Chemical EDA

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```
# Read in the cleaned dataset and select records of California and Florida
df <- read.csv("strawberry_cleaned.csv")

# Find states that used chemicals in growing strawberry
states_with_chemical_info <- df %>%
  filter(!is.na(Chemical_Info)) %>%
  distinct(State) %>%
  pull(State)

print(states_with_chemical_info)
```

```
## [1] "CALIFORNIA" "FLORIDA"
```

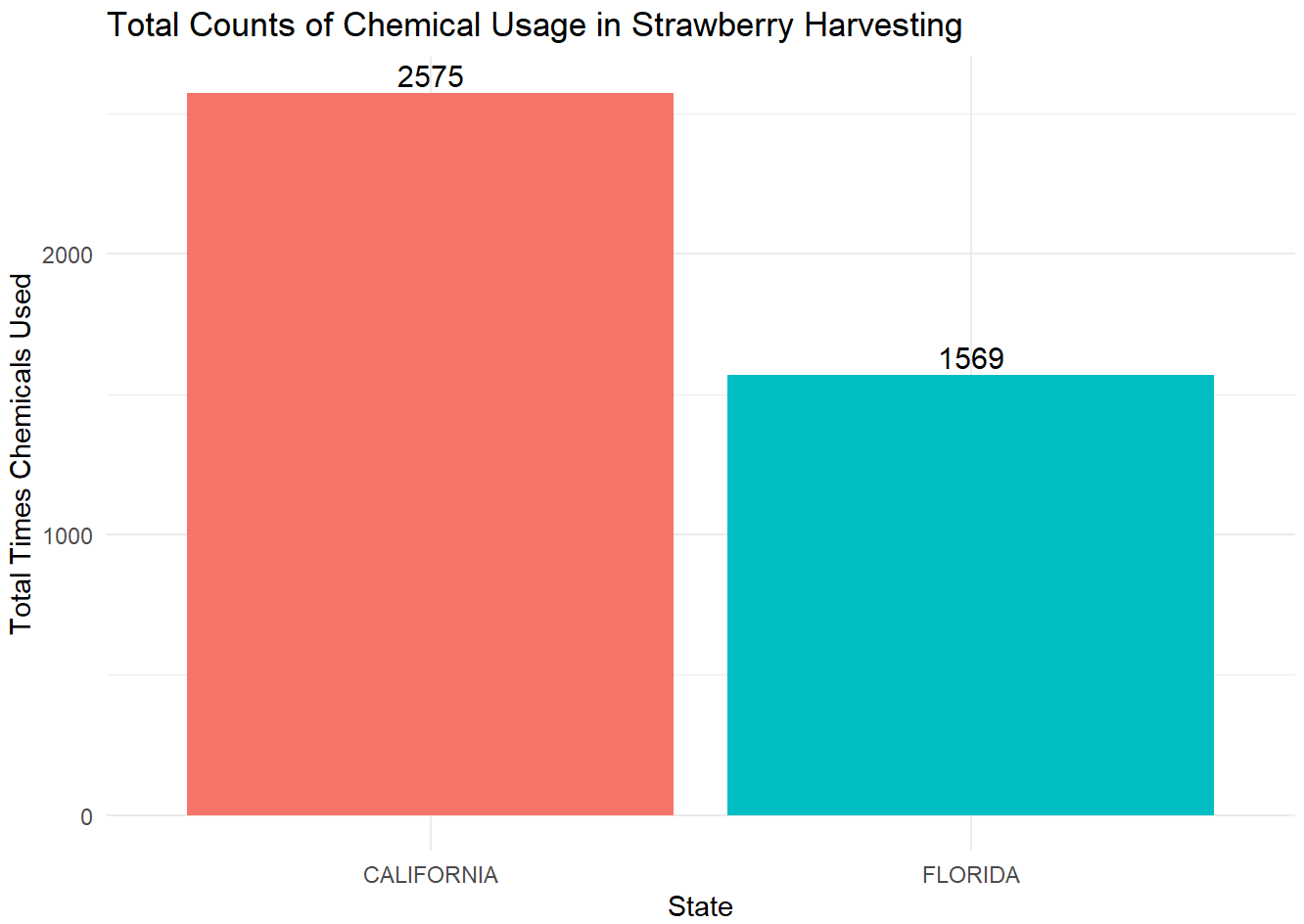
Only California and Florida used chemicals when growing strawberries, we can filter out only those two states and compare the frequency of chemical used:

```
df <- df %>%
  select(-1) %>%
  filter(State == "CALIFORNIA" | State == "FLORIDA")

# Draw a bar plot comparing the frequency
chem_state <- df %>%
  group_by(State) %>%
  summarise(Total_obs=n()) %>%
  arrange(desc(Total_obs))
print(chem_state)
```

```
## # A tibble: 2 × 2
##   State      Total_obs
##   <chr>          <int>
## 1 CALIFORNIA      2575
## 2 FLORIDA         1569
```

```
ggplot(chem_state, aes(x = State, y = Total_obs, fill = State)) +
  geom_bar(stat = "identity") +
  geom_text(aes(label = Total_obs), vjust = -0.3, size = 4) +
  theme_minimal() +
  labs(title = "Total Counts of Chemical Usage in Strawberry Harvesting",
       x = "State",
       y = "Total Times Chemicals Used") +
  theme(legend.position = "none")  # Remove legend
```



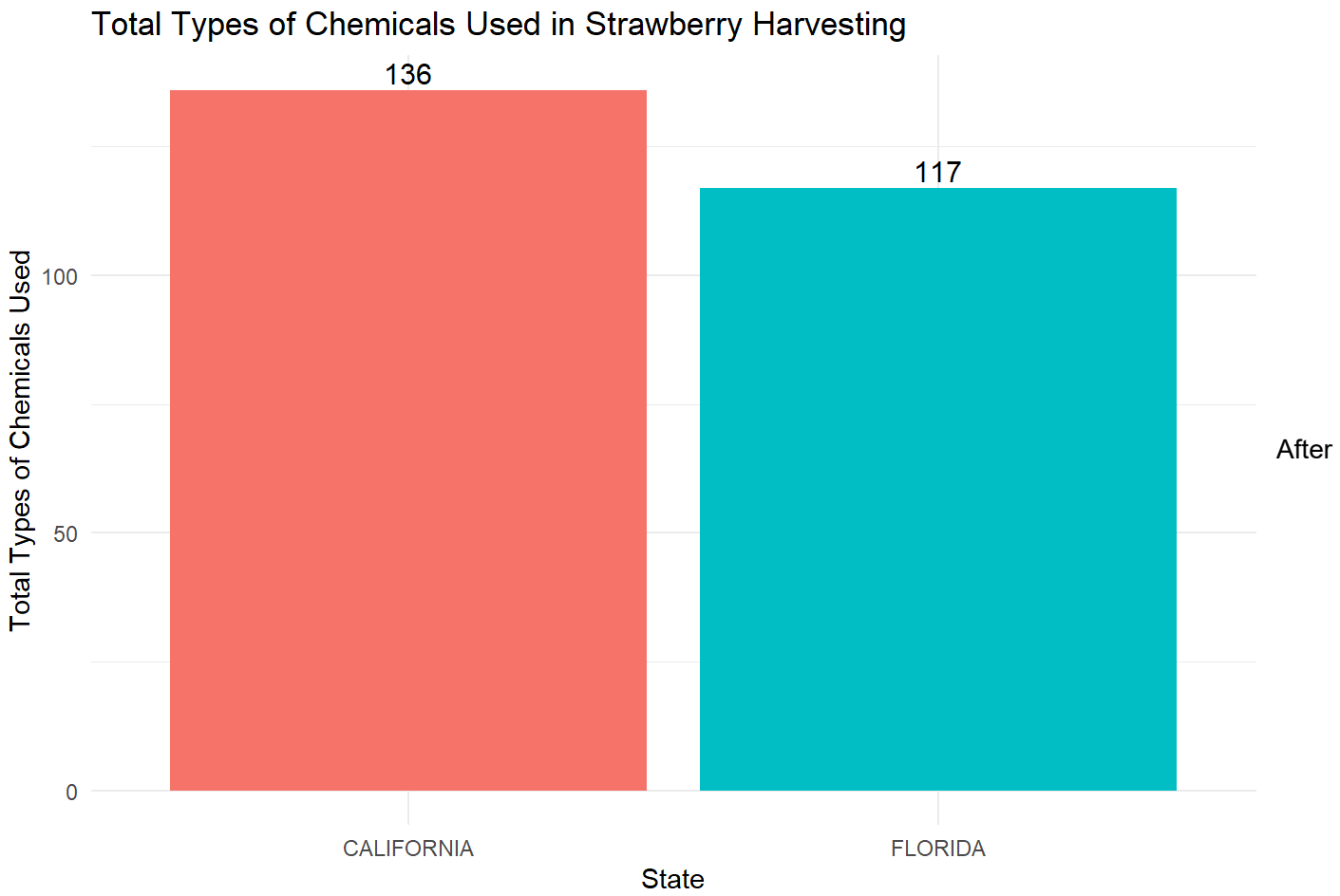
The frequency that California used chemicals is almost twice as the frequency of Florida.

```
# Split the California data and Florida data into two dataframes
df_cal <- df %>%
  filter(State == "CALIFORNIA")

df_flo <- df %>%
  filter(State == "FLORIDA")

# Find the distinct chemicals used in California and Florida
chem_comparison <- data.frame(
  State = c("CALIFORNIA", "FLORIDA"),
  Distinct_chemicals =
    c(length(unique(df_cal$Chemical_Info)),
      length(unique(df_flo$Chemical_Info)))
)


ggplot(chem_comparison, aes(x = State, y = Distinct_chemicals, fill = State)) +
  geom_bar(stat = "identity") +
  geom_text(aes(label = Distinct_chemicals), vjust = -0.3, size = 4) +
  theme_minimal() +
  labs(title = "Total Types of Chemicals Used in Strawberry Harvesting",
       x = "State",
       y = "Total Types of Chemicals Used") +
  theme(legend.position = "none")  # Remove Legend
```



finding the distinct chemicals in each state, California used 19 more types of chemicals than Florida, and there are 58 types of chemicals used in California but not in Florida:

```
# Find out chemicals used by California but not used by Florida
diff_chem1 <- setdiff(unique(df_cal$Chemical_Info), unique(df_flo$Chemical_Info))
print(diff_chem1)
```

```
##  [1] "CYCLANILIPROLE"
##  [2] "PERMETHRIN"
##  [3] "ISARIA FUMOSOROSEA STRAIN FE 9901"
##  [4] "BACILLUS AMYLOLIQUEFACIENS STRAIN D747"
##  [5] "BLAD"
##  [6] "BT SUBSP KURSTAKI EVB-113-19"
##  [7] "POLYOXIN D ZINC SALT"
##  [8] "QUINOLINE"
##  [9] "TRIFLOXYSTROBIN"
## [10] "PENDIMETHALIN"
## [11] "ACEQUINOCYL"
## [12] "AZADIRACHTIN"
## [13] "BEAUVERIA BASSIANA"
## [14] "BT KURSTAKI SA-11"
## [15] "CANOLA OIL"
## [16] "CHROMOBAC SUBTSUGAE PRAA4-1 CELLS AND SPENT MEDIA"
## [17] "ETOXAZOLE"
## [18] "FENBUTATIN-OXIDE"
## [19] "NEEM OIL"
## [20] "NEEM OIL, CLAR. HYD."
## [21] "PYRIDABEN"
## [22] "CAPSICUM OLEORESIN EXTRACT"
## [23] "GARLIC OIL"
## [24] "IRON PHOSPHATE"
## [25] "METALDEHYDE"
## [26] "METAM-SODIUM"
## [27] "BACILLUS AMYLOLIQUEFACIENS MBI 600"
## [28] "BACILLUS PUMILUS"
## [29] "COPPER OCTANOATE"
## [30] "POTASSIUM BICARBON."
## [31] "STREPTOMYCES LYDICUS"
## [32] "BT KURSTAKI EG7841"
## [33] "BT SUB AIZAWAI GC-91"
## [34] "BUPROFEZIN"
## [35] "BURKHOLDERIA A396 CELLS & MEDIA"
## [36] "HELICOVERPA ZEA NPV"
## [37] "PETROLEUM DISTILLATE"
## [38] "POTASSIUM SALTS"
## [39] "PYRIPROXYFEN"
## [40] "CAPRIC ACID"
## [41] "CAPRYLIC ACID"
## [42] "MINERAL OIL"
## [43] "PAECILOMYCES FUMOSOR"
## [44] "POTASSIUM SILICATE"
## [45] "BACILLUS SUBT. GB03"
## [46] "TRICHODERMA HARZ."
## [47] "GLUFOSINATE-AMMONIUM"
## [48] "SULFENTRAZONE"
## [49] "CHLORPYRIFOS"
## [50] "SOYBEAN OIL"
## [51] "ZETA-CYPERMETHRIN"
## [52] "AUREOBASIDIUM PULLULANS DSM 14940"
```

```
## [53] "AUREOBASIDIUM PULLULANS DSM 14941"
## [54] "BT KURSTAKI SA-12"
## [55] "GLIOCLADIUM VIRENS"
## [56] "TRICHODERMA VIRENS STRAIN G-41"
## [57] "EMAMECTIN BENZOATE"
## [58] "SPIROTETRAMAT"
```

on the other hand, there are 39 types of chemicals used in Florida but not in California:

```
diff_chem2 <- setdiff(unique(df_flo$Chemical_Info), unique(df_cal$Chemical_Info))
print(diff_chem2)
```

```
##  [1] "PYRIOFENONE"              "ZOXAMIDE"
##  [3] "METSULFURON-METHYL"       "PENOXSULAM"
##  [5] "S-METOLACHLOR"            "BETA-CYFLUTHRIN"
##  [7] "ETHYL 2E;4Z-DECADIENOATE" "OXAMYL"
##  [9] "CUPRAMMONIUM ACETATE"     "DODECADIEN-1-OL"
## [11] "FLUENSULFONE"             "GIBBERELLIC ACID"
## [13] "CHLOROTHALONIL"           "COPPER CHLORIDE HYD."
## [15] "CYMOXANIL"                "FAMOXADONE"
## [17] "MANCOZEB"                 "2,4-D, DIMETH. SALT"
## [19] "CLETHODIM"                "METHOMYL"
## [21] "CYTOKININS"               "INDOLEBUTYRIC ACID"
## [23] "COPPER ETHANOLAMINE"      "DIMETHENAMID"
## [25] "FLUROXYPYR 1-MHE"         "HALOSULFURON-METHYL"
## [27] "KANTOR"                   "FENAZAQUIN"
## [29] "ETHEPHON"                 "DODINE"
## [31] "FLUTOLANIL"               "2,4-D, TRIISO. SALT"
## [33] "CYPERMETHRIN"             "ALKYL. DIM. BENZ. AM"
## [35] "DECYLDIMETHYLOCTYL"       "DIDECYL DIM. AMMON."
## [37] "DIMETHYLDIOCTYL"          "MUSTARD OIL"
## [39] "DIMETHYL DISULFIDE DMDS"
```

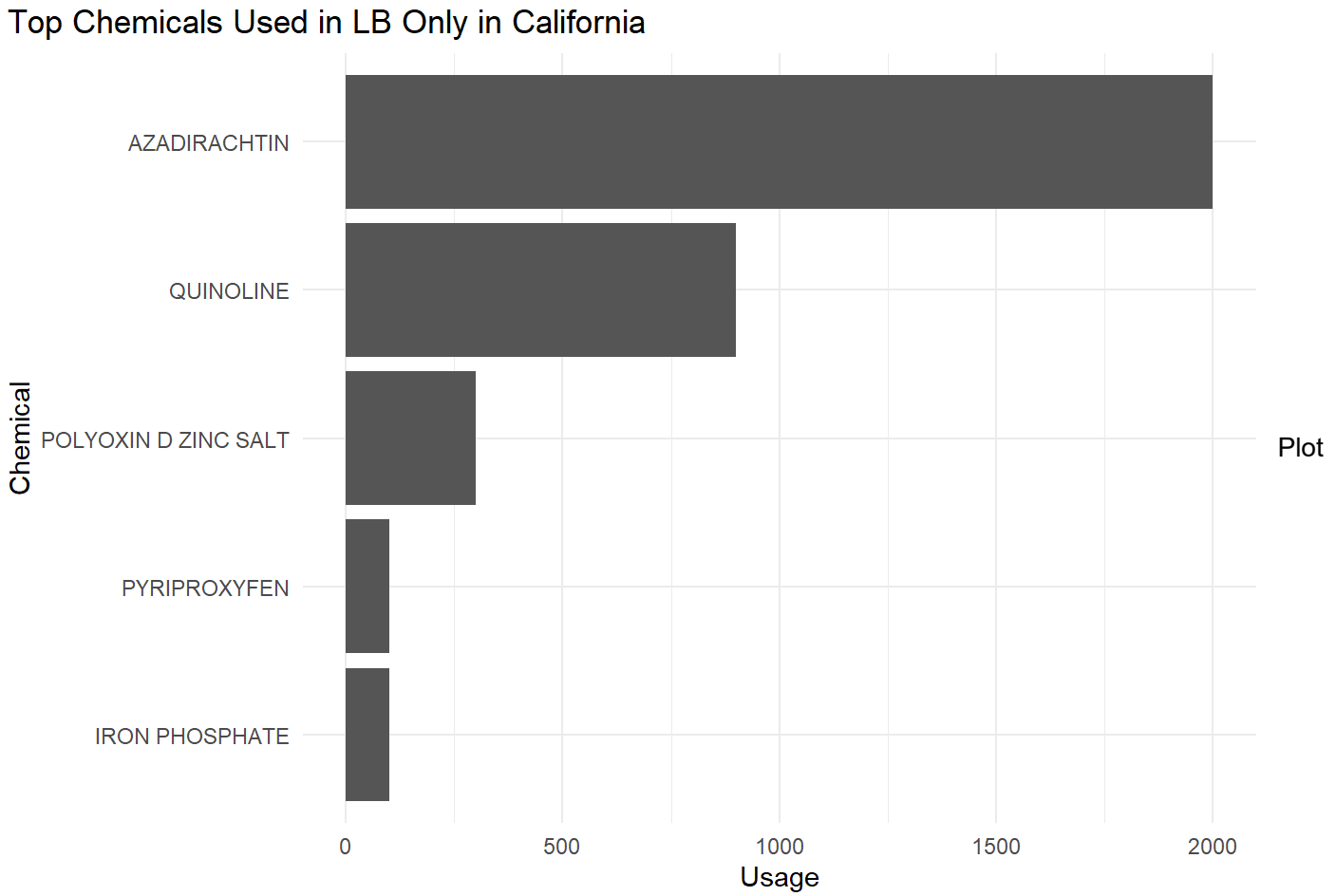
We can first explore those 58 chemicals used only in California:

```
# Select records with those 58 chemicals
df_chem_cal <- df_cal %>%
  filter(Chemical_Info %in% diff_chem1)

# Create a new column to record the frequency of each chemical used
chem_measure <- df_chem_cal %>%
  group_by(Measurement) %>%
  filter(Measurement == "MEASURED IN LB")

# Plot the top chemicals used in California
top_chem <- chem_measure %>%
  filter(!is.na(Value)) %>%
  group_by(Chemical_Info, Domain) %>%
  summarise(Value = sum(Value, na.rm = TRUE)) %>%
  arrange(desc(Value))

ggplot(top_chem, aes(x=reorder(Chemical_Info, Value), y=Value))+
  geom_bar(stat = "identity")+
  theme_minimal()+
  coord_flip()+
  labs(x = "Chemical", y = "Usage",
       title = "Top Chemicals Used in LB Only in California")+
  theme(plot.title.position = "plot")
```



above shows the most used chemicals in LB in strawberry harvesting, we can further explore the properties of those chemicals:

```
# Find the index of GHS classification
GHS_searcher<-function(result_json_object){
  # check if the chemicals in the database first
  if (is.null(result_json_object) ||
      is.null(result_json_object[["result"]]) ||
      is.null(result_json_object[["result"]][["Hierarchies"]]) ||
      is.null(result_json_object[["result"]][["Hierarchies"]][["Hierarchy"]])){
    return("did not find the chemical in the database")
  }

  result<-result_json_object
  for (i in 1:length(result[["result"]][["Hierarchies"]][["Hierarchy"]])){
    if(result[["result"]][["Hierarchies"]][["Hierarchy"]][[i]][["SourceName"]]=="GHS Classificat
ion (UNECE)"){
      return(i)
    }

  }
}

# Use the output from GHS_searcher to access the hazard information
hazards_retriever<-function(index,result_json_object){

  # Check if GHS_searcher did not find the index
  if (is.character(index) && index == "did not find the chemical in the database") {
    return(index)
  }

  result<-result_json_object
  hierarchy<-result[["result"]][["Hierarchies"]][["Hierarchy"]][[index]]
  i<-1
  output_list<-rep(NA,length(hierarchy[["Node"]]))
  while(str_detect(hierarchy[["Node"]][[i]][["Information"]][["Name"]],"H") & i<length(hierarchy
[["Node"]])){
    output_list[i]<-hierarchy[["Node"]][[i]][["Information"]][["Name"]]
    i<-i+1
  }
  return(output_list[!is.na(output_list)])
}

# Find the chemical information for the top chemicals
chem_vec <- top_chem$Chemical_Info
access_hazard <- function(chemical){
  results <- list()
  for (chem in chemical){
      result <- get_pug_rest(identifier = chem,
                             namespace = "name",
                             domain = "compound",
                             operation="classification",
                             output = "JSON")
      ghs_index <- GHS_searcher(result)
      hazards <- hazards_retriever(ghs_index, result)
```

```
      results[[chem]] <- list(
        chemical_name = chem,
        chemical_hazards = ifelse(hazards == "did not find the chemical in the database", charac
ter(0), hazards)
      )

  }

  return(results)
}


hazard_info <- access_hazard(chem_vec)
hazards_df <- do.call(rbind, lapply(hazard_info, function(x) {
  data.frame(
    chemical_name = x$chemical_name,
    hazards = paste(x$chemical_hazards, collapse = ";"),
    stringsAsFactors = FALSE
  )
}))


hazards_df %>%
  flextable() %>%
  theme_vanilla() %>%
  fontsize(size = 10) %>%
  fit_to_width(max_width = 8) %>%
  align(align = "left", part = "all")
```

chemical_name	hazards
AZADIRACHTIN	NA
QUINOLINE	H301: Toxic if swallowed [Danger Acute toxicity, oral];H300: Health Hazards;Hazard Statement Codes;H302: Harmful if swallowed [Warning Acute toxicity, oral];H311: Toxic in contact with skin [Danger Acute toxicity, dermal];H312: Harmful in contact with skin [Warning Acute toxicity, dermal];H315: Causes skin irritation [Warning Skin corrosion/irritation];H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation];H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation];H336: May cause drowsiness or dizziness [Warning Specific target organ toxicity, single exposure; Narcotic effects];H341: Suspected of causing genetic defects [Warning Germ cell mutagenicity];H350: May cause cancer [Danger Carcinogenicity];H351: Suspected of causing cancer [Warning Carcinogenicity];H370: Causes damage to organs [Danger Specific target organ toxicity, single exposure];H371: May cause damage to organs [Warning Specific target organ toxicity, single exposure];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H402: Harmful to aquatic life [Hazardous to the

chemical_name	hazards
	aquatic environment, acute hazard];H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard];H411: Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard];H412: Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
POLYOXIN D ZINC SALT	NA
IRON PHOSPHATE	H315: Causes skin irritation [Warning Skin corrosion/irritation];H300: Health Hazards;Hazard Statement Codes;H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation];H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]
PYRIPROXYFEN	H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;Hazard Statement Codes;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard];Hazardous to the aquatic environment, acute hazard;Environmental Hazards;Hazard Classes;Hazardous to the aquatic environment, long-term hazard; GHS09;Hazard Pictograms

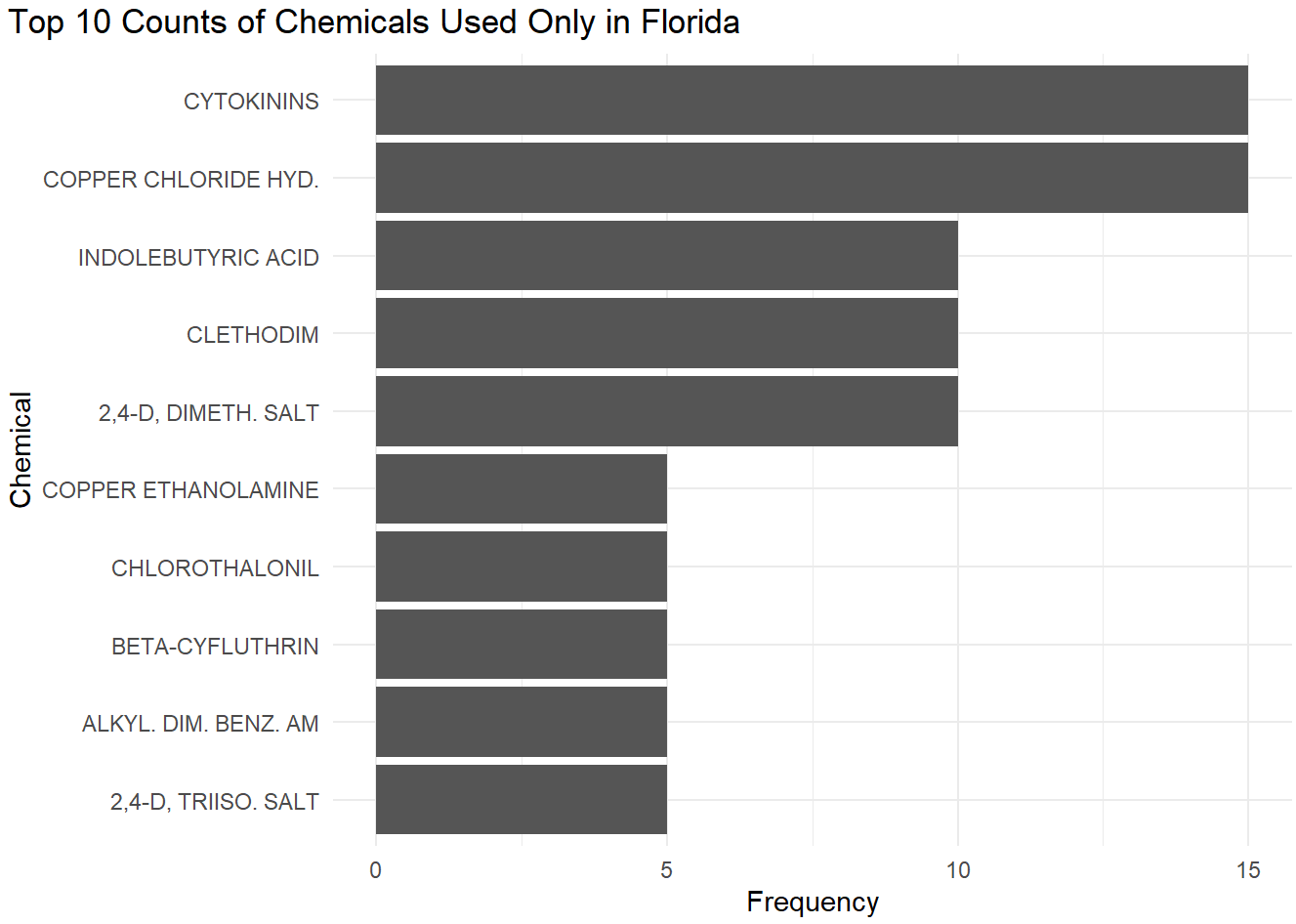
Through the chemical information presented in the above table, three out of the top five chemicals have harmful effect on the environment. Especially for QUINOLINE, which have a lot of harzardous information, especially causing damage to organs and toxic in contact. Also, most of those chemicals are very toxic to aquatic life, which will harm the sustainable development of the environment. Additionally, QUINOLINE belongs to fungicide group, iron phosphate belongs to other group, and PYRIPROXYFEN belongs to insecticide group. Thus, the suggestion to related authority is to decrease the usage of those three chemicals in growing strawberry. Although they can be used as pesticide and fungicide, they do more harm to the environment and humans.

Now, we can further analyze the top chemicals used in strawberry growing in Florida:

```
# Select records with Florida only chemicals
df_chem_flo <- df_flo %>%
  filter(Chemical_Info %in% diff_chem2)

# Create a new column to record the frequency of each chemical used
chem_freq_flo <- df_chem_flo %>%
  count(Chemical_Info) %>%
  arrange(desc(n))

# Plot the top 10 chemicals used in California
ggplot(chem_freq_flo[1: 10,], aes(x=reorder(Chemical_Info, n), y=n))+
  geom_bar(stat = "identity")+
  theme_minimal()+
  coord_flip()+
  labs(x = "Chemical", y = "Frequency",
       title = "Top 10 Counts of Chemicals Used Only in Florida")+
  theme(plot.title.position = "plot")
```



```
chem_vec_flo <- c("INDOLEBUTYRIC ACID",
                  "BETA-CYFLUTHRIN", "CHLOROTHALONIL")
hazard_info_flo <- access_hazard(chem_vec_flo)

hazards_df_flo <- do.call(rbind, lapply(hazard_info_flo, function(x) {
  data.frame(
    chemical_name = x$chemical_name,
    hazards = paste(x$chemical_hazards, collapse = ";"),
    stringsAsFactors = FALSE
  )
}))

hazards_df_flo %>%
  flextable() %>%
  theme_vanilla() %>%
  fontsize(size = 10) %>%
  width(j = "chemical_name", width = 2.5) %>%  # Set width for first column
  width(j = "hazards", width = 5) %>%  # Set width for second column
  align(align = "left", part = "all") %>%
  set_table_properties(layout = "autofit")
```

chemical_name	hazards
INDOLEBUTYRIC ACID	H301: Toxic if swallowed [Danger Acute toxicity, oral];H300: Health Hazards;Hazard Statement Codes;H315: Causes skin irritation [Warning Skin corrosion/irritation];H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation];H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation];H402: Harmful to aquatic life [Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H412: Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
BETA-CYFLUTHRIN	H300: Fatal if swallowed [Danger Acute toxicity, oral];H300: Health Hazards;Hazard Statement Codes;H330: Fatal if inhaled [Danger Acute toxicity, inhalation];H362: May cause harm to breast-fed children [Reproductive toxicity, effects on or via lactation];H370: Causes damage to organs [Danger Specific target organ toxicity, single exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
CHLOROTHALONIL	H317: May cause an allergic skin reaction [Warning Sensitization, Skin];H300: Health Hazards;Hazard Statement Codes;H318: Causes serious eye damage [Danger Serious eye damage/eye irritation];H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation];H330: Fatal if inhaled [Danger Acute toxicity, inhalation];H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled [Danger Sensitization, respiratory];H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation];H351: Suspected of causing cancer [Warning Carcinogenicity];H361: Suspected of damaging fertility or the unborn child [Warning Reproductive toxicity];H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure];H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard];H400: Environmental Hazards;H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

Through the table shown above, three out of top ten chemicals used only in Florida have hazard information. The most toxic chemical is the beta-cyfluthrin, which can be fatal if swallowed and inhaled, and it also has toxic effects to aquatic lives, which is bad for the environment.

In summary, by comparing the chemicals used in California and Florida, California used more types of chemicals than Florida, also, the counts of chemicals used in each state were also higher for California, which is almost two times higher compared to Florida. However, California and Florida both used chemicals that are toxic to the aquatic lives and environment when growing strawberry, and it is important to suggest to the goverment to restrict the amount of harmful chemicals used in insecticides and pesticides, and they should be changed to more environmental friendly substitutes.