# Microplastic1

October 27, 2024

[1]:

```python
#!/usr/bin/env python
# coding: utf-8

# In[14]:



import pandas as pd
# Define the file path provided by the user
file_path = r'~/Desktop/files/Microplastic.xlsx'

# Load the Excel file again to check the sheets and prepare for merging
xls = pd.ExcelFile(file_path)

# List all sheet names to understand the structure for further operations
sheet_names = xls.sheet_names
sheet_names
```

[1]:

```
['Table of Contents',
 'B.1. Chemical list key',
 'B.1. Chemicals list',
 'B.2. Health outcomes list',
 'B.3. Countries list']
```

[2]:

```python
# In[15]:

# Read the content of the Excel file to check the sheets available
xls = pd.ExcelFile(file_path)

# Display the sheet names
xls.sheet_names
```

[2]:

```
['Table of Contents',
 'B.1. Chemical list key',
 'B.1. Chemicals list',
 'B.2. Health outcomes list',
 'B.3. Countries list']
```

[3]:

```python
# In[16]:

# Read the relevant sheets
chemical_list_df = pd.read_excel(file_path, sheet_name='B.1. Chemicals list')
health_outcomes_df = pd.read_excel(file_path, sheet_name='B.2. Health outcomes␣
 ↪list')

# Clean the 'Chemical List' dataframe
chemical_list_cleaned = chemical_list_df[['Chemical class', 'Chemical name',␣
 ↪'CAS number', 'Function for SEM inclusion', 'Source', 'Found/Not␣
 ↪found','General function*','Sector of use*','Hazard rating*']].dropna()

# Clean the 'Health Outcomes List' dataframe (after renaming columns␣
 ↪appropriately)
health_outcomes_cleaned = health_outcomes_df.rename(columns={
    'Excel Table B.2. List of health outcome measures showing their ICD␣
 ↪classifications, corresponding search terms, and the health outcome measure␣
 ↪extracted and used for grouping in this systematic evidence map.': 'Health␣
 ↪outcome',
    'Unnamed: 6': 'Group'
})[['Health outcome', 'Group']].dropna()

# Merging the chemical list and health outcomes using 'concat'
merged_data = pd.concat([chemical_list_cleaned, health_outcomes_cleaned],␣
 ↪axis=1)

# Display the first few rows of the merged data
print(merged_data.head())
```

```
   Chemical class                                      Chemical name  \
0      Bisphenols  1,3-dibromo-5-[2-[3,5-dibromo-4-(2,3-dibromo-2…
1      Bisphenols  1,3-dibromo-5-[2-[3,5-dibromo-4-(2,3-dibromopr…
2      Bisphenols  2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)…
26           OPEs  (3-diphenoxyphosphoryloxyphenyl) diphenyl phos…
30           OPEs  2-[diethoxyphosphorylmethyl(2-hydroxyethyl)ami…

      CAS number Function for SEM inclusion  \
0   "97416-84-7"            Flame retardant
1   "21850-44-2"            Flame retardant
2      "79-94-7"            Flame retardant
26  "57583-54-7"            Flame retardant
30   "2781-11-5"            Flame retardant

                                               Source Found/Not found  \
0                           ECHA - EU Chemicals Agency       not found
1                           ECHA - EU Chemicals Agency       not found
2                           ECHA - EU Chemicals Agency           found
```

```
26  Added by expert based on structural similarity…          found
30  Added by expert based on chemical similarity w…      not found

                                    General function*  \
0             Colorant, Flame Retardant, Intermediates
1   Biocide, Colorant, Flame Retardant, Lubricant,…
2   Flame Retardant, Intermediates, Other Processi…
26  Colorant, Flame Retardant, Lubricant, Plasticizer
30                                     Flame Retardant

                                       Sector of use*     Hazard rating*  \
0   Building & Construction, Electrical and Electr…  No data available
1   Building & Construction, Electrical and Electr…  No data available
2   Automotive, Building & Construction, Electrica…               high
26  Automotive, Electrical and Electronic Equipmen…  No data available
30                                           Textiles  No data available

                                 Health outcome  \
0                                   ICD Level 0
1   01 Certain infectious or parasitic diseases
2   01 Certain infectious or parasitic diseases
26  01 Certain infectious or parasitic diseases
30  01 Certain infectious or parasitic diseases

                                     Group
0                                    Group
1   Other infectious or parasitic diseases
2   Other infectious or parasitic diseases
26                Viral infectious disease
30                Viral infectious disease
```

[4]:

```
# In[17]:

# Check for any missing, NaN, or empty values in the merged dataset
missing_values = merged_data.isnull().sum()

# Display the count of missing values in each column
print(missing_values)
```

```
Chemical class                955
Chemical name                 955
CAS number                    955
Function for SEM inclusion    955
Source                        955
Found/Not found               955
General function*             955
Sector of use*                955
Hazard rating*                955
```

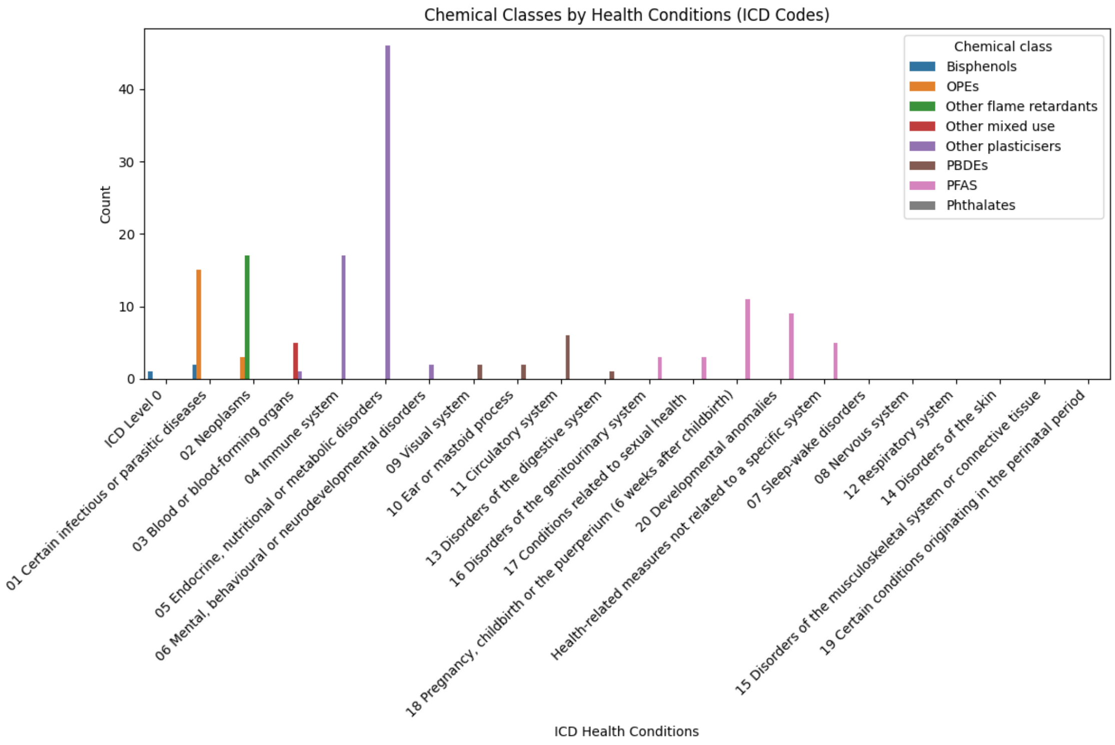
```
Health outcome                   36
Group                            36
dtype: int64
```

[5]:

```
# In[18]:

# Fill missing values with the mode (most frequent value) for each column
merged_data_filled = merged_data.apply(lambda x: x.fillna(x.mode()[0]))

# Display the first few rows of the filled dataset to verify
print(merged_data_filled.head())
```

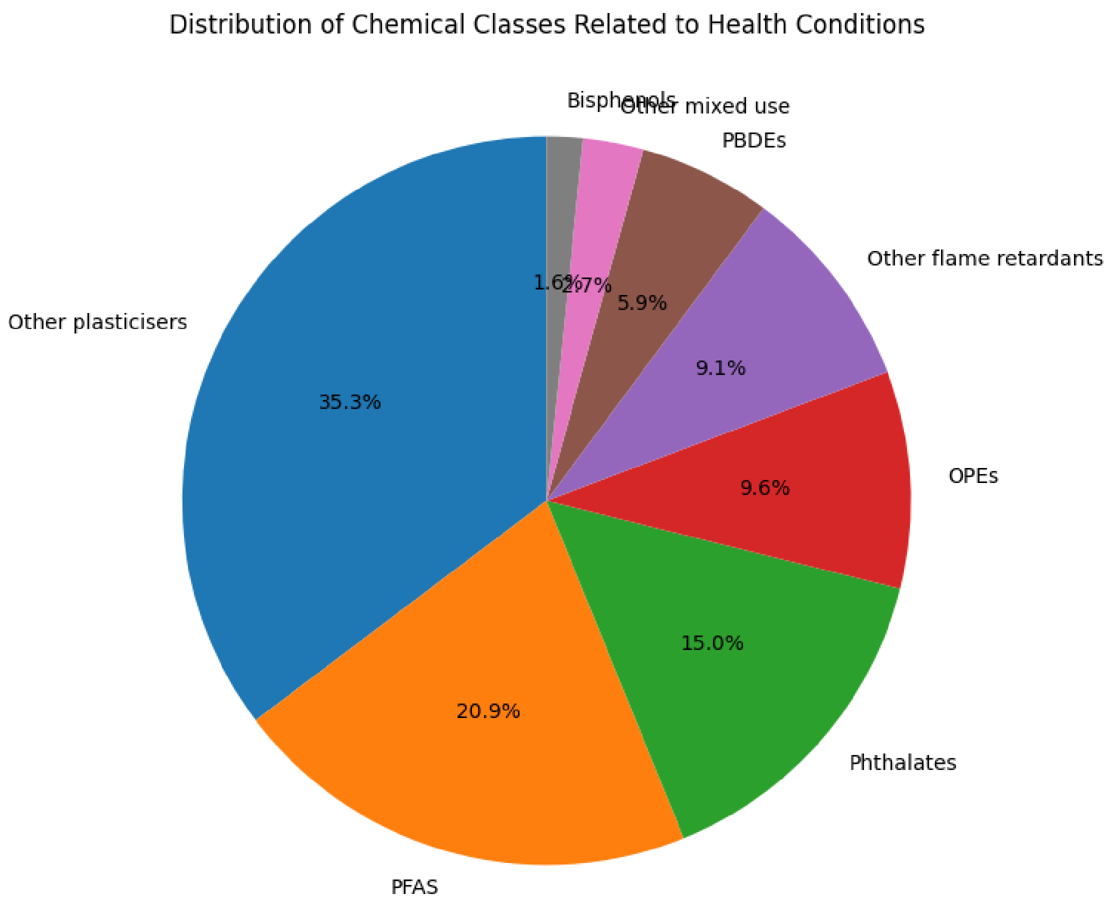
```
   Chemical class                                      Chemical name  \
0      Bisphenols  1,3-dibromo-5-[2-[3,5-dibromo-4-(2,3-dibromo-2…
1      Bisphenols  1,3-dibromo-5-[2-[3,5-dibromo-4-(2,3-dibromopr…
2      Bisphenols  2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)…
26           OPEs  (3-diphenoxyphosphoryloxyphenyl) diphenyl phos…
30           OPEs  2-[diethoxyphosphorylmethyl(2-hydroxyethyl)ami…

      CAS number Function for SEM inclusion  \
0   "97416-84-7"            Flame retardant
1   "21850-44-2"            Flame retardant
2      "79-94-7"            Flame retardant
26  "57583-54-7"            Flame retardant
30   "2781-11-5"            Flame retardant

                                               Source Found/Not found  \
0                           ECHA - EU Chemicals Agency       not found
1                           ECHA - EU Chemicals Agency       not found
2                           ECHA - EU Chemicals Agency           found
26  Added by expert based on structural similarity…           found
30  Added by expert based on chemical similarity w…       not found

                                    General function*  \
0            Colorant, Flame Retardant, Intermediates
1   Biocide, Colorant, Flame Retardant, Lubricant,…
2   Flame Retardant, Intermediates, Other Processi…
26  Colorant, Flame Retardant, Lubricant, Plasticizer
30                                    Flame Retardant

                                       Sector of use*     Hazard rating*  \
0   Building & Construction, Electrical and Electr…  No data available
1   Building & Construction, Electrical and Electr…  No data available
2   Automotive, Building & Construction, Electrica…               high
26  Automotive, Electrical and Electronic Equipmen…  No data available
30                                           Textiles  No data available

                                 Health outcome  \
0                                    ICD Level 0
1   01 Certain infectious or parasitic diseases
2   01 Certain infectious or parasitic diseases
26  01 Certain infectious or parasitic diseases
30  01 Certain infectious or parasitic diseases

                                     Group
0                                    Group
1   Other infectious or parasitic diseases
2   Other infectious or parasitic diseases
26                Viral infectious disease
30                Viral infectious disease
```

[6]:
```
# In[19]:

import seaborn as sns
import matplotlib.pyplot as plt

# Create a count plot (bar chart) to visualize the number of occurrences of␣
 ↪each chemical class by ICD code
plt.figure(figsize=(12, 8))
sns.countplot(data=merged_data, x='Health outcome', hue='Chemical class')
plt.title('Chemical Classes by Health Conditions (ICD Codes)')
plt.xticks(rotation=45, ha='right')
plt.xlabel('ICD Health Conditions')
plt.ylabel('Count')
plt.tight_layout()
plt.show()
```



[7]:

```
# In[20]:

# Plot pie chart for chemical class distribution
plt.figure(figsize=(8, 8))
merged_data['Chemical class'].value_counts().plot(kind='pie', autopct='%1.
 ↪1f%%', startangle=90)
plt.title("Distribution of Chemical Classes Related to Health Conditions")
plt.ylabel('')
plt.show()
```



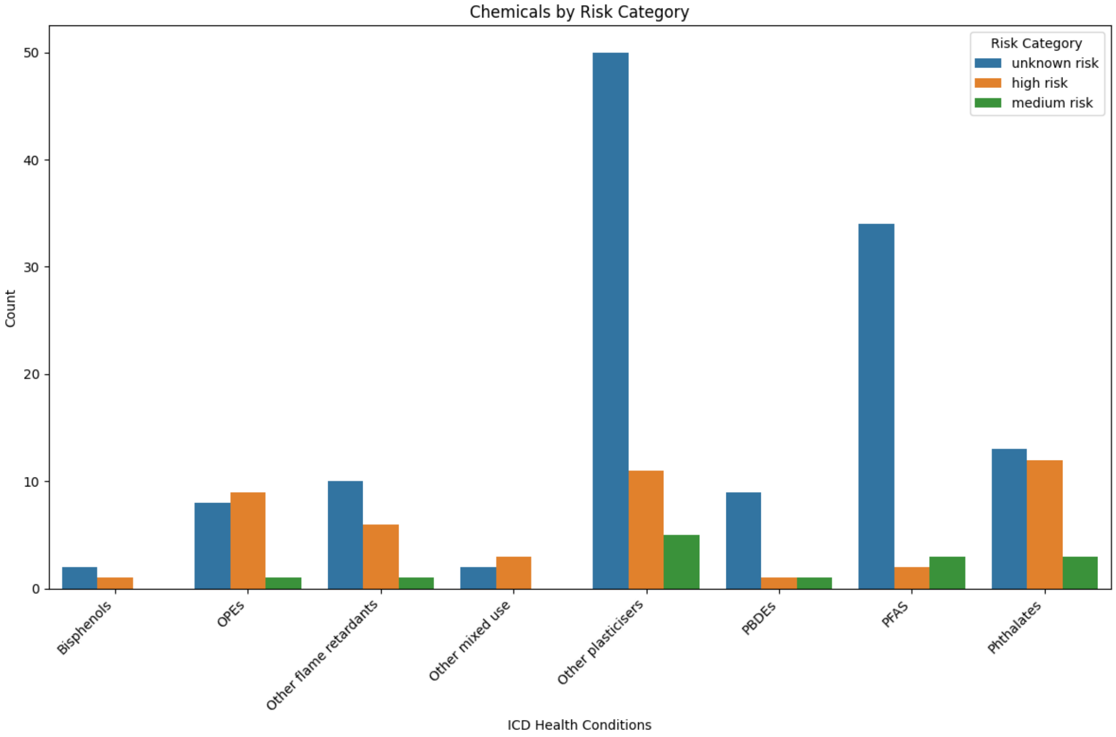
[8]:

```python
# In[21]:

##
def categorize_risk(hazard_rating):
    if hazard_rating == 'high':
        return 'high risk'
    elif hazard_rating == 'low':
        return 'low risk'
    elif hazard_rating == 'medium':
        return 'medium risk'
    elif hazard_rating == 'No data available':
        return 'unknown risk'
    else:
        return 'unknown risk'  # Optional: Handle unexpected cases

# Apply the function and create a new column
```

```
merged_data['Risk Category'] = merged_data['Hazard rating*'].
 ↪apply(categorize_risk)
##

# Display the first few rows to verify
print(merged_data[['Chemical name', 'Risk Category']].head())
```

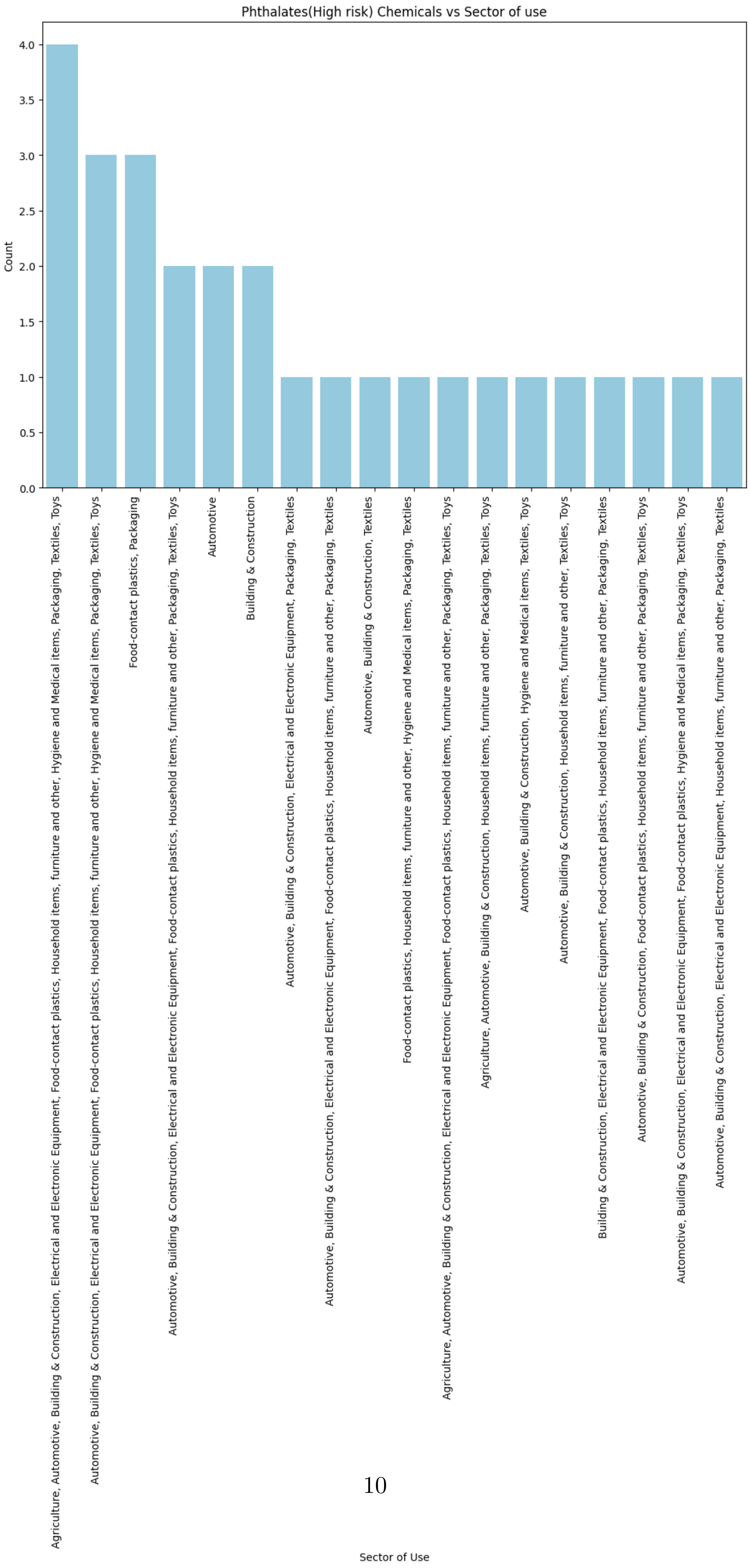
```
                                        Chemical name Risk Category
0   1,3-dibromo-5-[2-[3,5-dibromo-4-(2,3-dibromo-2…  unknown risk
1   1,3-dibromo-5-[2-[3,5-dibromo-4-(2,3-dibromopr…  unknown risk
2   2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)…     high risk
26  (3-diphenoxyphosphoryloxyphenyl) diphenyl phos…  unknown risk
30  2-[diethoxyphosphorylmethyl(2-hydroxyethyl)ami…  unknown risk
```

[9]:
```
# In[22]:

# Create a bar chart of chemicals by risk category and health outcomes
plt.figure(figsize=(12, 8))
sns.countplot(data=merged_data, x='Chemical class', hue='Risk Category')
plt.title("Chemicals by Risk Category")
plt.xticks(rotation=45, ha='right')
plt.xlabel('ICD Health Conditions')
plt.ylabel('Count')
plt.tight_layout()
plt.show()
```



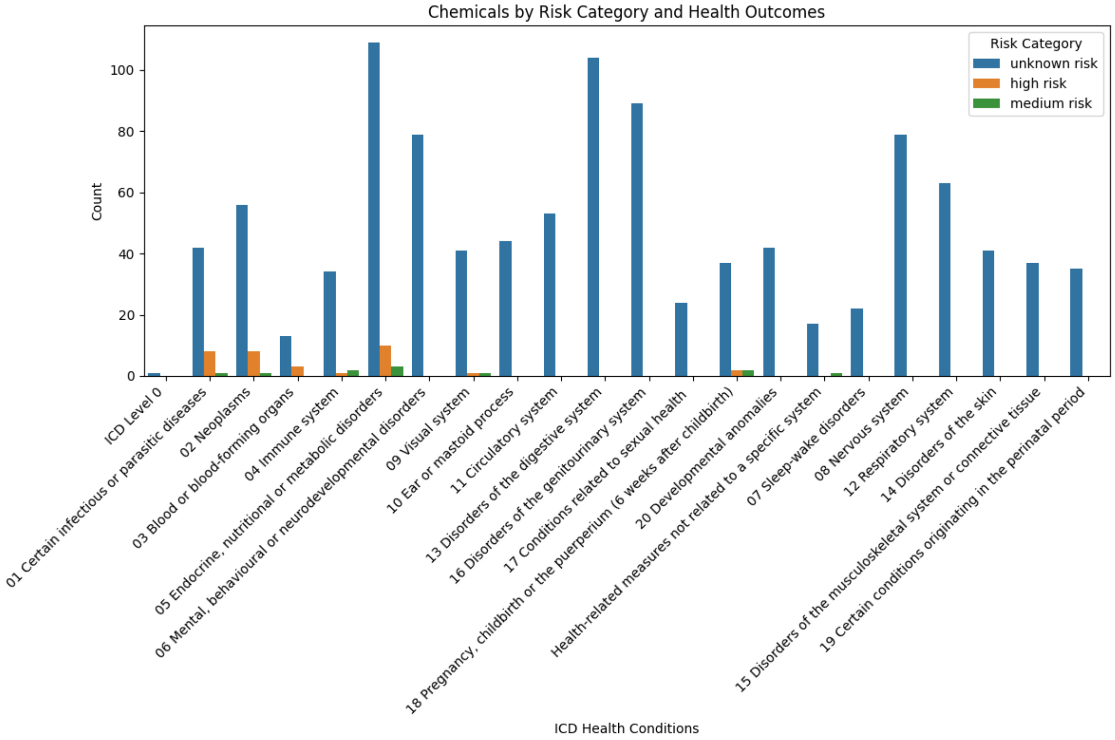
[18]:

```
# chemical class with the highest risk effect

Phthalates = merged_data[merged_data['Chemical class'] == 'Phthalates']

# Create a bar chart of phthalates chemicals by sector of use
# Calculate the counts of each sector
sector_counts = Phthalates['Sector of use*'].value_counts().index.tolist()
plt.figure(figsize=(12, 8))
sns.countplot(data=Phthalates, x='Sector of use*', color='skyblue',␣
 ↪order=sector_counts)
plt.title("Phthalates(High risk) Chemicals vs Sector of use")
plt.xticks(rotation=90, ha='right')
plt.xlabel('Sector of Use')
plt.ylabel('Count')
plt.show()
```


Phthalates(High risk) Chemicals vs Sector of use
Count
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Agriculture, Automotive, Building & Construction, Electrical and Electronic Equipment, Food-contact plastics, Household items, furniture and other, Hygiene and Medical items, Packaging, Textiles, Toys
Automotive, Building & Construction, Electrical and Electronic Equipment, Food-contact plastics, Household items, furniture and other, Hygiene and Medical items, Packaging, Textiles, Toys
Food-contact plastics, Packaging
Automotive, Building & Construction, Electrical and Electronic Equipment, Food-contact plastics, Household items, furniture and other, Packaging, Textiles, Toys
Automotive
Building & Construction
Automotive, Building & Construction, Electrical and Electronic Equipment, Packaging, Textiles
Automotive, Building & Construction, Electrical and Electronic Equipment, Food-contact plastics, Household items, furniture and other, Packaging, Textiles
Automotive, Building & Construction, Textiles
Food-contact plastics, Household items, furniture and other, Hygiene and Medical items, Packaging, Textiles
Agriculture, Automotive, Building & Construction, Electrical and Electronic Equipment, Food-contact plastics, Household items, furniture and other, Packaging, Textiles, Toys
Agriculture, Automotive, Building & Construction, Household items, furniture and other, Packaging, Textiles, Toys
Automotive, Building & Construction, Hygiene and Medical items, Textiles, Toys
Automotive, Building & Construction, Household items, furniture and other, Textiles, Toys
Building & Construction, Electrical and Electronic Equipment, Food-contact plastics, Household items, furniture and other, Packaging, Textiles
Automotive, Building & Construction, Food-contact plastics, Household items, furniture and other, Packaging, Textiles, Toys
Automotive, Building & Construction, Electrical and Electronic Equipment, Food-contact plastics, Hygiene and Medical items, Packaging, Textiles, Toys
Automotive, Building & Construction, Electrical and Electronic Equipment, Household items, furniture and other, Packaging, Textiles
Sector of Use

[ ]:

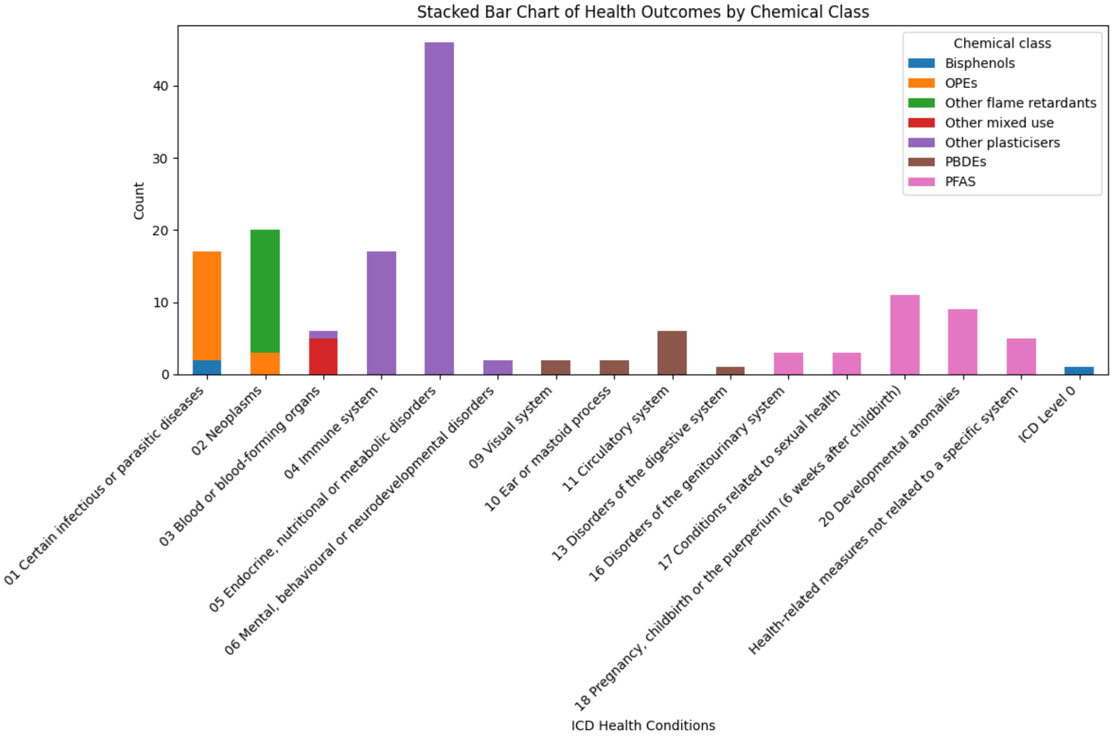
```
# In[22]:

# Create a bar chart of chemicals by risk category and health outcomes
plt.figure(figsize=(12, 8))
sns.countplot(data=merged_data, x='Health outcome', hue='Risk Category')
plt.title("Chemicals by Risk Category and Health Outcomes")
plt.xticks(rotation=45, ha='right')
plt.xlabel('ICD Health Conditions')
plt.ylabel('Count')
plt.tight_layout()
plt.show()
```



[ ]:

```
# In[23]:

# Group the data by 'Health outcome' and 'Chemical class'
grouped_data = merged_data.groupby(['Health outcome', 'Chemical class']).size().
 ↪unstack(fill_value=0)

# Plot a stacked bar chart
grouped_data.plot(kind='bar', stacked=True, figsize=(12, 8))
```

```
plt.title("Stacked Bar Chart of Health Outcomes by Chemical Class")
plt.xlabel('ICD Health Conditions')
plt.ylabel('Count')
plt.xticks(rotation=45, ha='right')
plt.tight_layout()
plt.show()
```



[ ]:
```
# In[45]:

print(merged_data.columns)
```

```
Index(['Chemical class', 'Chemical name', 'CAS number',
       'Function for SEM inclusion', 'Source', 'Found/Not found',
       'General function*', 'Sector of use*', 'Hazard rating*',
       'Health outcome', 'Group', 'Risk Category'],
      dtype='object')
```

[ ]:
```
# In[46]:

# Create a binary target variable based on 'Risk Category'
# Assuming 'High Risk' indicates responsibility for health issues
merged_data['Responsible'] = merged_data['Risk Category'].apply(lambda x: 1 if␣
 ↪x == 'high risk' else 0)
```

```python
# Encode the features

from sklearn.preprocessing import LabelEncoder

# Instances for LabelEncoder
le_chemical = LabelEncoder()
le_health = LabelEncoder()

# Fit and transform the features
merged_data['Chemical class_encoded'] = le_chemical.
 ↪fit_transform(merged_data['Chemical class'])
merged_data['Health outcome_encoded'] = le_health.
 ↪fit_transform(merged_data['Health outcome'])

# Prepare features (X) and target (y)
X = merged_data[['Chemical class_encoded', 'Health outcome_encoded']]  #␣
 ↪Features
y = merged_data['Responsible']  # Target variable: whether the chemical is␣
 ↪responsible

# Split the data into training and test sets
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
 ↪random_state=42)

# Train a Random Forest model (or any other model you prefer)
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score, classification_report

rf_classifier = RandomForestClassifier(random_state=42)
rf_classifier.fit(X_train, y_train)

# Make predictions
y_pred = rf_classifier.predict(X_test)

# Evaluate the model
accuracy = accuracy_score(y_test, y_pred)
print(f"Random Forest Accuracy: {accuracy:.2f}")

# Print detailed classification report
print(classification_report(y_test, y_pred))
```

```
Random Forest Accuracy: 0.97
              precision    recall  f1-score   support

           0       0.98      1.00      0.99       223
           1       0.50      0.17      0.25         6

    accuracy                           0.97       229
   macro avg       0.74      0.58      0.62       229
weighted avg       0.97      0.97      0.97       229
```

[ ]:

```python
# In[51]:

print(merged_data['Risk Category'].value_counts())
# or check other columns that could serve as a target
```

```
Risk Category
unknown risk    1083
high risk         45
medium risk       14
Name: count, dtype: int64
```

[ ]:

```python
# In[53]:

from sklearn.neighbors import KNeighborsClassifier

# Initialize KNN model
knn_model = KNeighborsClassifier(n_neighbors=5)

# Train model
knn_model.fit(X_train, y_train)

# Predict
y_pred = knn_model.predict(X_test)

# Accuracy and classification report
accuracy = accuracy_score(y_test, y_pred)
print(f"KNN Accuracy: {accuracy:.2f}")
print(classification_report(y_test, y_pred))
```

```
KNN Accuracy: 0.97
              precision    recall  f1-score   support

           0       0.98      0.98      0.98       223
           1       0.33      0.33      0.33         6

    accuracy                           0.97       229
   macro avg       0.66      0.66      0.66       229
weighted avg       0.97      0.97      0.97       229
```

[ ]:

```python
# In[54]:

from sklearn.tree import DecisionTreeClassifier

# Initialize Decision Tree model
dt_model = DecisionTreeClassifier(random_state=42)

# Train model
dt_model.fit(X_train, y_train)

# Predict
y_pred = dt_model.predict(X_test)

# Accuracy and classification report
accuracy = accuracy_score(y_test, y_pred)
print(f"Decision Tree Accuracy: {accuracy:.2f}")
print(classification_report(y_test, y_pred))
```

```
Decision Tree Accuracy: 0.97
              precision    recall  f1-score   support

           0       0.97      1.00      0.98       223
           1       0.00      0.00      0.00         6

    accuracy                           0.97       229
   macro avg       0.49      0.50      0.49       229
weighted avg       0.95      0.97      0.96       229

              precision    recall  f1-score   support

           0       0.97      1.00      0.98       223
           1       0.00      0.00      0.00         6

    accuracy                           0.97       229
   macro avg       0.49      0.50      0.49       229
weighted avg       0.95      0.97      0.96       229
```