               0                   0
## 25                               1                   0
## 26                               0                   0
##    Pyridine, 2,4,6-trimethyl- Quinazoline, 4-methyl- Quinoline, 3-methyl-
## 1                           0                       0                    0
## 2                           0                       0                    0
## 3                           0                       0                    0
## 4                           0                       0                    0
## 5                           0                       0                    0
## 6                           0                       1                    0
## 7                           0                       0                    0
## 8                           0                       1                    0
## 9                           0                       0                    0
## 10                          0                       1                    0
## 11                          0                       1                    0
## 12                          1                       0                    0
## 13                          0                       0                    0
## 14                          0                       0                    0
## 15                          0                       0                    0
## 16                          0                       0                    0
## 17                          0                       0                    1
## 18                          0                       0                    1
## 19                          1                       0                    0
## 20                          0                       0                    0
## 21                          0                       1                    1
## 22                          0                       1                    1
## 23                          0                       0                    1
## 24                          0                       0                    0
## 25                          0                       1                    1
## 26                          0                       0                    1
##    Quinoline, 4-methyl- S-Methyl methanethiosulphonate Styrene Tetracosane
## 1                     0                               0       1           0
## 2                     1                               0       0           0
## 3                     1                               0       1           0
## 4                     0                               0       1           0
## 5                     1                               0       0           1
```

```
## 6                     1                                0       0           0
## 7                     0                                0       1           0
## 8                     1                                0       0           0
## 9                     0                                0       1           0
## 10                    0                                0       0           0
## 11                    0                                0       1           0
## 12                    0                                0       0           0
## 13                    0                                0       0           0
## 14                    0                                0       0           0
## 15                    0                                0       0           0
## 16                    0                                0       1           0
## 17                    0                                0       0           0
## 18                    0                                0       0           0
## 19                    1                                0       0           0
## 20                    1                                0       0           0
## 21                    0                                0       0           0
## 22                    0                                0       0           0
## 23                    0                                0       0           0
## 24                    0                                1       0           0
## 25                    0                                1       1           0
## 26                    0                                0       1           0
##    Tetradecanal Tetradecane Undecanal
## 1             0           0         0
## 2             0           0         1
## 3             0           0         1
## 4             0           0         0
## 5             2           0         1
## 6             0           0         1
## 7             0           0         0
## 8             1           0         1
## 9             0           0         0
## 10            0           0         1
## 11            0           0         1
## 12            0           0         1
## 13            0           0         0
## 14            0           1         1
## 15            0           1         0
## 16            0           0         0
## 17            0           0         1
## 18            0           0         1
## 19            0           0         0
## 20            0           0         1
## 21            0           1         1
## 22            0           1         1
## 23            0           0         1
## 24            0           0         0
## 25            1           0         1
## 26            0           0         1
```

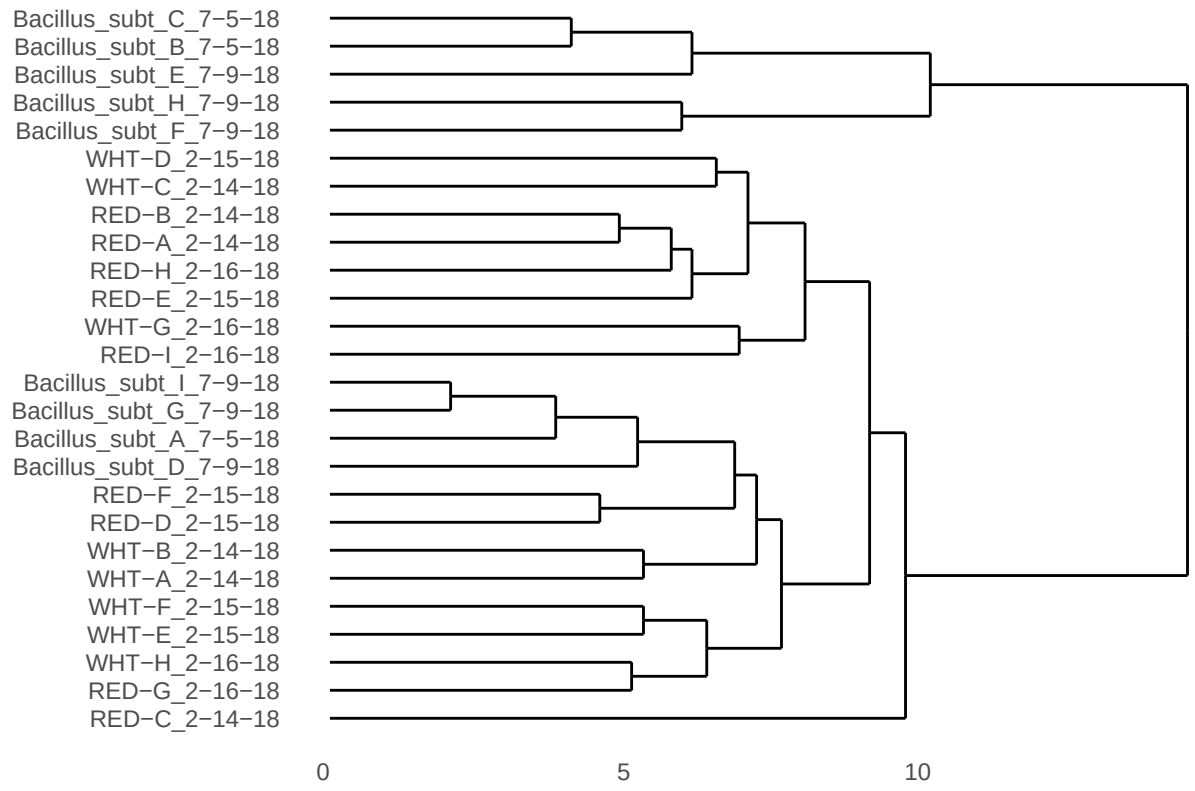
```
rownames(volatiles.table) <- volatiles.table$Sample
#volatiles.table
#write.table(volatiles.table, "vol_table.txt", sep="\t")
```

```
# Create dendro
volatile.dendro <- as.dendrogram(hclust(d = dist(x = volatiles.table)))
```

```
## Warning in dist(x = volatiles.table): NAs introduced by coercion
```

```
dendro.plot <- ggdendrogram(data = volatile.dendro, rotate = TRUE)

# Preview the plot
dendro.plot
```




```
pdf("over75_vol_dendro.pdf", height = 8, width = 16)
  dendro.plot
dev.off()
```

```
## pdf
##   2
```

```
#make heatmap
volatiles
```

```
## # A tibble: 1,105 x 3
##    Sample                variable              value
##    <chr>                 <chr>                 <dbl>
```

```
##  1 Bacillus_subt_A_7-5-18 1-Hexanol, 2-ethyl-      6.65
##  2 Bacillus_subt_A_7-5-18 2-Acetylthiazole         5.38
##  3 Bacillus_subt_A_7-5-18 2-Dodecanone             7.28
##  4 Bacillus_subt_A_7-5-18 2-Dodecanone             6.80
##  5 Bacillus_subt_A_7-5-18 2-Nonanol                2.01
##  6 Bacillus_subt_A_7-5-18 2-Nonanone               3.76
##  7 Bacillus_subt_A_7-5-18 2-Tridecanone            3.10
##  8 Bacillus_subt_A_7-5-18 2-Undecanol             16.7
##  9 Bacillus_subt_A_7-5-18 2-Undecanone            16.2
## 10 Bacillus_subt_A_7-5-18 2,4-Di-tert-butylphenol  1.20
## # ... with 1,095 more rows
```

```
volatiles.matrix <- as.matrix(volatiles)
volatiles.df <- as.data.frame(volatiles.matrix)
volatiles.df
```

```
##                      Sample
## 1    Bacillus_subt_A_7-5-18
## 2    Bacillus_subt_A_7-5-18
## 3    Bacillus_subt_A_7-5-18
## 4    Bacillus_subt_A_7-5-18
## 5    Bacillus_subt_A_7-5-18
## 6    Bacillus_subt_A_7-5-18
## 7    Bacillus_subt_A_7-5-18
## 8    Bacillus_subt_A_7-5-18
## 9    Bacillus_subt_A_7-5-18
## 10   Bacillus_subt_A_7-5-18
## 11   Bacillus_subt_A_7-5-18
## 12   Bacillus_subt_A_7-5-18
## 13   Bacillus_subt_A_7-5-18
## 14   Bacillus_subt_A_7-5-18
## 15   Bacillus_subt_A_7-5-18
## 16   Bacillus_subt_A_7-5-18
## 17   Bacillus_subt_A_7-5-18
## 18   Bacillus_subt_A_7-5-18
## 19   Bacillus_subt_A_7-5-18
## 20   Bacillus_subt_A_7-5-18
## 21   Bacillus_subt_A_7-5-18
## 22   Bacillus_subt_A_7-5-18
## 23   Bacillus_subt_A_7-5-18
## 24   Bacillus_subt_A_7-5-18
## 25   Bacillus_subt_A_7-5-18
## 26   Bacillus_subt_A_7-5-18
## 27   Bacillus_subt_B_7-5-18
## 28   Bacillus_subt_B_7-5-18
## 29   Bacillus_subt_B_7-5-18
## 30   Bacillus_subt_B_7-5-18
## 31   Bacillus_subt_B_7-5-18
## 32   Bacillus_subt_B_7-5-18
## 33   Bacillus_subt_B_7-5-18
## 34   Bacillus_subt_B_7-5-18
## 35   Bacillus_subt_B_7-5-18
## 36   Bacillus_subt_B_7-5-18
## 37   Bacillus_subt_B_7-5-18
```

```
## 38   Bacillus_subt_B_7-5-18
## 39   Bacillus_subt_B_7-5-18
## 40   Bacillus_subt_B_7-5-18
## 41   Bacillus_subt_B_7-5-18
## 42   Bacillus_subt_B_7-5-18
## 43   Bacillus_subt_B_7-5-18
## 44   Bacillus_subt_B_7-5-18
## 45   Bacillus_subt_B_7-5-18
## 46   Bacillus_subt_B_7-5-18
## 47   Bacillus_subt_B_7-5-18
## 48   Bacillus_subt_B_7-5-18
## 49   Bacillus_subt_B_7-5-18
## 50   Bacillus_subt_B_7-5-18
## 51   Bacillus_subt_B_7-5-18
## 52   Bacillus_subt_B_7-5-18
## 53   Bacillus_subt_B_7-5-18
## 54   Bacillus_subt_B_7-5-18
## 55   Bacillus_subt_B_7-5-18
## 56   Bacillus_subt_B_7-5-18
## 57   Bacillus_subt_B_7-5-18
## 58   Bacillus_subt_B_7-5-18
## 59   Bacillus_subt_B_7-5-18
## 60   Bacillus_subt_B_7-5-18
## 61   Bacillus_subt_B_7-5-18
## 62   Bacillus_subt_B_7-5-18
## 63   Bacillus_subt_B_7-5-18
## 64   Bacillus_subt_B_7-5-18
## 65   Bacillus_subt_B_7-5-18
## 66   Bacillus_subt_B_7-5-18
## 67   Bacillus_subt_B_7-5-18
## 68   Bacillus_subt_B_7-5-18
## 69   Bacillus_subt_B_7-5-18
## 70   Bacillus_subt_B_7-5-18
## 71   Bacillus_subt_B_7-5-18
## 72   Bacillus_subt_B_7-5-18
## 73   Bacillus_subt_B_7-5-18
## 74   Bacillus_subt_B_7-5-18
## 75   Bacillus_subt_B_7-5-18
## 76   Bacillus_subt_B_7-5-18
## 77   Bacillus_subt_B_7-5-18
## 78   Bacillus_subt_C_7-5-18
## 79   Bacillus_subt_C_7-5-18
## 80   Bacillus_subt_C_7-5-18
## 81   Bacillus_subt_C_7-5-18
## 82   Bacillus_subt_C_7-5-18
## 83   Bacillus_subt_C_7-5-18
## 84   Bacillus_subt_C_7-5-18
## 85   Bacillus_subt_C_7-5-18
## 86   Bacillus_subt_C_7-5-18
## 87   Bacillus_subt_C_7-5-18
## 88   Bacillus_subt_C_7-5-18
## 89   Bacillus_subt_C_7-5-18
## 90   Bacillus_subt_C_7-5-18
## 91   Bacillus_subt_C_7-5-18
```

```
## 92   Bacillus_subt_C_7-5-18
## 93   Bacillus_subt_C_7-5-18
## 94   Bacillus_subt_C_7-5-18
## 95   Bacillus_subt_C_7-5-18
## 96   Bacillus_subt_C_7-5-18
## 97   Bacillus_subt_C_7-5-18
## 98   Bacillus_subt_C_7-5-18
## 99   Bacillus_subt_C_7-5-18
## 100  Bacillus_subt_C_7-5-18
## 101  Bacillus_subt_C_7-5-18
## 102  Bacillus_subt_C_7-5-18
## 103  Bacillus_subt_C_7-5-18
## 104  Bacillus_subt_C_7-5-18
## 105  Bacillus_subt_C_7-5-18
## 106  Bacillus_subt_C_7-5-18
## 107  Bacillus_subt_C_7-5-18
## 108  Bacillus_subt_C_7-5-18
## 109  Bacillus_subt_C_7-5-18
## 110  Bacillus_subt_C_7-5-18
## 111  Bacillus_subt_C_7-5-18
## 112  Bacillus_subt_C_7-5-18
## 113  Bacillus_subt_C_7-5-18
## 114  Bacillus_subt_C_7-5-18
## 115  Bacillus_subt_C_7-5-18
## 116  Bacillus_subt_C_7-5-18
## 117  Bacillus_subt_C_7-5-18
## 118  Bacillus_subt_C_7-5-18
## 119  Bacillus_subt_C_7-5-18
## 120  Bacillus_subt_C_7-5-18
## 121  Bacillus_subt_C_7-5-18
## 122  Bacillus_subt_C_7-5-18
## 123  Bacillus_subt_C_7-5-18
## 124  Bacillus_subt_C_7-5-18
## 125  Bacillus_subt_C_7-5-18
## 126  Bacillus_subt_C_7-5-18
## 127  Bacillus_subt_C_7-5-18
## 128  Bacillus_subt_C_7-5-18
## 129  Bacillus_subt_C_7-5-18
## 130  Bacillus_subt_C_7-5-18
## 131  Bacillus_subt_C_7-5-18
## 132  Bacillus_subt_C_7-5-18
## 133  Bacillus_subt_C_7-5-18
## 134  Bacillus_subt_C_7-5-18
## 135  Bacillus_subt_D_7-9-18
## 136  Bacillus_subt_D_7-9-18
## 137  Bacillus_subt_D_7-9-18
## 138  Bacillus_subt_D_7-9-18
## 139  Bacillus_subt_D_7-9-18
## 140  Bacillus_subt_D_7-9-18
## 141  Bacillus_subt_D_7-9-18
## 142  Bacillus_subt_D_7-9-18
## 143  Bacillus_subt_D_7-9-18
## 144  Bacillus_subt_D_7-9-18
## 145  Bacillus_subt_D_7-9-18
```

```
## 146  Bacillus_subt_D_7-9-18
## 147  Bacillus_subt_D_7-9-18
## 148  Bacillus_subt_D_7-9-18
## 149  Bacillus_subt_D_7-9-18
## 150  Bacillus_subt_D_7-9-18
## 151  Bacillus_subt_D_7-9-18
## 152  Bacillus_subt_D_7-9-18
## 153  Bacillus_subt_D_7-9-18
## 154  Bacillus_subt_D_7-9-18
## 155  Bacillus_subt_D_7-9-18
## 156  Bacillus_subt_D_7-9-18
## 157  Bacillus_subt_D_7-9-18
## 158  Bacillus_subt_D_7-9-18
## 159  Bacillus_subt_D_7-9-18
## 160  Bacillus_subt_D_7-9-18
## 161  Bacillus_subt_D_7-9-18
## 162  Bacillus_subt_D_7-9-18
## 163  Bacillus_subt_D_7-9-18
## 164  Bacillus_subt_D_7-9-18
## 165  Bacillus_subt_D_7-9-18
## 166  Bacillus_subt_D_7-9-18
## 167  Bacillus_subt_D_7-9-18
## 168  Bacillus_subt_D_7-9-18
## 169  Bacillus_subt_D_7-9-18
## 170  Bacillus_subt_D_7-9-18
## 171  Bacillus_subt_E_7-9-18
## 172  Bacillus_subt_E_7-9-18
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## 175  Bacillus_subt_E_7-9-18
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## 178  Bacillus_subt_E_7-9-18
## 179  Bacillus_subt_E_7-9-18
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## 184  Bacillus_subt_E_7-9-18
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## 186  Bacillus_subt_E_7-9-18
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## 253  Bacillus_subt_F_7-9-18
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## 307  Bacillus_subt_G_7-9-18
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## 373  Bacillus_subt_H_7-9-18
## 374  Bacillus_subt_H_7-9-18
## 375  Bacillus_subt_H_7-9-18
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## 382  Bacillus_subt_H_7-9-18
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## 410           RED-A_2-14-18
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## 412           RED-A_2-14-18
## 413           RED-A_2-14-18
## 414           RED-A_2-14-18
## 415           RED-A_2-14-18
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## 417          RED-A_2-14-18
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## 423          RED-A_2-14-18
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## 426          RED-A_2-14-18
## 427          RED-A_2-14-18
## 428          RED-A_2-14-18
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## 431          RED-A_2-14-18
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## 439          RED-A_2-14-18
## 440          RED-A_2-14-18
## 441          RED-A_2-14-18
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## 443          RED-A_2-14-18
## 444          RED-A_2-14-18
## 445          RED-A_2-14-18
## 446          RED-A_2-14-18
## 447          RED-A_2-14-18
## 448          RED-A_2-14-18
## 449          RED-A_2-14-18
## 450          RED-A_2-14-18
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## 453          RED-A_2-14-18
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## 461          RED-B_2-14-18
## 462          RED-B_2-14-18
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## 469          RED-B_2-14-18
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## 484          RED-B_2-14-18
## 485          RED-B_2-14-18
## 486          RED-B_2-14-18
## 487          RED-B_2-14-18
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## 522          RED-C_2-14-18
## 523          RED-C_2-14-18
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## 623          RED-G_2-16-18
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## 674          RED-H_2-16-18
## 675          RED-H_2-16-18
## 676          RED-H_2-16-18
## 677          RED-H_2-16-18
## 678          RED-H_2-16-18
## 679          RED-H_2-16-18
## 680          RED-H_2-16-18
## 681          RED-H_2-16-18
## 682          RED-H_2-16-18
## 683          RED-H_2-16-18
## 684          RED-H_2-16-18
## 685          RED-H_2-16-18
```

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## 686          RED-H_2-16-18
## 687          RED-H_2-16-18
## 688          RED-H_2-16-18
## 689          RED-H_2-16-18
## 690          RED-H_2-16-18
## 691          RED-H_2-16-18
## 692          RED-H_2-16-18
## 693          RED-H_2-16-18
## 694          RED-H_2-16-18
## 695          RED-H_2-16-18
## 696          RED-H_2-16-18
## 697          RED-I_2-16-18
## 698          RED-I_2-16-18
## 699          RED-I_2-16-18
## 700          RED-I_2-16-18
## 701          RED-I_2-16-18
## 702          RED-I_2-16-18
## 703          RED-I_2-16-18
## 704          RED-I_2-16-18
## 705          RED-I_2-16-18
## 706          RED-I_2-16-18
## 707          RED-I_2-16-18
## 708          RED-I_2-16-18
## 709          RED-I_2-16-18
## 710          RED-I_2-16-18
## 711          RED-I_2-16-18
## 712          RED-I_2-16-18
## 713          RED-I_2-16-18
## 714          RED-I_2-16-18
## 715          RED-I_2-16-18
## 716          RED-I_2-16-18
## 717          RED-I_2-16-18
## 718          RED-I_2-16-18
## 719          RED-I_2-16-18
## 720          RED-I_2-16-18
## 721          RED-I_2-16-18
## 722          RED-I_2-16-18
## 723          RED-I_2-16-18
## 724          RED-I_2-16-18
## 725          RED-I_2-16-18
## 726          RED-I_2-16-18
## 727          RED-I_2-16-18
## 728          RED-I_2-16-18
## 729          RED-I_2-16-18
## 730          RED-I_2-16-18
## 731          RED-I_2-16-18
## 732          RED-I_2-16-18
## 733          RED-I_2-16-18
## 734          RED-I_2-16-18
## 735          RED-I_2-16-18
## 736          RED-I_2-16-18
## 737          RED-I_2-16-18
## 738          RED-I_2-16-18
## 739          RED-I_2-16-18
```

```
## 740          RED-I_2-16-18
## 741          RED-I_2-16-18
## 742          RED-I_2-16-18
## 743          RED-I_2-16-18
## 744          RED-I_2-16-18
## 745          RED-I_2-16-18
## 746          RED-I_2-16-18
## 747          RED-I_2-16-18
## 748          WHT-A_2-14-18
## 749          WHT-A_2-14-18
## 750          WHT-A_2-14-18
## 751          WHT-A_2-14-18
## 752          WHT-A_2-14-18
## 753          WHT-A_2-14-18
## 754          WHT-A_2-14-18
## 755          WHT-A_2-14-18
## 756          WHT-A_2-14-18
## 757          WHT-A_2-14-18
## 758          WHT-A_2-14-18
## 759          WHT-A_2-14-18
## 760          WHT-A_2-14-18
## 761          WHT-A_2-14-18
## 762          WHT-A_2-14-18
## 763          WHT-A_2-14-18
## 764          WHT-A_2-14-18
## 765          WHT-A_2-14-18
## 766          WHT-A_2-14-18
## 767          WHT-A_2-14-18
## 768          WHT-A_2-14-18
## 769          WHT-A_2-14-18
## 770          WHT-A_2-14-18
## 771          WHT-A_2-14-18
## 772          WHT-A_2-14-18
## 773          WHT-A_2-14-18
## 774          WHT-A_2-14-18
## 775          WHT-A_2-14-18
## 776          WHT-A_2-14-18
## 777          WHT-A_2-14-18
## 778          WHT-A_2-14-18
## 779          WHT-A_2-14-18
## 780          WHT-A_2-14-18
## 781          WHT-A_2-14-18
## 782          WHT-A_2-14-18
## 783          WHT-A_2-14-18
## 784          WHT-A_2-14-18
## 785          WHT-A_2-14-18
## 786          WHT-A_2-14-18
## 787          WHT-A_2-14-18
## 788          WHT-A_2-14-18
## 789          WHT-A_2-14-18
## 790          WHT-B_2-14-18
## 791          WHT-B_2-14-18
## 792          WHT-B_2-14-18
## 793          WHT-B_2-14-18
```

```
## 794          WHT-B_2-14-18
## 795          WHT-B_2-14-18
## 796          WHT-B_2-14-18
## 797          WHT-B_2-14-18
## 798          WHT-B_2-14-18
## 799          WHT-B_2-14-18
## 800          WHT-B_2-14-18
## 801          WHT-B_2-14-18
## 802          WHT-B_2-14-18
## 803          WHT-B_2-14-18
## 804          WHT-B_2-14-18
## 805          WHT-B_2-14-18
## 806          WHT-B_2-14-18
## 807          WHT-B_2-14-18
## 808          WHT-B_2-14-18
## 809          WHT-B_2-14-18
## 810          WHT-B_2-14-18
## 811          WHT-B_2-14-18
## 812          WHT-B_2-14-18
## 813          WHT-B_2-14-18
## 814          WHT-B_2-14-18
## 815          WHT-B_2-14-18
## 816          WHT-B_2-14-18
## 817          WHT-B_2-14-18
## 818          WHT-B_2-14-18
## 819          WHT-B_2-14-18
## 820          WHT-B_2-14-18
## 821          WHT-B_2-14-18
## 822          WHT-B_2-14-18
## 823          WHT-B_2-14-18
## 824          WHT-B_2-14-18
## 825          WHT-B_2-14-18
## 826          WHT-B_2-14-18
## 827          WHT-B_2-14-18
## 828          WHT-B_2-14-18
## 829          WHT-B_2-14-18
## 830          WHT-B_2-14-18
## 831          WHT-B_2-14-18
## 832          WHT-B_2-14-18
## 833          WHT-C_2-14-18
## 834          WHT-C_2-14-18
## 835          WHT-C_2-14-18
## 836          WHT-C_2-14-18
## 837          WHT-C_2-14-18
## 838          WHT-C_2-14-18
## 839          WHT-C_2-14-18
## 840          WHT-C_2-14-18
## 841          WHT-C_2-14-18
## 842          WHT-C_2-14-18
## 843          WHT-C_2-14-18
## 844          WHT-C_2-14-18
## 845          WHT-C_2-14-18
## 846          WHT-C_2-14-18
## 847          WHT-C_2-14-18
```

```
## 848          WHT-C_2-14-18
## 849          WHT-C_2-14-18
## 850          WHT-C_2-14-18
## 851          WHT-C_2-14-18
## 852          WHT-C_2-14-18
## 853          WHT-C_2-14-18
## 854          WHT-C_2-14-18
## 855          WHT-C_2-14-18
## 856          WHT-C_2-14-18
## 857          WHT-C_2-14-18
## 858          WHT-C_2-14-18
## 859          WHT-C_2-14-18
## 860          WHT-C_2-14-18
## 861          WHT-C_2-14-18
## 862          WHT-C_2-14-18
## 863          WHT-C_2-14-18
## 864          WHT-C_2-14-18
## 865          WHT-C_2-14-18
## 866          WHT-C_2-14-18
## 867          WHT-C_2-14-18
## 868          WHT-C_2-14-18
## 869          WHT-C_2-14-18
## 870          WHT-C_2-14-18
## 871          WHT-C_2-14-18
## 872          WHT-C_2-14-18
## 873          WHT-C_2-14-18
## 874          WHT-C_2-14-18
## 875          WHT-C_2-14-18
## 876          WHT-C_2-14-18
## 877          WHT-C_2-14-18
## 878          WHT-C_2-14-18
## 879          WHT-C_2-14-18
## 880          WHT-C_2-14-18
## 881          WHT-C_2-14-18
## 882          WHT-C_2-14-18
## 883          WHT-C_2-14-18
## 884          WHT-D_2-15-18
## 885          WHT-D_2-15-18
## 886          WHT-D_2-15-18
## 887          WHT-D_2-15-18
## 888          WHT-D_2-15-18
## 889          WHT-D_2-15-18
## 890          WHT-D_2-15-18
## 891          WHT-D_2-15-18
## 892          WHT-D_2-15-18
## 893          WHT-D_2-15-18
## 894          WHT-D_2-15-18
## 895          WHT-D_2-15-18
## 896          WHT-D_2-15-18
## 897          WHT-D_2-15-18
## 898          WHT-D_2-15-18
## 899          WHT-D_2-15-18
## 900          WHT-D_2-15-18
## 901          WHT-D_2-15-18
```

```
## 902          WHT-D_2-15-18
## 903          WHT-D_2-15-18
## 904          WHT-D_2-15-18
## 905          WHT-D_2-15-18
## 906          WHT-D_2-15-18
## 907          WHT-D_2-15-18
## 908          WHT-D_2-15-18
## 909          WHT-D_2-15-18
## 910          WHT-D_2-15-18
## 911          WHT-D_2-15-18
## 912          WHT-D_2-15-18
## 913          WHT-D_2-15-18
## 914          WHT-D_2-15-18
## 915          WHT-D_2-15-18
## 916          WHT-D_2-15-18
## 917          WHT-D_2-15-18
## 918          WHT-D_2-15-18
## 919          WHT-D_2-15-18
## 920          WHT-D_2-15-18
## 921          WHT-D_2-15-18
## 922          WHT-D_2-15-18
## 923          WHT-D_2-15-18
## 924          WHT-D_2-15-18
## 925          WHT-D_2-15-18
## 926          WHT-D_2-15-18
## 927          WHT-D_2-15-18
## 928          WHT-D_2-15-18
## 929          WHT-D_2-15-18
## 930          WHT-E_2-15-18
## 931          WHT-E_2-15-18
## 932          WHT-E_2-15-18
## 933          WHT-E_2-15-18
## 934          WHT-E_2-15-18
## 935          WHT-E_2-15-18
## 936          WHT-E_2-15-18
## 937          WHT-E_2-15-18
## 938          WHT-E_2-15-18
## 939          WHT-E_2-15-18
## 940          WHT-E_2-15-18
## 941          WHT-E_2-15-18
## 942          WHT-E_2-15-18
## 943          WHT-E_2-15-18
## 944          WHT-E_2-15-18
## 945          WHT-E_2-15-18
## 946          WHT-E_2-15-18
## 947          WHT-E_2-15-18
## 948          WHT-E_2-15-18
## 949          WHT-E_2-15-18
## 950          WHT-E_2-15-18
## 951          WHT-E_2-15-18
## 952          WHT-E_2-15-18
## 953          WHT-E_2-15-18
## 954          WHT-E_2-15-18
## 955          WHT-E_2-15-18
```

```
## 956          WHT-E_2-15-18
## 957          WHT-E_2-15-18
## 958          WHT-E_2-15-18
## 959          WHT-E_2-15-18
## 960          WHT-E_2-15-18
## 961          WHT-E_2-15-18
## 962          WHT-E_2-15-18
## 963          WHT-E_2-15-18
## 964          WHT-E_2-15-18
## 965          WHT-E_2-15-18
## 966          WHT-E_2-15-18
## 967          WHT-E_2-15-18
## 968          WHT-E_2-15-18
## 969          WHT-E_2-15-18
## 970          WHT-F_2-15-18
## 971          WHT-F_2-15-18
## 972          WHT-F_2-15-18
## 973          WHT-F_2-15-18
## 974          WHT-F_2-15-18
## 975          WHT-F_2-15-18
## 976          WHT-F_2-15-18
## 977          WHT-F_2-15-18
## 978          WHT-F_2-15-18
## 979          WHT-F_2-15-18
## 980          WHT-F_2-15-18
## 981          WHT-F_2-15-18
## 982          WHT-F_2-15-18
## 983          WHT-F_2-15-18
## 984          WHT-F_2-15-18
## 985          WHT-F_2-15-18
## 986          WHT-F_2-15-18
## 987          WHT-F_2-15-18
## 988          WHT-F_2-15-18
## 989          WHT-F_2-15-18
## 990          WHT-F_2-15-18
## 991          WHT-F_2-15-18
## 992          WHT-F_2-15-18
## 993          WHT-F_2-15-18
## 994          WHT-F_2-15-18
## 995          WHT-F_2-15-18
## 996          WHT-F_2-15-18
## 997          WHT-G_2-16-18
## 998          WHT-G_2-16-18
## 999          WHT-G_2-16-18
## 1000         WHT-G_2-16-18
## 1001         WHT-G_2-16-18
## 1002         WHT-G_2-16-18
## 1003         WHT-G_2-16-18
## 1004         WHT-G_2-16-18
## 1005         WHT-G_2-16-18
## 1006         WHT-G_2-16-18
## 1007         WHT-G_2-16-18
## 1008         WHT-G_2-16-18
## 1009         WHT-G_2-16-18
```

```
## 1010          WHT-G_2-16-18
## 1011          WHT-G_2-16-18
## 1012          WHT-G_2-16-18
## 1013          WHT-G_2-16-18
## 1014          WHT-G_2-16-18
## 1015          WHT-G_2-16-18
## 1016          WHT-G_2-16-18
## 1017          WHT-G_2-16-18
## 1018          WHT-G_2-16-18
## 1019          WHT-G_2-16-18
## 1020          WHT-G_2-16-18
## 1021          WHT-G_2-16-18
## 1022          WHT-G_2-16-18
## 1023          WHT-G_2-16-18
## 1024          WHT-G_2-16-18
## 1025          WHT-G_2-16-18
## 1026          WHT-G_2-16-18
## 1027          WHT-G_2-16-18
## 1028          WHT-G_2-16-18
## 1029          WHT-G_2-16-18
## 1030          WHT-G_2-16-18
## 1031          WHT-G_2-16-18
## 1032          WHT-G_2-16-18
## 1033          WHT-G_2-16-18
## 1034          WHT-G_2-16-18
## 1035          WHT-G_2-16-18
## 1036          WHT-G_2-16-18
## 1037          WHT-G_2-16-18
## 1038          WHT-G_2-16-18
## 1039          WHT-G_2-16-18
## 1040          WHT-G_2-16-18
## 1041          WHT-G_2-16-18
## 1042          WHT-G_2-16-18
## 1043          WHT-G_2-16-18
## 1044          WHT-G_2-16-18
## 1045          WHT-G_2-16-18
## 1046          WHT-G_2-16-18
## 1047          WHT-G_2-16-18
## 1048          WHT-G_2-16-18
## 1049          WHT-G_2-16-18
## 1050          WHT-G_2-16-18
## 1051          WHT-G_2-16-18
## 1052          WHT-G_2-16-18
## 1053          WHT-G_2-16-18
## 1054          WHT-G_2-16-18
## 1055          WHT-G_2-16-18
## 1056          WHT-G_2-16-18
## 1057          WHT-G_2-16-18
## 1058          WHT-G_2-16-18
## 1059          WHT-G_2-16-18
## 1060          WHT-G_2-16-18
## 1061          WHT-G_2-16-18
## 1062          WHT-G_2-16-18
## 1063          WHT-G_2-16-18
```

```
## 1064          WHT-H_2-16-18
## 1065          WHT-H_2-16-18
## 1066          WHT-H_2-16-18
## 1067          WHT-H_2-16-18
## 1068          WHT-H_2-16-18
## 1069          WHT-H_2-16-18
## 1070          WHT-H_2-16-18
## 1071          WHT-H_2-16-18
## 1072          WHT-H_2-16-18
## 1073          WHT-H_2-16-18
## 1074          WHT-H_2-16-18
## 1075          WHT-H_2-16-18
## 1076          WHT-H_2-16-18
## 1077          WHT-H_2-16-18
## 1078          WHT-H_2-16-18
## 1079          WHT-H_2-16-18
## 1080          WHT-H_2-16-18
## 1081          WHT-H_2-16-18
## 1082          WHT-H_2-16-18
## 1083          WHT-H_2-16-18
## 1084          WHT-H_2-16-18
## 1085          WHT-H_2-16-18
## 1086          WHT-H_2-16-18
## 1087          WHT-H_2-16-18
## 1088          WHT-H_2-16-18
## 1089          WHT-H_2-16-18
## 1090          WHT-H_2-16-18
## 1091          WHT-H_2-16-18
## 1092          WHT-H_2-16-18
## 1093          WHT-H_2-16-18
## 1094          WHT-H_2-16-18
## 1095          WHT-H_2-16-18
## 1096          WHT-H_2-16-18
## 1097          WHT-H_2-16-18
## 1098          WHT-H_2-16-18
## 1099          WHT-H_2-16-18
## 1100          WHT-H_2-16-18
## 1101          WHT-H_2-16-18
## 1102          WHT-H_2-16-18
## 1103          WHT-H_2-16-18
## 1104          WHT-H_2-16-18
## 1105          WHT-H_2-16-18
##                                                 variable        value
## 1                                  1-Hexanol, 2-ethyl-    6.6500345
## 2                                     2-Acetylthiazole    5.3754333
## 3                                         2-Dodecanone    7.2773113
## 4                                         2-Dodecanone    6.7952937
## 5                                            2-Nonanol    2.0108762
## 6                                           2-Nonanone    3.7570653
## 7                                        2-Tridecanone    3.1030794
## 8                                          2-Undecanol   16.6965492
## 9                                         2-Undecanone   16.2493839
## 10                          2,4-Di-tert-butylphenol    1.2022303
## 11                                     Acetophenone    4.3196327
```

```
## 12                                      Benzene, 1,3-dimethyl-    1.2699423
## 13                                               Benzothiazole    1.7051156
## 14                                               Benzyl alcohol   5.6580648
## 15                                               Benzyl nitrile   1.3152989
## 16                                    Butylated Hydroxytoluene    2.4171401
## 17                               Cyclopentasiloxane, decamethyl-  4.3433226
## 18                                                     Decanal    2.6586334
## 19                                          Dibutyl phthalate    4.0149588
## 20                                                   Dodecanal   1.7306880
## 21                                                   Nonanal     1.6114139
## 22                                                    Phenol    10.2452610
## 23                                        Phenylethyl Alcohol    8.7019358
## 24                                   Pyrazine, 2-ethyl-5-methyl-  0.4197620
## 25                                       Pyrazine, 2,5-dimethyl-  72.6067621
## 26                                                    Styrene    7.4828002
## 27                                         1-Hexanol, 2-ethyl-   17.6188336
## 28   1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester    5.2753408
## 29                                     1,3,5,7-Cyclooctatetraene  11.6149372
## 30                                           2-Acetylthiazole   13.8875485
## 31                                                  2-Decanol    4.7156945
## 32                                                  2-Decanol    1.7644606
## 33                                                 2-Decanone    7.7215999
## 34                                                 2-Dodecanol   4.3075456
## 35                                                2-Dodecanone  56.2808981
## 36                                                2-Dodecanone  49.3141984
## 37                                                2-Dodecanone   7.9084549
## 38                                                 2-Heptanone  30.4159185
## 39                                           2-Heptanone, 4-methyl-  1.6550352
## 40                                           2-Heptanone, 5-methyl-  10.1800148
## 41                                           2-Heptanone, 6-methyl-  20.0517098
## 42                                                  2-Nonanol   13.7311892
## 43                                                 2-Nonanone    2.0090620
## 44                          2-Pentadecanone, 6,10,14-trimethyl-   3.7735580
## 45                                                2-Tridecanone   4.5340674
## 46                                                  2-Undecanol   3.0646101
## 47                                                 2-Undecanone  76.5065510
## 48                                     2,4-Di-tert-butylphenol    4.7198144
## 49                                    5-Hepten-2-one, 6-methyl-   3.4631139
## 50                          5,9-Undecadien-2-one, 6,10-dimethyl-   3.5273979
## 51                                                Acetophenone   16.9137176
## 52                                                Benzophenone    3.7535148
## 53                                                Benzothiazole   3.0062528
## 54                                                Benzyl alcohol  12.0113530
## 55                                    Butanoic acid, 2-methyl-   89.1684545
## 56                                    Butanoic acid, 2-methyl-   54.6742991
## 57                                    Butylated Hydroxytoluene   13.5142496
## 58                               Cyclohexasiloxane, dodecamethyl-  22.2301655
## 59                                                     Decanal   17.0781791
## 60                                          Dibutyl phthalate   21.5006189
## 61                                                   Dodecanal    8.1870675
## 62                             Ethanone, 1-(1H-pyrrol-2-yl)-     5.0960446
## 63                                                  Hexadecane    5.8548469
## 64                                                  Homosalate    7.5690780
## 65                                                  Nonadecane    9.6173790
```

```
## 66                                                Nonadecane    8.5785582
## 67                                                Nonadecane    7.6046293
## 68                                                Nonadecane    5.1543247
## 69                                                  Nonanal    9.2774648
## 70                                    Octadecane, 2-methyl-    4.6908092
## 71                                                  Phenol   58.0673620
## 72                                     Phenylethyl Alcohol   23.3281495
## 73                                 Pyrazine, 2-ethyl-5-methyl-    6.3275237
## 74                                 Pyrazine, 2-ethyl-6-methyl-    3.4076961
## 75                                     Pyrazine, 2,5-dimethyl-  257.5152757
## 76                                    Quinoline, 4-methyl-    2.0570060
## 77                                                 Undecanal    2.2408101
## 78                                      1-Hexanol, 2-ethyl-   26.0304185
## 79   1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester    5.6969650
## 80                                          2-Acetylthiazole   15.6007987
## 81                                                2-Decanol    6.9168614
## 82                                                2-Decanol    3.2019037
## 83                                               2-Decanone   27.2688741
## 84                                              2-Dodecanol   14.5092481
## 85                                              2-Dodecanol    5.2419060
## 86                                             2-Dodecanone   74.0214275
## 87                                             2-Dodecanone   62.3946735
## 88                                             2-Dodecanone   10.5721017
## 89                                             2-Dodecanone    5.1009865
## 90                                              2-Heptanone   35.9337628
## 91                                  2-Heptanone, 4-methyl-    2.9329050
## 92                                  2-Heptanone, 5-methyl-    9.7369420
## 93                                  2-Heptanone, 6-methyl-   11.2484003
## 94                                              2-Nonanol   16.9867210
## 95                                             2-Nonanone    5.4012247
## 96                       2-Pentadecanone, 6,10,14-trimethyl-    1.7288602
## 97                                          2-Tridecanone    8.2849691
## 98                                            2-Undecanol    1.7696954
## 99                                           2-Undecanone   85.6594893
## 100                                2,4-Di-tert-butylphenol    1.2810519
## 101                               5-Hepten-2-one, 6-methyl-    5.0980120
## 102                                           Acetophenone   19.9122526
## 103                                           Benzaldehyde    5.8562564
## 104                                           Benzophenone    3.6756221
## 105                                          Benzothiazole    2.3874828
## 106                                         Benzyl alcohol   12.5460786
## 107                                         Benzyl nitrile    4.7360531
## 108                              Butanoic acid, 2-methyl-   60.7921356
## 109                              Butanoic acid, 2-methyl-   42.8027293
## 110                              Butylated Hydroxytoluene   18.9803320
## 111                 Cyclohexasiloxane, dodecamethyl-    2.4653752
## 112                  Cyclotetrasiloxane, octamethyl-   40.8301504
## 113                                           Decanal   13.0263630
## 114                                Dibutyl phthalate   13.2991510
## 115                                           Dodecanal    7.4018190
## 116                       Ethanone, 1-(1H-pyrrol-2-yl)-    7.4891637
## 117                            Ethanone, 1-(2-furanyl)-    1.1209390
## 118                                         Heneicosane    2.4780050
## 119                                        Hexanoic acid    4.6006318
```

```
## 120                                                Homosalate    6.3306272
## 121                                                  Mequinol    1.0552223
## 122                                                Nonadecane    5.4010127
## 123                                                Nonadecane    5.2885963
## 124                                                Nonadecane    4.3038990
## 125                                                Nonadecane    4.0264555
## 126                                                  Nonanal    7.7612351
## 127                                                   Phenol   57.1058092
## 128                                       Phenylethyl Alcohol   26.9545029
## 129                                  Pyrazine, 2-ethyl-6-methyl-    3.4115749
## 130                                     Pyrazine, 2,5-dimethyl-   23.3128396
## 131                                Pyrazine, 3-ethyl-2,5-dimethyl-    8.4726124
## 132                                      Quinoline, 4-methyl-    2.3414263
## 133                                                   Styrene   17.8927573
## 134                                                Undecanal    1.7161530
## 135                                       1-Hexanol, 2-ethyl-    9.8924589
## 136                                       1,2-Benzisothiazole    2.2436773
## 137                                          2-Acetylthiazole    4.1340859
## 138                                                 2-Decanol    2.1719553
## 139                                              2-Dodecanone    1.3769484
## 140                                              2-Heptanone    8.9928027
## 141                                    2-Heptanone, 5-methyl-    4.2741641
## 142                                    2-Heptanone, 6-methyl-    3.4245927
## 143                                                 2-Nonanol    4.4031767
## 144                                              2-Nonanone    5.2880483
## 145                                              2-Undecanol   61.1016402
## 146                                             2-Undecanone   38.6435223
## 147                  5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-    1.5692492
## 148                                             Acetophenone    7.3663525
## 149                                             Benzaldehyde    2.2783580
## 150                                              Benzyl alcohol    3.8088126
## 151                                              Benzyl nitrile    1.3809379
## 152                                  Butanoic acid, 2-methyl-   89.9400090
## 153                                  Butanoic acid, 2-methyl-   31.1796447
## 154                                  Butylated Hydroxytoluene    1.3833714
## 155                        Cyclooctasiloxane, hexadecamethyl-    2.4488962
## 156                           Cyclotetrasiloxane, octamethyl-    9.3866746
## 157                                                 Decanal   12.4146765
## 158                                       Dibutyl phthalate    3.8784364
## 159                                                 Dodecanal    1.7560419
## 160                                               Heptadecane    2.0805199
## 161                        Heptadecane, 2,6,10,15-tetramethyl-    2.9555456
## 162                                               Nonadecane    2.1675859
## 163                                                  Nonanal    7.1022544
## 164                                    Octadecane, 2-methyl-    1.5405147
## 165                                                  Octanal    4.6752910
## 166                                                   Phenol   30.9346703
## 167                                       Phenylethyl Alcohol    6.7198787
## 168                                    Pyrazine, 2,5-dimethyl-    6.3972000
## 169                                Pyrazine, 3-ethyl-2,5-dimethyl-    2.8426084
## 170                                                   Styrene    5.7524973
## 171  1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester    6.6529145
## 172                                    1,3,5,7-Cyclooctatetraene   21.0549243
## 173                                          2-Acetylthiazole   22.8410653
```

```
## 174                                      2-Decanone    3.7409159
## 175                                     2-Dodecanone   45.3880817
## 176                                     2-Dodecanone   37.4247288
## 177                                     2-Dodecanone    4.0212040
## 178                                  2-Ethyl-1-hexanol  106.7993291
## 179                               2-Heptanone, 4-methyl-    4.6794350
## 180                               2-Heptanone, 6-methyl-    4.8480445
## 181                                       2-Nonanol   11.7274977
## 182                                      2-Nonanone   18.9975548
## 183                 2-Pentadecanone, 6,10,14-trimethyl-    6.7909454
## 184                                   2-Tridecanone    2.7006361
## 185                                     2-Undecanol  219.8963142
## 186                                     2-Undecanol    9.7981699
## 187                                    2-Undecanone  151.3395269
## 188                          5-Isoquinolinecarbonitrile    1.4695588
## 189                                    Acetophenone   22.9942389
## 190                                    Benzaldehyde    6.4009942
## 191                               Benzeneacetaldehyde    2.2898686
## 192                                    Benzophenone    3.4021169
## 193                                    Benzothiazole    7.3013852
## 194                                 Benzyl alcohol   36.6750435
## 195                                 Benzyl nitrile    5.2618876
## 196                           Butanoic acid, 2-methyl-  112.0928717
## 197                           Butanoic acid, 2-methyl-   79.7067448
## 198                           Butanoic acid, 2-methyl-   72.4817908
## 199                           Butanoic acid, 2-methyl-   50.1326663
## 200                          Butylated Hydroxytoluene    4.8622370
## 201                                       Caprolactam   13.9051132
## 202                     Cyclohexasiloxane, dodecamethyl-    2.5745402
## 203                    Cyclooctasiloxane, hexadecamethyl-    3.0122059
## 204                       Cyclotetrasiloxane, octamethyl-   43.0280020
## 205                                         Decanal   31.9573613
## 206                              Dibutyl phthalate   23.8102989
## 207                                  Diphenylamine    4.8376093
## 208                                      Dodecanal    6.6488058
## 209                 Ethanone, 1-(1H-pyrrol-2-yl)-    8.0669169
## 210                                   Heneicosane    1.3356828
## 211                                     Homosalate   15.9354159
## 212                                       Mequinol    1.2002467
## 213                                     Nonadecane   15.8335905
## 214                                     Nonadecane   11.3959895
## 215                                     Nonadecane    7.6763095
## 216                                     Nonadecane    5.5532409
## 217                                        Nonanal   18.5864724
## 218                                         Phenol  101.1294214
## 219                              Phenylethyl Alcohol   30.0225734
## 220                    Pyrazine, 2-ethyl-6-methyl-    2.2533194
## 221                       Pyrazine, 2,5-dimethyl-  268.3348949
## 222                  Pyrazine, 3-ethyl-2,5-dimethyl-    8.8135346
## 223                           Quinoline, 4-methyl-    2.8126623
## 224                                    Tetracosane    7.4401273
## 225                                   Tetradecanal    2.7961777
## 226                                   Tetradecanal    1.8442003
## 227                                      Undecanal    5.5783378
```

```
## 228                                1-Isoquinolinecarbonitrile    1.8125685
## 229 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester    1.8291309
## 230                                     1,2-Benzisothiazole    4.3655214
## 231                   2-(3-Methylbutyl)-3,5-dimethylpyrazine    1.6163618
## 232                                       2-Acetylthiazole   14.3994609
## 233                           2-Butenoic acid, 2-methyl-, (Z)-    2.0340757
## 234                                              2-Decanol   13.3529659
## 235                                              2-Decanol    7.9999045
## 236                                              2-Decanol    2.6430401
## 237                                            2-Dodecanol    7.3189748
## 238                                           2-Dodecanone   24.5797235
## 239                                           2-Dodecanone    4.5205383
## 240                                           2-Dodecanone    3.9014327
## 241                                         2-Ethyl-1-hexanol   19.4110971
## 242                                            2-Heptanone   11.0629652
## 243                                  2-Heptanone, 5-methyl-    8.2028998
## 244                                  2-Heptanone, 6-methyl-   10.0143780
## 245                       2-Methyl-3-isopropylpyrazine    3.4180823
## 246                                              2-Nonanol   16.2008371
## 247                                             2-Nonanone    0.0000000
## 248                                          2-Tetradecanol   16.4054320
## 249                                           2-Tridecanone    6.0766516
## 250                                           2-Tridecanone    3.2588136
## 251                                             2-Undecanol    1.8625977
## 252                                             2-Undecanol    1.6416852
## 253                                            2-Undecanone  102.7276983
## 254                               5-Hepten-2-one, 6-methyl-    7.3608447
## 255                 5,9-Undecadien-2-one, 6,10-dimethyl-    6.1801477
## 256                                          Acetophenone   21.9602170
## 257                             Benzene, (1-methyldecyl)-    2.1936438
## 258                             Benzene, (1-methylnonyl)-    1.6326564
## 259                                          Benzophenone    3.9605852
## 260                                       Benzyl alcohol   14.7600825
## 261                                       Benzyl nitrile    4.0495846
## 262                              Butanoic acid, 2-methyl-  297.1855304
## 263                              Butanoic acid, 2-methyl-  255.5469226
## 264                              Butanoic acid, 2-methyl-  171.7572986
## 265                              Butanoic acid, 2-methyl-  171.5066970
## 266                              Butanoic acid, 2-methyl-  145.2670342
## 267                              Butanoic acid, 2-methyl-  129.2538365
## 268                              Butanoic acid, 2-methyl-  100.9046441
## 269                              Butanoic acid, 2-methyl-   60.9543472
## 270                              Butanoic acid, 2-methyl-   39.2631060
## 271                  Butanoic acid, 3-bromo-3-methyl-    4.8446117
## 272                              Butanoic acid, 3-methyl-  195.5899345
## 273                              Butanoic acid, 3-methyl-  117.7723740
## 274                              Butanoic acid, 3-methyl-  115.6378605
## 275                              Butylated Hydroxytoluene    5.9696219
## 276                                          Caprolactam    2.9891146
## 277                                              Decanal   41.1838265
## 278                                     Dibutyl phthalate    5.2381131
## 279                                         Diphenylamine    3.7767195
## 280                                              Dodecanal    5.4945205
## 281                        Ethanone, 1-(1H-pyrrol-2-yl)-    7.8999626
```

```
## 282                                          Heptadecane    2.7260058
## 283                                             Mequinol    1.0512603
## 284                                           Nonadecane    2.7459971
## 285                                           Nonadecane    2.0951777
## 286                                              Nonanal   20.5613017
## 287                                              Octanal   11.7766871
## 288                                               Phenol  153.9824645
## 289                                    Phenylethyl Alcohol   30.2390712
## 290                        Pyrazine, 2-ethyl-6-methyl-    1.8683596
## 291                            Pyrazine, 2,5-dimethyl-  344.7420609
## 292                            Pyrazine, 2,5-dimethyl-    9.4984172
## 293                  Pyrazine, 3-ethyl-2,5-dimethyl-   13.4728999
## 294                               Pyrazine, trimethyl-   29.5233956
## 295                           Quinazoline, 4-methyl-    1.5938189
## 296                             Quinoline, 4-methyl-    2.8023074
## 297                                          Undecanal    5.2454645
## 298                           1-Hexanol, 2-ethyl-    3.1619170
## 299                              2-Acetylthiazole    2.0646915
## 300                                 2-Tridecanone    1.8628138
## 301                                   2-Undecanol   11.6153746
## 302                                  2-Undecanone    8.9851968
## 303                                  Acetophenone    2.3382203
## 304                                Benzyl alcohol    3.3170546
## 305                  Cyclopentasiloxane, decamethyl-    3.1406278
## 306                                         Decanal    3.3371213
## 307                                Dibutyl phthalate    2.3756059
## 308                                       Nonadecane    1.3253602
## 309                                          Nonanal    2.5074034
## 310                                           Phenol   12.8051693
## 311                                Phenylethyl Alcohol    3.3371089
## 312                            Pyrazine, 2,5-dimethyl-   26.4096427
## 313                                          Styrene    3.7631542
## 314                        1-Isoquinolinecarbonitrile    2.8028573
## 315  1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester   10.8410236
## 316                                 2-Acetylthiazole   19.4526941
## 317                    2-Butenoic acid, 2-methyl-, (Z)-    2.7495252
## 318                                         2-Decanol   13.9349258
## 319                                         2-Decanol    8.4806146
## 320                                         2-Decanol    2.1497471
## 321                                        2-Decanone   10.2175821
## 322                                        2-Dodecanol    8.2719544
## 323                                       2-Dodecanone   57.6719461
## 324                                       2-Dodecanone   41.7181647
## 325                                       2-Dodecanone    7.6995580
## 326                                       2-Dodecanone    7.1758655
## 327                                       2-Dodecanone    2.4220934
## 328                                    2-Ethyl-1-hexanol   21.9979834
## 329                                 2-Heptanone, 4-methyl-    4.7492379
## 330                                 2-Heptanone, 5-methyl-    8.8184748
## 331                                 2-Heptanone, 6-methyl-   10.4640352
## 332                                         2-Nonanol   16.8321357
## 333                                        2-Nonanone    4.7495238
## 334                  2-Pentadecanone, 6,10,14-trimethyl-    8.2712470
## 335                                      2-Tetradecanol    7.0000122
```

```
## 336                                        2-Tridecanone    9.6036232
## 337                                          2-Undecanol  202.5499610
## 338                                          2-Undecanol   20.1967416
## 339                                         2-Undecanone  108.0430771
## 340                          5-Hepten-2-one, 6-methyl-    10.0373010
## 341               5,9-Undecadien-2-one, 6,10-dimethyl-    9.8026988
## 342                           9H-Fluorene, 9-methylene-    8.6350966
## 343                                        Acetophenone   23.9444361
## 344                                        Benzaldehyde    9.0239192
## 345                                        Benzophenone    7.0149767
## 346                                       Benzothiazole    2.6679636
## 347                                     Benzyl alcohol   24.0315942
## 348                                     Benzyl nitrile    5.1732333
## 349                          Butanoic acid, 2-methyl-  442.3495753
## 350                          Butanoic acid, 2-methyl-  271.3274104
## 351                          Butanoic acid, 2-methyl-  239.4303078
## 352                          Butanoic acid, 2-methyl-  184.3016494
## 353                          Butanoic acid, 2-methyl-  141.1966067
## 354                          Butanoic acid, 2-methyl-  107.0487572
## 355                          Butanoic acid, 2-methyl-   67.2499424
## 356                          Butanoic acid, 2-methyl-   53.6590070
## 357              Butanoic acid, 3-bromo-3-methyl-    6.8922351
## 358                          Butanoic acid, 3-methyl-  201.3439391
## 359                          Butanoic acid, 3-methyl-  174.0705841
## 360                          Butanoic acid, 3-methyl-  145.4487641
## 361                          Butanoic acid, 3-methyl-  115.9803085
## 362                          Butanoic acid, 3-methyl-  107.9741202
## 363                          Butylated Hydroxytoluene    4.0734415
## 364                                         Caprolactam   11.3111922
## 365              Cyclohexasiloxane, dodecamethyl-    1.9465111
## 366                                            Decanal   42.8493443
## 367                                 Dibutyl phthalate   26.5990394
## 368                                     Diphenylamine    2.6818031
## 369                                        Dodecanal    2.5829545
## 370                 Ethanone, 1-(1H-pyrrol-2-yl)-   10.0725596
## 371                                         Hexadecane    9.5689839
## 372                                         Homosalate   17.6392511
## 373                                         Nonadecane   18.4203723
## 374                                         Nonadecane   13.3626715
## 375                                         Nonadecane    4.7422332
## 376                                            Nonanal   23.8565997
## 377                                         Octadecane    2.5494493
## 378                           Octadecane, 2-methyl-    3.7881772
## 379                                            Octanal   13.3559822
## 380                                             Phenol  179.0365068
## 381                               Phenylethyl Alcohol   39.0457475
## 382                  Pyrazine, 2-ethyl-5-methyl-   15.3939008
## 383                  Pyrazine, 2-ethyl-6-methyl-    2.5570296
## 384                      Pyrazine, 2,5-dimethyl-  362.3266589
## 385 Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-    3.0215678
## 386            Pyrazine, 3-ethyl-2,5-dimethyl-   15.4314755
## 387                        Pyrazine, trimethyl-   18.9489047
## 388                     Quinazoline, 4-methyl-    3.8715255
## 389                       Quinoline, 4-methyl-    3.6156125
```

```
## 390                                  Tetradecanal    3.9392861
## 391                                     Undecanal    6.7819772
## 392                          1-Hexanol, 2-ethyl-    1.9377118
## 393                             2-Acetylthiazole    1.3859288
## 394                                 2-Dodecanone    1.3034054
## 395                                  2-Undecanol    6.1454250
## 396                                 2-Undecanone    3.9405616
## 397                                 Acetophenone    1.2460300
## 398                                Benzyl alcohol    1.8857495
## 399          Cyclopentasiloxane, decamethyl-    3.4524964
## 400          Cyclotetrasiloxane, octamethyl-    6.2014475
## 401                                     Decanal    1.9830436
## 402                           Dibutyl phthalate    1.4403867
## 403                                     Nonanal    1.8086712
## 404                                      Phenol    6.2365222
## 405                          Phenylethyl Alcohol    1.3379664
## 406                 Pyrazine, 2,5-dimethyl-   18.3928557
## 407                                     Styrene    2.0797417
## 408                          1-Hexanol, 2-ethyl-    8.6531823
## 409                                  1-Nonanol    3.1320763
## 410                       1-Phenyl-2-propanone    8.3666581
## 411          1,3-Cyclopentadiene, 5-methyl-   68.9530612
## 412                                 2-Heptanone   58.2828787
## 413                                2-Tridecanone   11.9304613
## 414                                 2-Undecanone    8.1747317
## 415                  2,4,4-Trimethyl-1-hexene   16.0955324
## 416              2,4,6-Cycloheptatrien-1-one    9.1668172
## 417                                 Acetophenone   12.9676654
## 418                                      Anisole  459.7465773
## 419                                Benzaldehyde    7.5833237
## 420             Benzene, 1-chloro-2-methoxy-    4.8383428
## 421           Benzene, 1-isocyano-2-methyl-    6.3940428
## 422            Benzene, 1-methoxy-4-methyl-    8.0077813
## 423                 Benzene, 1,3-dimethyl-    3.0577415
## 424                           Benzophenone    4.4085171
## 425                          Benzothiazole    3.2954604
## 426          Bicyclo[4.2.0]octa-1,3,5-triene   14.2804652
## 427                 Butylated Hydroxytoluene    3.9832746
## 428                               Caprolactam    6.4413997
## 429          Cyclohexasiloxane, dodecamethyl-    7.1649849
## 430          Cyclopentasiloxane, decamethyl-   21.4129014
## 431                                     Decanal   68.4585199
## 432                           Dibutyl phthalate    5.7893614
## 433                           Diethyl Phthalate   28.7674167
## 434                         Dimethyl trisulfide   59.2541216
## 435           Ethanone, 1-(1H-pyrrol-2-yl)-   11.9484283
## 436            Ethanone, 1-(2-aminophenyl)-   13.2053773
## 437                Ethanone, 1-(2-furanyl)-    2.1175934
## 438                                Heptadecane    2.9103486
## 439              Methane, oxybis[dichloro-    6.4129277
## 440                                Nonadecane    4.6381782
## 441                                Nonadecane    3.4713133
## 442                                   Nonanal   64.3106262
## 443                                   Octanal   30.8987184
```

```
## 444                                                 Phenol  680.4461633
## 445                                          Phenol, 2-iodo-    5.6086718
## 446                                        Phenol, 2-methoxy-   95.4485687
## 447                                          Phenol, 3-ethyl-    3.4821953
## 448                                       Phenylethyl Alcohol  141.4386474
## 449                                  Pyrazine, 2-ethyl-5-methyl-   16.5933014
## 450                                  Pyrazine, 2-ethyl-6-methyl-    3.3387659
## 451                                     Pyrazine, 2,5-dimethyl- 1142.9020819
## 452                  Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-    2.6901969
## 453                           Pyrazine, 3-ethyl-2,5-dimethyl-   15.7825960
## 454                                   Quinazoline, 4-methyl-    4.7068097
## 455                                               Undecanal    5.3612489
## 456                                     1-Hexanol, 2-ethyl-    8.4859440
## 457                                               1-Nonanol    4.0185303
## 458                                    1-Phenyl-2-propanone    4.9586103
## 459  1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester    1.5990470
## 460                           1,3-Cyclopentadiene, 5-methyl-   85.6390608
## 461                                              2-Heptanone   45.8300465
## 462                                                2-Nonanol    1.5863984
## 463                                               2-Nonanone    3.7794509
## 464                                  2-Pyrrolidinone, 1-methyl-    1.1001868
## 465                                             2-Tridecanone   11.0251223
## 466                                             2-Undecanone    9.0467261
## 467                                2,4,6-Cycloheptatrien-1-one    7.6902916
## 468                      5,9-Undecadien-2-one, 6,10-dimethyl-    3.4675568
## 469                                             Acetophenone   14.6512837
## 470                                                  Anisole  283.1868761
## 471                               Benzene, 1-chloro-2-methoxy-    2.7169673
## 472                               Benzene, 1-methoxy-4-methyl-    4.6644299
## 473                                             Benzophenone    3.3296847
## 474                                            Benzothiazole    1.4116127
## 475                                           Benzyl nitrile    3.4367910
## 476                                Butylated Hydroxytoluene    5.3436229
## 477                                              Caprolactam   12.3925674
## 478                                          Cyclohept-4-enone    9.2844268
## 479                         Cyclohexasiloxane, dodecamethyl-    7.8838677
## 480                                          Cyclooctene, (Z)-    2.6484326
## 481                          Cyclopentasiloxane, decamethyl-   44.8181997
## 482                                    Cyclopropane, pentyl-    0.5581797
## 483                          Cyclotetrasiloxane, octamethyl-   47.9597554
## 484                                               Decanal   91.7330039
## 485                                        Dibutyl phthalate    5.9431409
## 486                                        Diethyl Phthalate   34.7043225
## 487                                       Dimethyl trisulfide   23.8496534
## 488                          Ethanone, 1-(1H-pyrrol-2-yl)-    6.8038667
## 489                               Furan, 2-ethyl-5-methyl-    0.6061785
## 490                                             Homosalate    4.3224256
## 491                                             Nonadecane    4.8624568
## 492                                             Nonadecane    2.5721708
## 493                                                Nonanal   55.6263315
## 494                                                Octanal   28.1028631
## 495                                                 Phenol  434.4276935
## 496                                          Phenol, 2-iodo-    3.8783080
## 497                                        Phenol, 2-methoxy-   51.4021731
```

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## 498                                    Phenol, 3-ethyl-    1.6337791
## 499                                Phenylethyl Alcohol  112.7700944
## 500                      Pyrazine, 2-ethyl-6-methyl-    2.5177398
## 501                         Pyrazine, 2,5-dimethyl-  701.8826881
## 502 Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-    1.8917362
## 503           Pyrazine, 3-ethyl-2,5-dimethyl-   10.8227407
## 504                    Quinazoline, 4-methyl-    1.9915277
## 505                                    Styrene   10.5776721
## 506                                  Undecanal    7.3476380
## 507                                  1-Nonanol    5.0563658
## 508                       1-Phenyl-2-propanone    9.0035169
## 509                       1,2-Benzisothiazole    5.2832461
## 510           1,3-Cyclopentadiene, 5-methyl-   45.8879648
## 511                1,3,5,7-Cyclooctatetraene   36.1938793
## 512                      2-Ethyl-1-hexanol   40.6383783
## 513                          2-Tridecanone   12.0458968
## 514             2,4,6-Cycloheptatrien-1-one   17.7206542
## 515                      3-Aminoacetophenone   10.8615058
## 516                                  Anisole 1012.5634058
## 517             Benzene, 1-chloro-2-methoxy-    4.5738975
## 518             Benzene, 1-methoxy-4-methyl-   12.8226816
## 519                           Benzophenone    4.4348772
## 520                       Benzyl nitrile    9.1917022
## 521                  Butanoic acid, 2-methyl-  146.5561267
## 522                  Butanoic acid, 2-methyl-  143.6706523
## 523                  Butanoic acid, 2-methyl-   96.6812549
## 524                  Butanoic acid, 2-methyl-   86.9090136
## 525                  Butanoic acid, 2-methyl-   28.6921665
## 526                  Butanoic acid, 2-methyl-   10.5742026
## 527                  Butylated Hydroxytoluene    7.2960693
## 528                       Cyclohept-4-enone   15.2571098
## 529          Cyclohexasiloxane, dodecamethyl-   10.9166412
## 530                       Cyclooctene, (Z)-    5.9635829
## 531                                  Decanal  232.8347647
## 532                       Dibutyl phthalate   13.7327371
## 533                       Diethyl Phthalate    9.5824453
## 534                      Dimethyl trisulfide   35.6574138
## 535        Ethanone, 1-(1H-pyrrol-2-yl)-   41.6065018
## 536             Formamide, N,N-dibutyl-   26.9157483
## 537           Heptadecane, 2,6-dimethyl-    5.7839966
## 538                           Nonadecane    6.0927024
## 539                           Nonadecane    4.3741416
## 540                              Nonanal  209.6942003
## 541                              Octanal   63.2045465
## 542                   Octane, 1-chloro-   11.6685904
## 543                                Phenol  933.1921556
## 544                    Phenol, 2-methoxy-  366.4634937
## 545                   Phenylethyl Alcohol   86.8667310
## 546              Pyrazine, 2-ethyl-5-methyl-   17.5492908
## 547              Pyrazine, 2-ethyl-6-methyl-    4.2697481
## 548                 Pyrazine, 2,5-dimethyl- 1702.6889391
## 549           Pyrazine, 3-ethyl-2,5-dimethyl-   18.3766086
## 550                Pyridine, 2,4,6-trimethyl-    4.0779040
## 551                                  Undecanal   18.7925733
```

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## 552                                1,3,5,7-Cyclooctatetraene    3.8438404
## 553                                 2,3,3-Trimethyl-1-hexene   11.3649907
## 554                                 2,4,4-Trimethyl-1-hexene   19.1830271
## 555                                 2,4,4-Trimethyl-1-hexene   17.2952152
## 556                                5-Hepten-2-one, 6-methyl-   10.3020585
## 557                                             Benzaldehyde    4.9002909
## 558                           Benzene, 3-cyclohexen-1-yl-    4.4721832
## 559                       Cyclohexasiloxane, dodecamethyl-    4.8988713
## 560        Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-   36.7090280
## 561                       Cyclopentasiloxane, decamethyl-   24.3568764
## 562                       Cyclotetrasiloxane, octamethyl-   16.1892184
## 563                       Cyclotetrasiloxane, octamethyl-    8.7822703
## 564                                              Decanal    8.9852868
## 565                                               Phenol   41.1375765
## 566                                   Phenylethyl Alcohol   39.7331235
## 567                                 Pyrazine, 2,5-dimethyl-   82.1273267
## 568                                 Pyrazine, 2,5-dimethyl-   32.2695051
## 569                          1,3-Cyclopentadiene, 5-methyl-   34.4588735
## 570                                             2-Heptanone   42.2132979
## 571                            2-Methyl-3-isopropylpyrazine   16.3376727
## 572                                           2-Tridecanone    5.3723251
## 573                                           2-Undecanone    7.2414109
## 574                                2,4-Di-tert-butylphenol    8.5852337
## 575                               2,4,4-Trimethyl-1-hexene    8.3197064
## 576                             2,4,6-Cycloheptatrien-1-one    7.0416717
## 577                                  3-Aminoacetophenone    8.4039072
## 578                          3-Penten-1-ol, 2,2,4-trimethyl-   37.0430576
## 579                              5-Decen-1-ol, acetate, (E)-   13.6904186
## 580                                5-Hepten-2-one, 6-methyl-    5.3120000
## 581              5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-    6.9043447
## 582                                           Acetophenone   17.2116229
## 583                                                Anisole  679.1442827
## 584                             Benzene, 1-isocyano-2-methyl-    6.9926935
## 585                             Benzene, 1-methoxy-4-methyl-    7.9277859
## 586                             Benzene, 3-cyclohexen-1-yl-    4.4719101
## 587                                           Benzophenone    2.6727709
## 588                                  Benzyl methyl ketone    8.9300674
## 589                          Bicyclo[4.2.0]octa-1,3,5-triene   16.5629860
## 590                                 Butylated Hydroxytoluene    4.8190914
## 591                                               Caprolactam    4.8281082
## 592                          Cyclohexasiloxane, dodecamethyl-    8.5221453
## 593                                       Cyclooctene, (Z)-    2.3621496
## 594                          Cyclopentasiloxane, decamethyl-   33.2451445
## 595                          Cyclotetrasiloxane, octamethyl-   69.8356009
## 596                                             D-Limonene   51.3382598
## 597                                                Decanal   38.7699773
## 598                                     Dibutyl phthalate    9.0820210
## 599                                     Diethyl Phthalate    3.5612305
## 600                                   Dimethyl trisulfide   39.3885624
## 601                             Ethanone, 1-(1H-pyrrol-2-yl)-   14.2229144
## 602                                             Nonadecane    4.8265292
## 603                                             Nonadecane    4.2467365
## 604                                                Nonanal   55.4971643
## 605                                               Phenol   70.5164135
```

```
## 606                                    Phenol, 2-methoxy-  103.7700912
## 607                                  Phenylethyl Alcohol   57.9550308
## 608                       Pyrazine, 2-ethyl-5-methyl-   15.8209404
## 609                       Pyrazine, 2-ethyl-6-methyl-    1.7258930
## 610                          Pyrazine, 2,5-dimethyl- 1660.6082104
## 611                     Pyrazine, 3-ethyl-2,5-dimethyl-   11.8879541
## 612                                       Tetradecane    2.3392090
## 613                                        Undecanal    3.1100902
## 614                  Cyclohexasiloxane, dodecamethyl-   10.8100963
## 615                   Cyclopentasiloxane, decamethyl-   11.0151026
## 616                   Cyclotetrasiloxane, octamethyl-    1.8503900
## 617                                       Nonadecane    1.6239626
## 618                                       Tetradecane    1.3924478
## 619                                         1-Nonanol    2.7189277
## 620                        2,3,3-Trimethyl-1-hexene   11.7282555
## 621                        2,4,4-Trimethyl-1-hexene   21.1598868
## 622                        2,4,4-Trimethyl-1-hexene   11.9727563
## 623                  4,8,12,16-tetraoxaeicosan-1-ol    8.1297693
## 624                       5-Hepten-2-one, 6-methyl-    1.6748076
## 625                                    Acetophenone    1.6659351
## 626                                         Anisole   84.7934938
## 627                       Benzaldehyde, 3-ethyl-    1.2846816
## 628                    Benzene, 3-cyclohexen-1-yl-    2.9605389
## 629                                    Benzyl nitrile    1.8276971
## 630                  Cyclohexasiloxane, dodecamethyl-    8.2537710
## 631                   Cyclopentasiloxane, decamethyl-   44.5223715
## 632                   Cyclotetrasiloxane, octamethyl-   33.0057132
## 633                                         Decanal    9.0516948
## 634                                  Dibutyl phthalate    1.9250960
## 635                Ethanone, 1-(3,4-dimethylphenyl)-   15.8054853
## 636                     Ethanone, 1-(4-ethylphenyl)-    6.1829464
## 637                                       Eucalyptol    8.2809087
## 638                                         Limonene   23.6424509
## 639                                          Nonanal   13.0988569
## 640                                           Phenol   34.9575799
## 641                                  Phenol, 2-methoxy-    5.1309476
## 642                                  Phenylethyl Alcohol   20.0461951
## 643       Propanol, [(butoxymethylethoxy)methylethoxy]-    8.1237318
## 644       Propanol, [(butoxymethylethoxy)methylethoxy]-    3.3412369
## 645                          Pyrazine, 2,5-dimethyl-   81.6849212
## 646                          Pyrazine, 2,5-dimethyl-   29.3406157
## 647                                          Styrene    3.0765510
## 648                                         1-Nonanol    3.8572212
## 649                               1-Phenyl-2-propanone    4.7702936
## 650                   1,3-Cyclopentadiene, 5-methyl-   79.6490327
## 651                1,3,5-Cycloheptatriene, 1-methoxy-    3.6402337
## 652                          1,3,5,7-Cyclooctatetraene   21.2903101
## 653                                       2-Heptanone   57.6002914
## 654                                     2-Tridecanone    9.3491260
## 655                                     2-Undecanone    6.8454602
## 656                          2,4-Di-tert-butylphenol    4.6662924
## 657                       2,4,6-Cycloheptatrien-1-one    1.6825589
## 658                       5-Decen-1-ol, acetate, (E)-   19.8920851
## 659                5,9-Undecadien-2-one, 6,10-dimethyl-    7.4206692
```

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## 660                                          Acetophenone   13.4717173
## 661                                              Anisole  205.5621971
## 662                                          Benzaldehyde    9.2861515
## 663                          Benzene, 1-chloro-2-methoxy-    4.9102299
## 664                               Benzene, 1,3-dimethyl-    3.4251951
## 665                           Benzene, 3-cyclohexen-1-yl-    2.0756780
## 666                                  Benzeneacetaldehyde    8.6840020
## 667                                          Benzophenone    4.1599497
## 668                                         Benzothiazole    1.4938440
## 669                                        Benzyl nitrile    5.5034789
## 670                             Butylated Hydroxytoluene    9.5717729
## 671                                           Caprolactam   31.9463650
## 672          Carbamodithioic acid, diethyl-, methyl ester    2.1867194
## 673                    Cyclohexasiloxane, dodecamethyl-   10.5487362
## 674                    Cyclopentasiloxane, decamethyl-   67.5083257
## 675                    Cyclotetrasiloxane, octamethyl-   46.0853735
## 676                                           Decanal   47.9200734
## 677                                    Dibutyl phthalate    4.0444051
## 678                                    Diethyl Phthalate    5.1430962
## 679                                   Dimethyl trisulfide   20.7485086
## 680                     Ethanone, 1-(1H-pyrrol-2-yl)-   10.8305696
## 681                          Ethanone, 1-(2-furanyl)-    2.6640429
## 682                                         Eucalyptol    7.7818992
## 683                                         Nonadecane    2.9950707
## 684                                         Nonadecane    1.7868771
## 685                                            Nonanal   29.6845196
## 686                                            Octanal   28.7516825
## 687                                             Phenol  329.1948140
## 688                                       Phenol, 2-iodo-    6.8283551
## 689                                     Phenol, 2-methoxy-   29.3810320
## 690                                   Phenylethyl Alcohol  189.3598206
## 691                       Pyrazine, 2-ethyl-5-methyl-   20.5734482
## 692                       Pyrazine, 2-ethyl-5-methyl-    1.7559506
## 693                          Pyrazine, 2,5-dimethyl-  788.4867601
## 694                     Pyrazine, 3-ethyl-2,5-dimethyl-   10.4229160
## 695                               Quinoline, 3-methyl-    6.5246406
## 696                                          Undecanal    5.3609361
## 697                                1-Hexanol, 2-ethyl-   46.6985715
## 698                                1,2-Benzisothiazole    2.7802223
## 699                     1,3-Cyclopentadiene, 5-methyl-   74.7195971
## 700                     1,3-Cyclopentadiene, 5-methyl-   64.4645186
## 701                  1,3,5-Cycloheptatriene, 1-methoxy-    3.9497108
## 702                          1,3,5,7-Cyclooctatetraene   22.6278301
## 703                                2-Acetylthiazole    2.9638138
## 704                                     2-Heptanone   59.1452550
## 705                                   2-Tridecanone   13.2952678
## 706                                   2-Undecanone    9.2111746
## 707                       2,4,4-Trimethyl-1-hexene   19.0408760
## 708                       2,4,4-Trimethyl-1-hexene   12.0044002
## 709                     2,4,6-Cycloheptatrien-1-one    1.7513903
## 710                   4,8,12,16-tetraoxaeicosan-1-ol   12.2942529
## 711          5,9-Undecadien-2-one, 6,10-dimethyl-    6.4296154
## 712                                          Acetophenone   21.3254512
## 713                                              Anisole  190.9815616
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## 714                                        Benzaldehyde  12.3922200
## 715                           Benzene, 1-chloro-2-methoxy-   4.9286519
## 716                         Benzene, 1-isocyano-2-methyl-   6.6142609
## 717                           Benzene, 3-cyclohexen-1-yl-   1.2024825
## 718                                  Benzeneacetaldehyde  44.7352428
## 719                                        Benzophenone   6.1502412
## 720                                     Benzyl alcohol   3.7397436
## 721                                Benzyl methyl ketone   6.5881420
## 722                             Butylated Hydroxytoluene   6.5866241
## 723                                        Caprolactam  20.0294754
## 724                       Cyclohexasiloxane, dodecamethyl-  17.5710696
## 725                        Cyclopentasiloxane, decamethyl-  60.2405997
## 726                        Cyclotetrasiloxane, octamethyl-  53.4329093
## 727                                           Decanal  58.8878033
## 728                                    Dibutyl phthalate   4.1529264
## 729                                  Dimethyl trisulfide  10.2625846
## 730                                       Diphenylamine   2.9230618
## 731                         Ethanone, 1-(1H-pyrrol-2-yl)-  12.9251965
## 732                              Ethanone, 1-(2-furanyl)-   3.1574137
## 733                          Ethanone, 1-(4-ethylphenyl)-  15.1133369
## 734                          Ethanone, 1-(4-ethylphenyl)-  10.8685191
## 735                                         Nonadecane   2.9849807
## 736                                         Nonadecane   2.6728795
## 737                                            Nonanal  30.0464482
## 738                                             Phenol 354.0758458
## 739                                       Phenol, 2-iodo-  10.5315452
## 740                                     Phenol, 2-methoxy-  33.3635551
## 741                                   Phenylethyl Alcohol 209.9468888
## 742          Propanol, [(butoxymethylethoxy)methylethoxy]-  12.7502593
## 743          Propanol, [(butoxymethylethoxy)methylethoxy]-   6.1547433
## 744                               Pyrazine, 2,5-dimethyl- 940.9323939
## 745                      Pyrazine, 3-ethyl-2,5-dimethyl-  14.0099967
## 746                                 Quinoline, 3-methyl-   7.8052768
## 747                                         Undecanal   6.1644990
## 748                                  1-Hexanol, 2-ethyl-   8.4600102
## 749                                1-Phenyl-2-propanone  10.0545000
## 750                           1,3,5,7-Cyclooctatetraene  12.0294130
## 751                          2-Pyrrolidinone, 1-methyl-   4.0387815
## 752                                       2-Undecanone   4.0338157
## 753                            2,3,3-Trimethyl-1-hexene  10.6782601
## 754                             2,4-Di-tert-butylphenol   4.0385686
## 755                            2,4,4-Trimethyl-1-hexene  10.8418483
## 756                         2,4,6-Cycloheptatrien-1-one  11.6401207
## 757                                       Acetophenone  13.4031064
## 758                                       Benzaldehyde   7.3351232
## 759                                       Benzophenone   3.1121629
## 760                                      Benzothiazole   2.2838332
## 761                                     Benzyl alcohol  18.8194093
## 762                                     Benzyl nitrile   4.0330195
## 763                           Butanoic acid, 2-methyl-  37.2822805
## 764                           Butanoic acid, 2-methyl-  34.0864557
## 765                                        Caprolactam   3.3772118
## 766                                      Cyclohexanone  19.4886492
## 767                        Cyclopentasiloxane, decamethyl-   8.9239012
```

```
## 768                                        Decanal   25.9868509
## 769                                Dibutyl phthalate    6.9934555
## 770                                Diethyl Phthalate   11.3116356
## 771                              Dimethyl trisulfide 1701.9910430
## 772                   Disulfide, isopentyl methyl    3.8275904
## 773                 Ethanone, 1-(1H-pyrrol-2-yl)-    9.3783343
## 774                  Ethanone, 1-(2-aminophenyl)-   10.3282521
## 775               Ethanone, 1-(3,4-dimethylphenyl)-    1.6501316
## 776                       Furan, 2-ethyl-5-methyl-    0.2639191
## 777          Glutaric acid, di(isobutyl) ester    2.4648650
## 778                                    Mequinol    2.2669267
## 779                  Methane, oxybis[dichloro-    5.2127087
## 780                                    Nonanal   34.0400615
## 781                                     Phenol  572.0768965
## 782                           Phenylethyl Alcohol   70.0905158
## 783                Pyrazine, 2-ethyl-5-methyl-   20.9022846
## 784                Pyrazine, 2-ethyl-5-methyl-    2.2903089
## 785                   Pyrazine, 2,5-dimethyl- 1060.2210933
## 786            Pyrazine, 3-ethyl-2,5-dimethyl-   12.4309297
## 787                       Pyrazine, trimethyl-   26.7262704
## 788                 Pyridine, 2,4,6-trimethyl-    3.6447024
## 789                       Quinoline, 4-methyl-    3.5301230
## 790                                  1-Hexanol    1.7668294
## 791                        1-Hexanol, 2-ethyl-    6.0464493
## 792                                  1-Nonanol    2.7345353
## 793                1,3,5,7-Cyclooctatetraene    7.2104632
## 794                         2-Acetylthiazole    3.9638100
## 795                              2-Heptanone   16.8097973
## 796                              2-Nonanone    3.2536169
## 797                            2-Tridecanone    4.9490826
## 798                            2-Undecanone    4.6274563
## 799               2,3,3-Trimethyl-1-hexene    6.9829061
## 800                2,4-Di-tert-butylphenol    1.9597091
## 801               2,4,4-Trimethyl-1-hexene   12.4340520
## 802            2,4,6-Cycloheptatrien-1-one    8.0226823
## 803                           Acetophenone   10.0396115
## 804                           Benzaldehyde   10.1322468
## 805                           Benzophenone    2.9167931
## 806                          Benzothiazole    1.1651123
## 807                         Benzyl alcohol   12.9858096
## 808                     Benzyl methyl ketone   20.0427369
## 809                          Benzyl nitrile    3.0677428
## 810                Butylated Hydroxytoluene    1.1726184
## 811                             Caprolactam    2.4951390
## 812                          Cyclohexanone   14.4177958
## 813          Cyclohexasiloxane, dodecamethyl-    2.8806130
## 814          Cyclopentasiloxane, decamethyl-   18.6789222
## 815                                    Decanal   35.5015266
## 816                          Dibutyl phthalate    3.1799767
## 817                          Diethyl Phthalate   44.3046405
## 818                        Dimethyl trisulfide  566.0029789
## 819                                  Dodecanal    2.1002036
## 820            Ethanone, 1-(1H-pyrrol-2-yl)-    6.6343268
## 821                 Ethanone, 1-(2-furanyl)-    0.8716399
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```
## 822                                        Mequinol    1.7420731
## 823                                        Nonanal    23.5755777
## 824                                         Phenol   389.2102470
## 825                              Phenylethyl Alcohol    82.9102371
## 826                  Pyrazine, 2-ethyl-5-methyl-    21.2345868
## 827                  Pyrazine, 2-ethyl-5-methyl-     2.9271300
## 828                      Pyrazine, 2,5-dimethyl- 1117.5181450
## 829                      Pyrazine, 2,5-dimethyl-    49.6859488
## 830            Pyrazine, 3-ethyl-2,5-dimethyl-    12.7966383
## 831                        Quinoline, 4-methyl-     1.8108327
## 832                                    Undecanal     2.5613268
## 833                     1-Hexanol, 2-ethyl-    12.1437457
## 834                                    1-Nonanol     8.8679199
## 835                    1-Phenyl-2-propanone    35.6701736
## 836                                    1-Undecanol     2.7142327
## 837                       2-Acetylthiazole     8.8916322
## 838                            2-Heptanone    25.2355644
## 839                          2-Tridecanone     6.3236943
## 840             2,3,3-Trimethyl-1-hexene    10.4346533
## 841              2,4-Di-tert-butylphenol     9.5223275
## 842             2,4,4-Trimethyl-1-hexene    20.3269997
## 843             2,4,4-Trimethyl-1-hexene    12.9943879
## 844          2,4,6-Cycloheptatrien-1-one    26.4960974
## 845 5,9-Undecadien-2-one, 6,10-dimethyl-     6.1757942
## 846                          Acetophenone    24.1015255
## 847                          Benzaldehyde    18.7510144
## 848                          Benzophenone     6.2882388
## 849                         Benzothiazole     3.3254236
## 850                        Benzyl alcohol    33.6762106
## 851                        Benzyl nitrile     7.5982542
## 852     Bicyclo[4.2.0]octa-1,3,5-triene    19.1814521
## 853            Butanoic acid, 2-methyl-    25.0466866
## 854                          Caprolactam     8.5909779
## 855                        Cyclohexanone    21.2974020
## 856  Cyclooctasiloxane, hexadecamethyl-     2.0773461
## 857     Cyclopentasiloxane, decamethyl-    14.3480681
## 858                              Decanal   138.0258725
## 859                 Dibutyl phthalate    10.9872320
## 860                 Diethyl Phthalate    75.5909677
## 861               Dimethyl trisulfide   623.8906541
## 862           Disulfide, isopentyl methyl     2.3799070
## 863                           Dodecanal     8.9089032
## 864        Ethanone, 1-(2-aminophenyl)-    23.2387269
## 865           Ethanone, 1-(2-furanyl)-     3.3167332
## 866            Methane, oxybis[dichloro-     7.3577463
## 867                          Nonadecane     5.3146462
## 868                          Nonadecane     4.4392315
## 869                          Nonadecane     3.1768429
## 870                             Nonanal   107.9513250
## 871                             Octanal    46.2563667
## 872                      Octane, 1-chloro-     5.1969604
## 873                               Phenol  1032.8152281
## 874                      Phenylethyl Alcohol   121.5477032
## 875           Pyrazine, 2-ethyl-6-methyl-    53.9355694
```

```
## 876                          Pyrazine, 2-ethyl-6-methyl-    7.5254440
## 877                              Pyrazine, 2,5-dimethyl- 2222.1532010
## 878                       Pyrazine, 3-ethyl-2,5-dimethyl-   26.3234657
## 879                                Pyrazine, trimethyl-   50.5346717
## 880                             Quinazoline, 4-methyl-    2.1160938
## 881                               Quinoline, 3-methyl-    3.4288649
## 882                                        Tetradecane    2.0940823
## 883                                          Undecanal   11.3967822
## 884                                          1-Decanol    3.3125142
## 885                                          1-Hexanol    5.0313973
## 886                                          1-Nonanol    4.4039272
## 887                           1,2-Benzisothiazole    2.5476472
## 888                                         2-Decanone    3.0677135
## 889                                        2-Heptanone   52.3114321
## 890                                          2-Nonanol    4.5354189
## 891                                       2-Tridecanone    8.0594995
## 892                                       2-Undecanone   12.3463122
## 893                          2,4-Di-tert-butylphenol    5.6943425
## 894                        2,4,4-Trimethyl-1-hexene   20.6646859
## 895                     2,4,6-Cycloheptatrien-1-one   12.5291186
## 896                             3-Aminoacetophenone   16.1951171
## 897          5,9-Undecadien-2-one, 6,10-dimethyl-    5.8351854
## 898                                       Acetophenone   22.7390807
## 899                                       Benzaldehyde   17.3141540
## 900                Benzene, 3-cyclohexen-1-yl-    1.7080267
## 901                                       Benzophenone    4.5407215
## 902                                    Benzyl alcohol   38.4517465
## 903                          Benzyl methyl ketone   13.3346227
## 904                                    Benzyl nitrile    5.6435471
## 905                Bicyclo[4.2.0]octa-1,3,5-triene   23.6318648
## 906                       Butylated Hydroxytoluene    2.8836098
## 907                                        Caprolactam    3.8563165
## 908             Cyclopentasiloxane, decamethyl-   21.5528244
## 909                                           Decanal   76.8038769
## 910                                Dibutyl phthalate    9.7861396
## 911                                Diethyl Phthalate    3.0948581
## 912                             Dimethyl trisulfide 1332.5319862
## 913                                         Dodecanal    5.7322463
## 914               Ethanone, 1-(1H-pyrrol-2-yl)-   12.5091856
## 915                    Furan, 2-ethyl-5-methyl-    1.1649388
## 916          Glutaric acid, di(isobutyl) ester    3.3115735
## 917                                         Limonene   39.0285536
## 918                                          Nonanal   56.5720388
## 919                                          Octanal   28.8454588
## 920                                           Phenol  351.7728998
## 921                             Phenylethyl Alcohol  154.8223701
## 922                Pyrazine, 2-ethyl-6-methyl-   21.4608347
## 923                Pyrazine, 2-ethyl-6-methyl-    3.4639222
## 924                    Pyrazine, 2,5-dimethyl-  968.5382909
## 925 Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-    1.8304523
## 926                      Quinazoline, 4-methyl-    3.6865706
## 927                        Quinoline, 3-methyl-    3.2235596
## 928                                        Tetradecane    2.2650861
## 929                                          Undecanal    6.0296257
```

```
## 930                                          1-Decanol    3.0264049
## 931                                          1-Nonanol    3.3161603
## 932                      2-Methyl-3-isopropylpyrazine    6.6420212
## 933                                       2-Undecanone    8.3626538
## 934                          2,4-Di-tert-butylphenol     3.2646313
## 935                        2,4,4-Trimethyl-1-hexene     13.9677314
## 936                        2,4,4-Trimethyl-1-hexene     8.2703246
## 937                      2,4,6-Cycloheptatrien-1-one    8.6334553
## 938                             3-Aminoacetophenone    10.0935158
## 939                      5-Decen-1-ol, acetate, (E)-    10.4483744
## 940                        5-Hepten-2-one, 6-methyl-    6.9454333
## 941                                       Acetophenone   13.3088128
## 942                                       Benzaldehyde   10.3487638
## 943                           Benzene, 1,3-dimethyl-     1.8068397
## 944                       Benzene, 3-cyclohexen-1-yl-    3.4800238
## 945                                       Benzophenone    2.7598513
## 946                                    Benzyl alcohol    24.3358908
## 947                          Benzyl methyl ketone        14.2289287
## 948                                    Benzyl nitrile     6.3099943
## 949                  Bicyclo[4.2.0]octa-1,3,5-triene     17.3574347
## 950                                       Caprolactam    2.6806168
## 951          Cyclohexane, 2-propyl-1,1,3-trimethyl-      26.7538093
## 952  Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-    37.2331630
## 953           Cyclooctasiloxane, hexadecamethyl-         2.8075499
## 954              Cyclopentasiloxane, decamethyl-         13.3126110
## 955              Cyclotetrasiloxane, octamethyl-         1.7886232
## 956                                          Decanal    29.0974780
## 957                                Dibutyl phthalate     5.5378614
## 958                               Dimethyl trisulfide   931.3704710
## 959                                          Dodecanal    2.4149478
## 960                 Ethanone, 1-(1H-pyrrol-2-yl)-        7.1518522
## 961                                       Nonadecane     2.7601525
## 962                                          Nonanal    38.3671567
## 963                                           Phenol    157.8900331
## 964                               Phenylethyl Alcohol   111.8971026
## 965                    Pyrazine, 2-ethyl-5-methyl-      14.9771649
## 966                        Pyrazine, 2,5-dimethyl-      466.9847533
## 967                        Pyrazine, 2,5-dimethyl-      118.8325966
## 968                           Quinoline, 3-methyl-      1.7808813
## 969                                          Undecanal    2.3854928
## 970                                          1-Decanol    1.4917846
## 971                      1,3,5,7-Cyclooctatetraene        9.4736414
## 972                                       2-Undecanone    3.2121630
## 973                        2,3,3-Trimethyl-1-hexene      11.3302929
## 974                        2,4,4-Trimethyl-1-hexene      17.8927730
## 975                        2,4,4-Trimethyl-1-hexene      9.4239391
## 976                      2,4,6-Cycloheptatrien-1-one     3.5178994
## 977                                       Acetophenone    7.2920969
## 978                                       Benzaldehyde    5.5421701
## 979                       Benzene, 3-cyclohexen-1-yl-     3.2522174
## 980                                       Benzophenone    2.2201683
## 981                                    Benzyl alcohol    13.8293909
## 982                          Benzyl methyl ketone        7.8635701
## 983          Cyclohexane, 2-propyl-1,1,3-trimethyl-      7.5456066
```

```
## 984                                        Cyclooctene, (Z)-    1.6700256
## 985                             Cyclopentasiloxane, decamethyl-    8.6768538
## 986                                               D-Limonene   32.4823004
## 987                                                  Decanal   11.8054428
## 988                                          Dibutyl phthalate    2.2282465
## 989                                       Dimethyl trisulfide  235.3843659
## 990                                       Dimethyl trisulfide   59.7644004
## 991                               Ethanone, 1-(1H-pyrrol-2-yl)-    3.9665393
## 992                                   Methane, oxybis[dichloro-   11.9595357
## 993                                                    Phenol   65.0956337
## 994                                       Phenylethyl Alcohol   76.0736052
## 995                                     Pyrazine, 2,5-dimethyl-  269.6420474
## 996                               S-Methyl methanethiosulphonate    2.5763974
## 997                                                  1-Decanol    5.5394575
## 998                                                  1-Nonanol    6.5594688
## 999  1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester    1.0172182
## 1000                            1,3-Cyclopentadiene, 5-methyl-  128.3494607
## 1001                            1,3-Cyclopentadiene, 5-methyl-   68.6295920
## 1002                                       2-Acetylthiazole   12.2903461
## 1003                                            2-Heptanone   82.2154296
## 1004                                              2-Nonanol    3.9516640
## 1005                                             2-Nonanone   17.4608796
## 1006                                          2-Tridecanone   10.8959993
## 1007                                          2-Undecanone   14.3025885
## 1008                                2,4-Di-tert-butylphenol    5.9332851
## 1009                               2,4,4-Trimethyl-1-hexene   10.5469305
## 1010                             2,4,6-Cycloheptatrien-1-one   13.0143968
## 1011                                    3-Aminoacetophenone   18.3528761
## 1012                              4,8,12,16-tetraoxaeicosan-1-ol   13.2678101
## 1013                  5,9-Undecadien-2-one, 6,10-dimethyl-    7.5667261
## 1014                                9H-Fluorene, 9-methylene-    1.7305960
## 1015                                          Acetophenone   23.3376087
## 1016                                          Benzaldehyde   19.3066785
## 1017                             Benzene, 3-cyclohexen-1-yl-    3.0786833
## 1018                                    Benzeneacetaldehyde   24.7006706
## 1019                                    Benzeneacetaldehyde   11.1670486
## 1020                                           Benzophenone    7.0250582
## 1021                                         Benzothiazole    3.0302778
## 1022                                        Benzyl alcohol   44.8071936
## 1023                                   Benzyl methyl ketone   13.5559010
## 1024                                        Benzyl nitrile    7.4342066
## 1025                                  Butanoic acid, 2-methyl-   39.8930635
## 1026                                  Butanoic acid, 2-methyl-   28.3257825
## 1027                                  Butylated Hydroxytoluene    5.8303349
## 1028                                          Caprolactam   18.8447931
## 1029           Carbamodithioic acid, diethyl-, methyl ester    1.8380078
## 1030                         Cyclohexasiloxane, dodecamethyl-   12.7363609
## 1031                          Cyclopentasiloxane, decamethyl-   66.1499641
## 1032                                   Cyclopropane, pentyl-    8.7798713
## 1033                                                 Decanal   86.5435879
## 1034                                    Dibutyl phthalate    3.9648092
## 1035                                    Diethyl Phthalate    2.0269512
## 1036                                  Dimethyl trisulfide   98.0044500
## 1037                                                Dodecanal    7.7247415
```

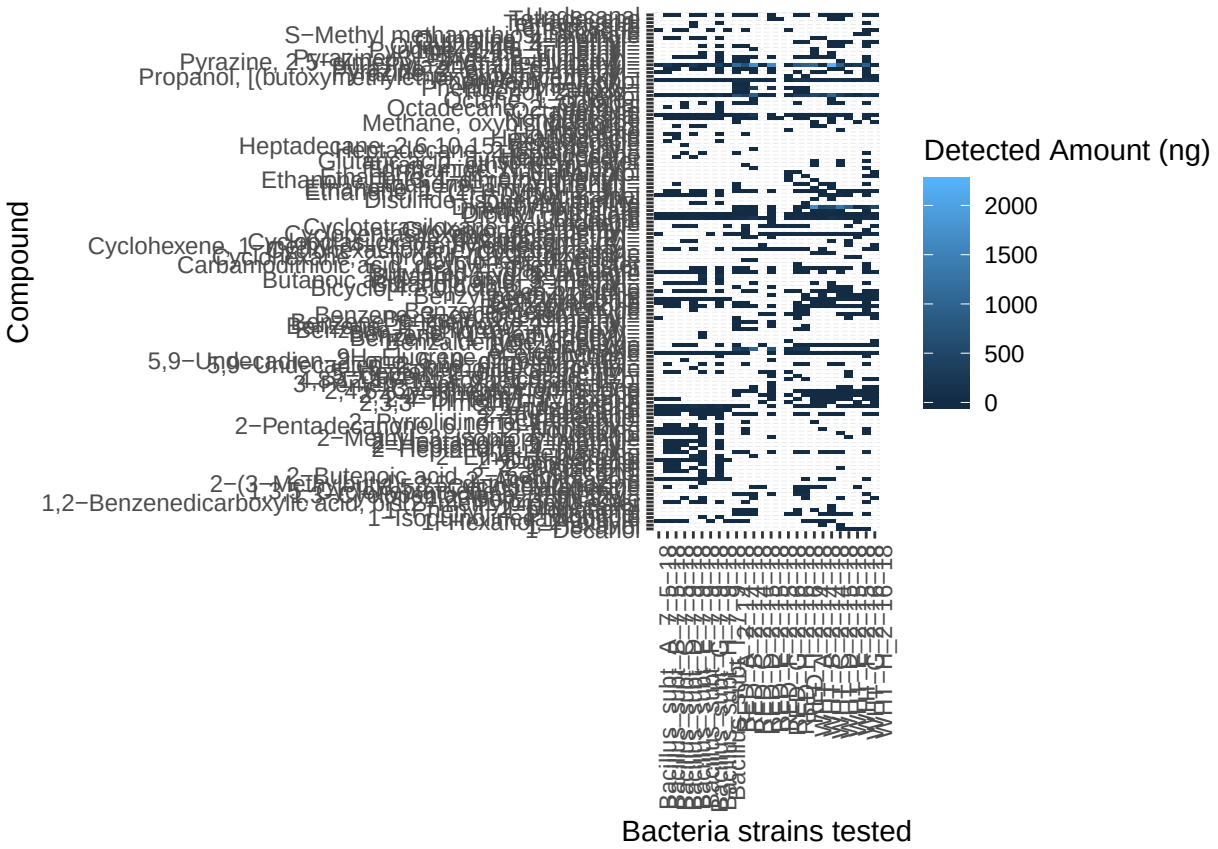
```
## 1038                                          Dodecanal    2.2699158
## 1039                          Ethanone, 1-(1H-pyrrol-2-yl)-   13.0569140
## 1040                               Ethanone, 1-(2-furanyl)-    0.9191914
## 1041                           Ethanone, 1-(4-ethylphenyl)-   19.0697151
## 1042                           Ethanone, 1-(4-ethylphenyl)-    5.8013770
## 1043                                Formamide, N,N-dibutyl-    9.8326622
## 1044                       Glutaric acid, di(isobutyl) ester    4.2017892
## 1045                                          Heptadecane    4.3023102
## 1046                                           Nonadecane    2.5753361
## 1047                                              Nonanal   48.2799169
## 1048                                              Octanal   26.4845057
## 1049                                               Phenol  258.0066366
## 1050                                    Phenylethyl Alcohol  176.7424256
## 1051          Propanol, [(butoxymethylethoxy)methylethoxy]-   14.5051822
## 1052          Propanol, [(butoxymethylethoxy)methylethoxy]-    5.9640675
## 1053                           Pyrazine, 2-ethyl-5-methyl-   17.9793927
## 1054                           Pyrazine, 2-ethyl-6-methyl-    1.1787218
## 1055                               Pyrazine, 2,5-dimethyl-  924.4342371
## 1056              Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-    2.0008619
## 1057                        Pyrazine, 3-ethyl-2,5-dimethyl-   20.7007969
## 1058                                 Quinazoline, 4-methyl-    1.3973549
## 1059                                  Quinoline, 3-methyl-    3.3033553
## 1060                       S-Methyl methanethiosulphonate    0.7133950
## 1061                                               Styrene   26.1031100
## 1062                                           Tetradecanal    2.3711336
## 1063                                             Undecanal    9.1349248
## 1064                                     1,2-Benzisothiazole    1.0271162
## 1065                                          2-Tridecanone    3.3701854
## 1066                                          2-Undecanone    6.3873329
## 1067                                2,3,3-Trimethyl-1-hexene   12.1751810
## 1068                                 2,4-Di-tert-butylphenol    2.6094449
## 1069                                2,4,4-Trimethyl-1-hexene   20.5139503
## 1070                                2,4,4-Trimethyl-1-hexene   11.0092699
## 1071                             2,4,6-Cycloheptatrien-1-one    0.6747200
## 1072                                   3-Aminoacetophenone    5.9589869
## 1073                          4,8,12,16-tetraoxaeicosan-1-ol    9.1498413
## 1074                                          Acetophenone    7.7752066
## 1075                                          Benzaldehyde    3.2778692
## 1076                                Benzaldehyde, 3-ethyl-    1.8006794
## 1077                                Benzene, 1,3-dimethyl-    1.3097645
## 1078                             Benzene, 3-cyclohexen-1-yl-    2.0492193
## 1079                                          Benzophenone    1.9964714
## 1080                                       Benzyl alcohol   16.0851841
## 1081                                  Benzyl methyl ketone    4.5085441
## 1082                                       Benzyl nitrile    2.9197533
## 1083                                Butylated Hydroxytoluene    1.6290448
## 1084                         Cyclohexasiloxane, dodecamethyl-    8.2962683
## 1085       Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-   25.2574340
## 1086                         Cyclopentasiloxane, decamethyl-   42.4446924
## 1087                         Cyclotetrasiloxane, octamethyl-   40.6697881
## 1088                                          Decanal   13.1485167
## 1089                                    Dibutyl phthalate    1.8814173
## 1090                                  Dimethyl trisulfide  484.2134826
## 1091                           Ethanone, 1-(1H-pyrrol-2-yl)-    4.4026845
```

```
## 1092                            Ethanone, 1-(4-ethylphenyl)-   16.9480324
## 1093                            Ethanone, 1-(4-ethylphenyl)-   10.7655526
## 1094                                              Eucalyptol    3.3859516
## 1095                               Methane, oxybis[dichloro-    4.4185442
## 1096                                                 Nonanal   13.2403580
## 1097                                                  Phenol  114.3847106
## 1098                                      Phenylethyl Alcohol   57.0826127
## 1099           Propanol, [(butoxymethylethoxy)methylethoxy]-    8.0289712
## 1100           Propanol, [(butoxymethylethoxy)methylethoxy]-    3.3630259
## 1101                                 Pyrazine, 2,5-dimethyl-  329.3825113
## 1102                                 Pyrazine, 2,5-dimethyl-   21.7504815
## 1103                                    Quinoline, 3-methyl-    1.8924160
## 1104                                                 Styrene   11.8555234
## 1105                                               Undecanal    1.2131730
```

```
volatiles.long <- melt(volatiles, id = c("Sample", "variable", "value"))


volatiles.long$value <- as.numeric(as.character(volatiles.long$value))
#write.table(volatiles.long, "vol_melt2.txt", sep="\t")


heatmap.plot <- ggplot(data = volatiles.long, aes(x = Sample, y = variable)) +
  geom_tile(aes(fill = value)) +
  scale_color_gradient2(na.value = "black") +  ylab("Compound") +
  xlab("Bacteria strains tested") +
  theme(axis.text.x = element_text(angle = 90, hjust = 1)) +
  labs(fill = "Detected Amount (ng)")
heatmap.plot
```

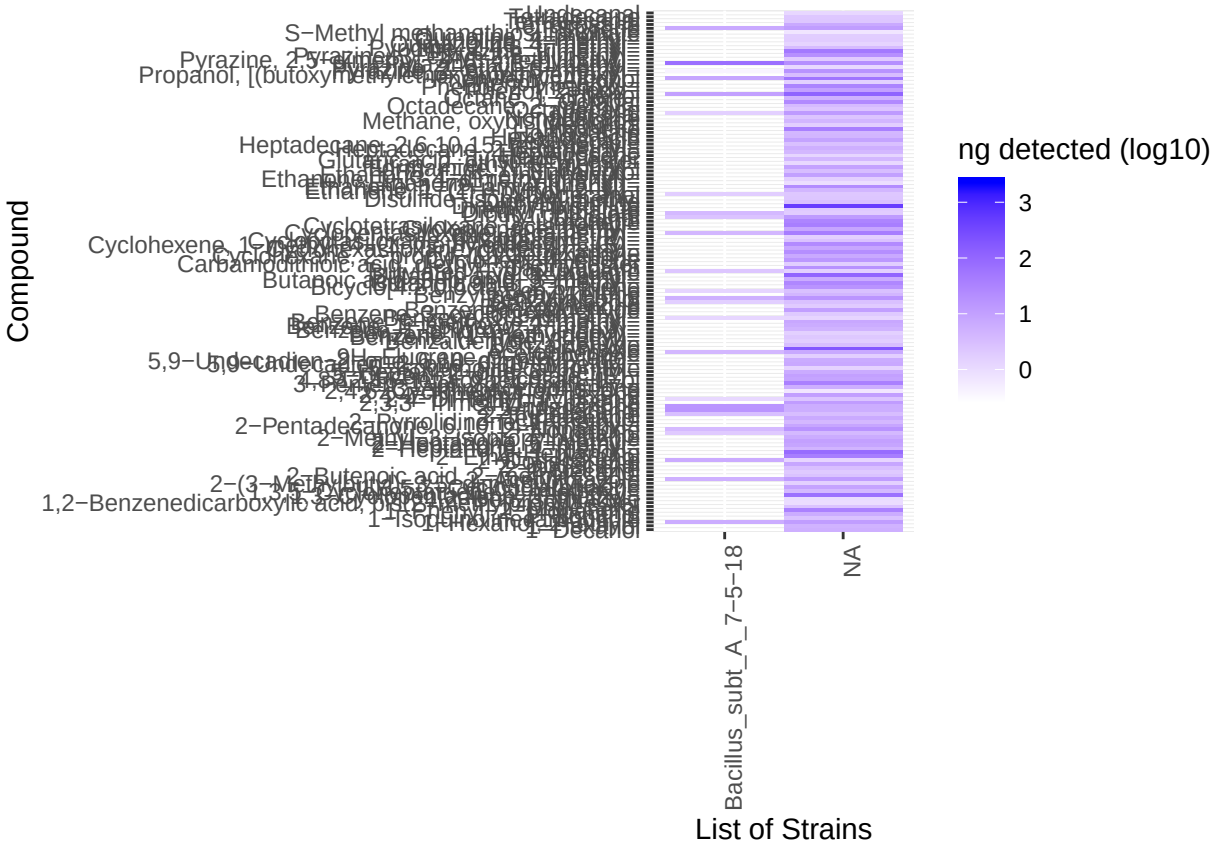



```
pdf("RSI_over85_noUnique_vol_heat.pdf", height = 32, width = 12)
  heatmap.plot
dev.off()
```

```
## pdf
##   2
```

```
#Order Branches
branch.order <- order.dendrogram(volatile.dendro)
volatiles.long$Sample <- factor(x = volatiles.long$Sample,
                                levels = unique(volatiles.long$Sample[branch.order]),
                                ordered = TRUE)
#make sorted heatmap
heatmap.plot.sorted <- ggplot(data = volatiles.long, aes(x = Sample, y = variable)) +
  geom_tile(aes(fill = log10(value))) +
  scale_fill_gradient(low = "white", high = "blue", na.value = "black") +  ylab("Compound") +
  xlab("List of Strains") +
  theme(axis.text.x = element_text(angle = 90, hjust = 1)) +
  labs(fill = "ng detected (log10)")

heatmap.plot.sorted
```




```
# Save sorted heatmap
pdf("heatmap_dendro_sorted.pdf", height = 12, width = 12)
heatmap.plot.sorted
dev.off()
```

```
## pdf
##   2
```

#“‘{r} #NMDS Plot #install.packages(“vegan”) library(vegan) library(readxl)

volatiles_names <- read_excel(“data.xlsx”, sheet = “Sheet3”) volatiles <- read_excel(“/data.xlsx”, sheet = “Sheet4”) rownames(volatiles) <- volatiles_names$X___1 volatiles volatiles.matrix=as.matrix(volatiles) volatiles.matrix test_NMDS=metaMDS(volatiles.matrix, k=2) example_NMDS=metaMDS(volatiles.matrix, # Our community-by-species matrix k=2) # The number of reduced dimensions stressplot(example_NMDS) plot(example_NMDS) treat=c(rep(“Bacillus”,9),rep(“Red”,8),rep(“White”,8)) ordiplot(example_NMDS,type=“n”) ordihull(example_NMDS,groups=treat,draw=“polygon”,col=“grey90”,label=F) orditorp(example_NMDS,display=“sites”,c air=0.01,cex=1.25)

pdf(“NMDS.pdf”, height = 12, width = 12) plot(example_NMDS) treat=c(rep(“Bacillus”,9),rep(“Red”,8),rep(“White”,8)) ordiplot(example_NMDS,type=“n”) ordihull(example_NMDS,groups=treat,draw=“polygon”,col=“grey90”,label=F) orditorp(example_NMDS,display=“sites”,col=c(rep(“blue”,9),rep(“red”,8),rep(“black”,8)), air=0.01,cex=1.25) dev.off()

“‘

Conclusions:

In conclusion we have shown that different environmental strains of Serratia can inhibit zygomycete growth, the variability in inhibition may be based on genetic differences as growth rate does not seem to affect inhibition by volatiles. We would like to explore why some strains of zygo's (e.g. Actinomucor elegans) grow so well under serratia's volatiles. More work needs to be done in other systems, especially outside of a petri dish. Spores/Conidia can sense the presence of volatiles and wait until favorable conditions, this would be an interesting follow-up experiment to learn about environmental cues that stop fungi from germinating from conidia. Looking into additional compounds to find more fungal responses or if there is a conserved fungal response. Anisole would be an interesting compound to follow up on, only found in Serratia marcescens (ADJS-Red). Not in Bacillus. Searching for new antifungals is important. Looking to the future, volatile profiles with multiple antifungal components may be important for the war against fungi.

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