EBU | European Business Institute LUXEMBOURG

COURSE: MASTER OF SCIENCE IN DATA SCIENCE AND AI

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PROJECT TITTLE: Investigating Genomic Patterns with Machine Learning in the Mycobacterium TB Complex: Deciphering the Dynamics of Antimicrobial Resistance

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Investigating Genomic Patterns with Machine Learning in the Mycobacterium TB Complex: Deciphering the Dynamics of Antimicrobial Resistance

Tuberculosis (TB) is one of the most dangerous diseases in the world today, and it poses a serious challenge to public health systems everywhere. Tuberculosis (TB) was responsible for 1.30 million deaths worldwide in 2022 (including HIV-positive individuals). The WHO reported 410 000 cases of multidrug-resistant or rifampicin-resistant tuberculosis (MDR/RR-TB) worldwide in 2022(WHO, 2023). Despite the development of new diagnostic tools, the number of cases of multidrug-resistant (MDR-TB) tuberculosis has increased, making drug-resistant tuberculosis (DR-TB) more difficult to diagnose. Finding genomic patterns that influence drug resistance is essential to combating antimicrobial resistance (AMR) in the Mycobacterium tuberculosis (TB) complex. The purpose of this work was to use machine learning to investigate and interpret the complex dynamics of antibiotic resistance in the Mycobacterium tuberculosis complex. To detect and predict drug-resistant tuberculosis patterns, data from the WHO was analyzed using machine learning RFE. Identifying important genetic variants associated with medication resistance is the primary objective; these variants will be ranked in order of significance using a tiered system. The study seeks to assess how well different drug variations predict antimicrobial response.

RESULTS OF THE ANALYSIS

This analysis shows that: on the correlation analysis that, INITIAL CONFIDENCE GRADING and FINAL CONFIDENCE GRADING are moderately positively correlated (0.279718) between the initial and final confidence gradings suggesting that the initial confidence grading has a notable influence on the final confidence grading.

On the first analysis, the presence of common genetic variants has a weak negative correlation (Correlation Coefficient: -0.04838) with the final confidence grading, with a highly significant p-value of 1.718e-10, implying that these variants may have a minor impact on the grading. In contrast, there is a moderate positive correlation (Correlation Coefficient: 0.27972) between the initial and final confidence gradings, with an extremely low p-value of 4.058e-310, indicating that the initial grading has a strong influence on the final outcome. Furthermore, the presence of certain genetic markers associated with resistance (Present_SOLO_R) demonstrates a moderate negative correlation (Correlation Coefficient: -0.11221) with the final confidence grading, accompanied by a highly significant p-value of 7.388e-50, indicating that these markers may negatively affect the grading process.

The F-statistic calculated from the ANOVA analysis is 49133.70, indicating a significant difference between the groups. The observed differences are statistically significant, as evidenced by the low p-value ($p < 0.001$). This implies that at least one of the groups is significantly different from the other. Based on these findings, we can conclude that the drug used has a significant influence on the final grading outcome suggesting that different drugs may result in varying levels of efficacy or resistance in treating MDR-TB. Understanding the impact of drug Selection in final grading is critical for optimizing treatment strategies and improving patient outcomes. The model achieved an overall accuracy of 98%, indicating a high degree of accuracy in predicting the final confidence grade.

• Classes with significant support have higher precision, recall, and F1-scores compared to others.

n• Class 2 ("Not assoc w R") has the highest precision, recall, and F1-score, indicating high prediction accuracy.

Based on model analysis on important features. The presence of common genetic variants (Common Variant (0.3599)) associated with drug resistance was the most important feature, indicating that genetic marker variations have a significant impact on drug resistance prediction. Furthermore, the presence of rifampicin resistance-related genetic markers is the third most important feature, emphasizing the need for genetic testing to identify drug-resistant tuberculosis strains (0.0854).This information can guide clinical decision-making and aid in the prioritization of interventions for drug-resistant tuberculosis cases

In [1]:
```
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
```

```
C:\Users\hp\anaconda3\lib\site-packages\scipy\__init__.py:155: UserWarning: A NumPy version >=1.18.5 and <1.25.
0 is required for this version of SciPy (detected version 1.26.4
  warnings.warn(f"A NumPy version >={np_minversion} and <{np_maxversion}"
```

In [2]:
```
df = pd.read_excel("C:/Users/hp/Downloads/WHO-UCN-GTB-PCI-2021.7-eng.xlsx", sheet_name ='Mutation_catalogue')
```

In [3]:
```
df.head()
```

Out[3]:

	Drug	Tier	Common Variant	Genome position	algorithm pass	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	...	RIF CC guide 2021	Ha GenoTy MTBDRpl V:
0	AMI	1.0	rrs_a1401g	1473246.0	1.0	918.0	966.0	50.0	15640.0	939.0	...	NaN	N
1	AMI	1.0	eis_c-14t	2715346.0	1.0	28.0	77.0	51.0	7325.0	32.0	...	NaN	N
2	AMI	1.0	rrs_g1484t	1473329.0	1.0	5.0	7.0	2.0	15688.0	6.0	...	NaN	N
3	AMI	1.0	rrs_c1402t	1473247.0	1.0	4.0	13.0	10.0	15680.0	5.0	...	NaN	N
4	AMI	2.0	whiB6_A77V	NaN	1.0	3.0	100.0	97.0	15593.0	3.0	...	NaN	N

5 rows × 52 columns

In [ ]:
```
df.info()
```

In [4]:
```
df.isnull().sum()#Checking for missing values
```

Out[4]:
```
Drug                                 0
Tier                                48
Common Variant                       0
Genome position                  10910
algorithm pass                       8
Present_SOLO_R                       8
Present_SOLO_SR                      8
Present_S                            8
Absent_S                             8
Present_R                            8
Absent_R                             8
PPV                                  8
PPV_lb                               8
PPV_ub                               8
PPV | SOLO                        1322
PPV | SOLO_lb                     1322
PPV | SOLO_ub                     1322
Sensitivity                          8
Sensitivity_lb                       8
Sensitivity_ub                       8
Specificity                          8
Specificity_lb                       8
Specificity_ub                       8
LR+                                  8
LR+_lb                               8
LR+_ub                               8
LR-                                 11
LR-_lb                               8
LR-_ub                               8
OR                                  11
OR_lb                                8
OR_ub                                8
OR SOLO                           9700
OR SOLO_lb                        9700
OR SOLO_ub                        9700
OR SOLO_FE-sig                       8
Neutral masked                       8
INITIAL CONFIDENCE GRADING           8
DATASET(S)                           8
Miotto et al. (PMID 29284687)    17085
NGS Guide 2018                   17140
Level of resistance to INH or MXF    17265
RIF CC guide 2021                17261
Hain GenoType MTBDRplus V2.0     17245
Nipro Genoscholar NTM+MDRTB II   17220
Cepheid Xpert MTB/RIF            17261
Cepheid Xpert MTB/RIF Ultra      17257
Hain GenoType MTBDRsl V2.0       17320
Cepheid Xpert MTB/XDR            17197
Nipro Genoscholar PZA-TB II      16893
Additional grading criteria      16460
FINAL CONFIDENCE GRADING             0
dtype: int64
```

In [5]:
```python
df.columns #Checking for the number of features
```

Out[5]:
```
Index(['Drug', 'Tier', 'Common Variant', 'Genome position', 'algorithm pass',
       'Present_SOLO_R', 'Present_SOLO_SR', 'Present_S', 'Absent_S',
       'Present_R', 'Absent_R', 'PPV', 'PPV_lb', 'PPV_ub', 'PPV | SOLO',
       'PPV | SOLO_lb', 'PPV | SOLO_ub', 'Sensitivity', 'Sensitivity_lb',
       'Sensitivity_ub', 'Specificity', 'Specificity_lb', 'Specificity_ub',
       'LR+', 'LR+_lb', 'LR+_ub', 'LR-', 'LR-_lb', 'LR-_ub', 'OR', 'OR_lb',
       'OR_ub', 'OR SOLO', 'OR SOLO_lb', 'OR SOLO_ub', 'OR SOLO_FE-sig',
       'Neutral masked', 'INITIAL CONFIDENCE GRADING', 'DATASET(S)',
       'Miotto et al. (PMID 29284687)', 'NGS Guide 2018',
       'Level of resistance to INH or MXF', 'RIF CC guide 2021',
       'Hain GenoType MTBDRplus V2.0', 'Nipro Genoscholar NTM+MDRTB II',
       'Cepheid Xpert MTB/RIF', 'Cepheid Xpert MTB/RIF Ultra',
       'Hain GenoType MTBDRsl V2.0', 'Cepheid Xpert MTB/XDR',
       'Nipro Genoscholar PZA-TB II', 'Additional grading criteria',
       'FINAL CONFIDENCE GRADING'],
      dtype='object')
```

In [6]:
```python
drop_columns = ['Genome position', 'algorithm pass', 'PPV', 'PPV_lb', 'PPV_ub',  'PPV | SOLO',
                 'PPV | SOLO_lb', 'PPV | SOLO_ub','Sensitivity', 'Sensitivity_lb', 'Sensitivity_ub',
                 'Specificity', 'Specificity_lb', 'Specificity_ub', 'LR+', 'LR+_lb', 'LR+_ub', 'LR-', 'LR-_lb',
                 'LR-_ub', 'OR', 'OR_lb', 'OR_ub', 'OR SOLO', 'OR SOLO_lb', 'OR SOLO_ub', 'OR SOLO_FE-sig',
                 'DATASET(S)', 'Miotto et al. (PMID 29284687)', 'NGS Guide 2018', 'Level of resistance to INH or
                 'RIF CC guide 2021', 'Hain GenoType MTBDRplus V2.0', 'Nipro Genoscholar NTM+MDRTB II',
                 'Cepheid Xpert MTB/RIF', 'Cepheid Xpert MTB/RIF Ultra', 'Hain GenoType MTBDRsl V2.0',
                 'Cepheid Xpert MTB/XDR', 'Nipro Genoscholar PZA-TB II', 'Additional grading criteria']

# Dropping the specified columns from the DataFrame
df.drop(columns=drop_columns, inplace=True)
```

In [7]:
```python
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 17396 entries, 0 to 17395
Data columns (total 12 columns):
 #   Column                     Non-Null Count  Dtype  
---  ------                     --------------  -----  
 0   Drug                       17396 non-null  object 
 1   Tier                       17348 non-null  float64
 2   Common Variant             17396 non-null  object 
 3   Present_SOLO_R             17388 non-null  float64
 4   Present_SOLO_SR            17388 non-null  float64
 5   Present_S                  17388 non-null  float64
 6   Absent_S                   17388 non-null  float64
 7   Present_R                  17388 non-null  float64
 8   Absent_R                   17388 non-null  float64
 9   Neutral masked             17388 non-null  float64
 10  INITIAL CONFIDENCE GRADING 17388 non-null  object 
 11  FINAL CONFIDENCE GRADING   17396 non-null  object 
dtypes: float64(8), object(4)
memory usage: 1.6+ MB
```

In [8]:
```
df.dtypes
```

Out[8]:
```
Drug                           object
Tier                          float64
Common Variant                 object
Present_SOLO_R                float64
Present_SOLO_SR               float64
Present_S                     float64
Absent_S                      float64
Present_R                     float64
Absent_R                      float64
Neutral masked                float64
INITIAL CONFIDENCE GRADING     object
FINAL CONFIDENCE GRADING       object
dtype: object
```

In [9]:
```
#Handle missing values in categorical columns by imputing with mode
categorical_cols = ['Drug', 'Common Variant', 'Neutral masked', 'INITIAL CONFIDENCE GRADING', 'FINAL CONFIDENCE
df[categorical_cols] = df[categorical_cols].fillna(df[categorical_cols].mode().iloc[0])

df.head()
```

Out[9]:

	Drug	Tier	Common Variant	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	Absent_R	Neutral masked	INITIAL CONFIDENCE GRADING	CONFI GR
0	AMI	1.0	rrs_a1401g	918.0	966.0	50.0	15640.0	939.0	349.0	0.0	Assoc w R	1) Ass
1	AMI	1.0	eis_c-14t	28.0	77.0	51.0	7325.0	32.0	632.0	0.0	Assoc w R	1) Ass
2	AMI	1.0	rrs_g1484t	5.0	7.0	2.0	15688.0	6.0	1282.0	0.0	Assoc w R	2) Assc
3	AMI	1.0	rrs_c1402t	4.0	13.0	10.0	15680.0	5.0	1283.0	0.0	Uncertain significance	2) Assc
4	AMI	2.0	whiB6_A77V	3.0	100.0	97.0	15593.0	3.0	141.0	0.0	Uncertain significance	3) Ur sign

In [10]:
```
df.info()
```

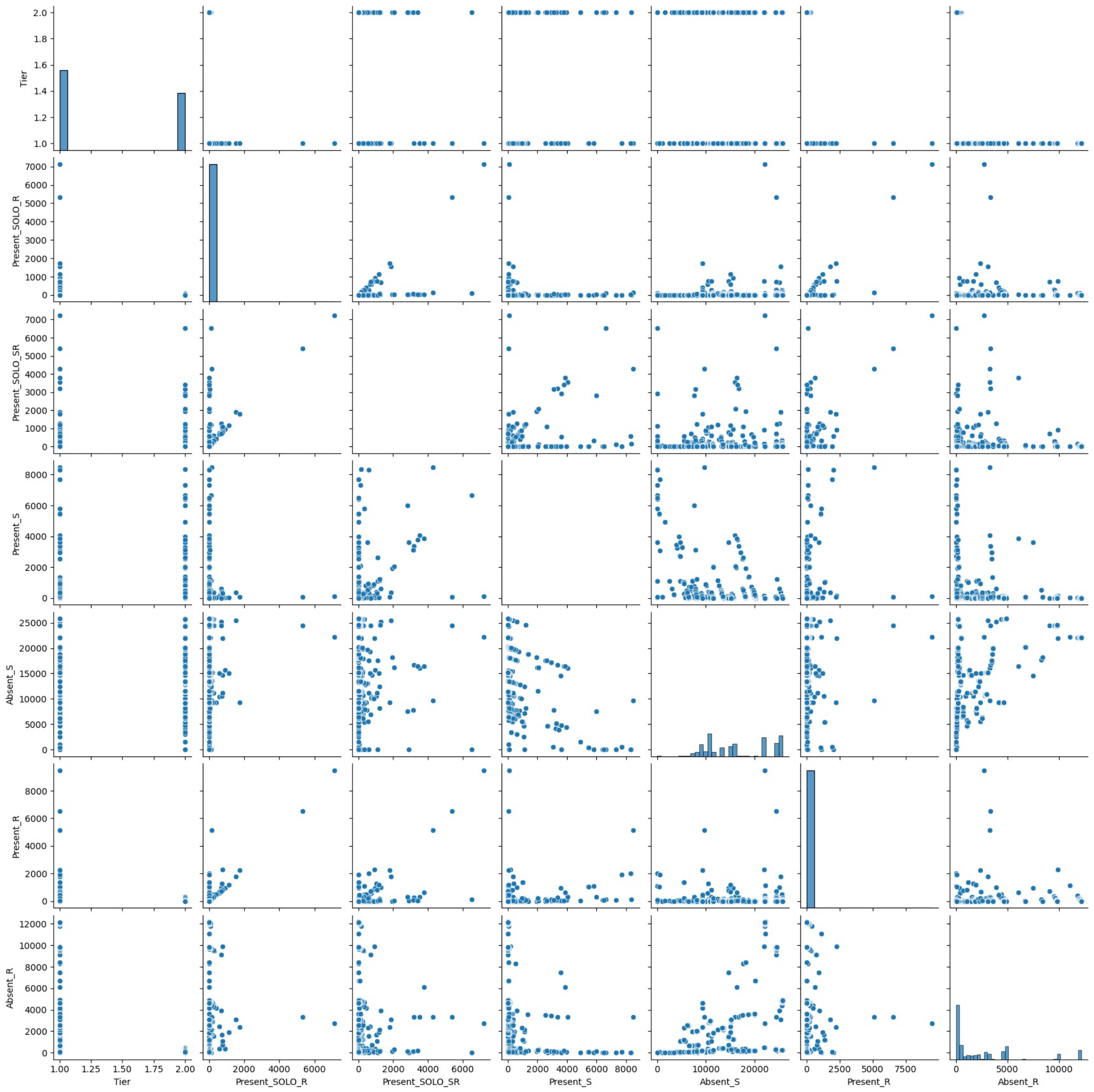
```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 17396 entries, 0 to 17395
Data columns (total 12 columns):
 #   Column                     Non-Null Count  Dtype  
---  ------                     --------------  -----  
 0   Drug                       17396 non-null  object 
 1   Tier                       17348 non-null  float64
 2   Common Variant             17396 non-null  object 
 3   Present_SOLO_R             17388 non-null  float64
 4   Present_SOLO_SR            17388 non-null  float64
 5   Present_S                  17388 non-null  float64
 6   Absent_S                   17388 non-null  float64
 7   Present_R                  17388 non-null  float64
 8   Absent_R                   17388 non-null  float64
 9   Neutral masked             17396 non-null  float64
 10  INITIAL CONFIDENCE GRADING 17396 non-null  object 
 11  FINAL CONFIDENCE GRADING   17396 non-null  object 
dtypes: float64(8), object(4)
memory usage: 1.6+ MB
```

In [11]:
```
unique_values = ['Drug', 'Common Variant', 'INITIAL CONFIDENCE GRADING', 'FINAL CONFIDENCE GRADING']

# Calculate the number of unique values for the specified columns
unique_count = df[unique_values].nunique()

unique_count
```

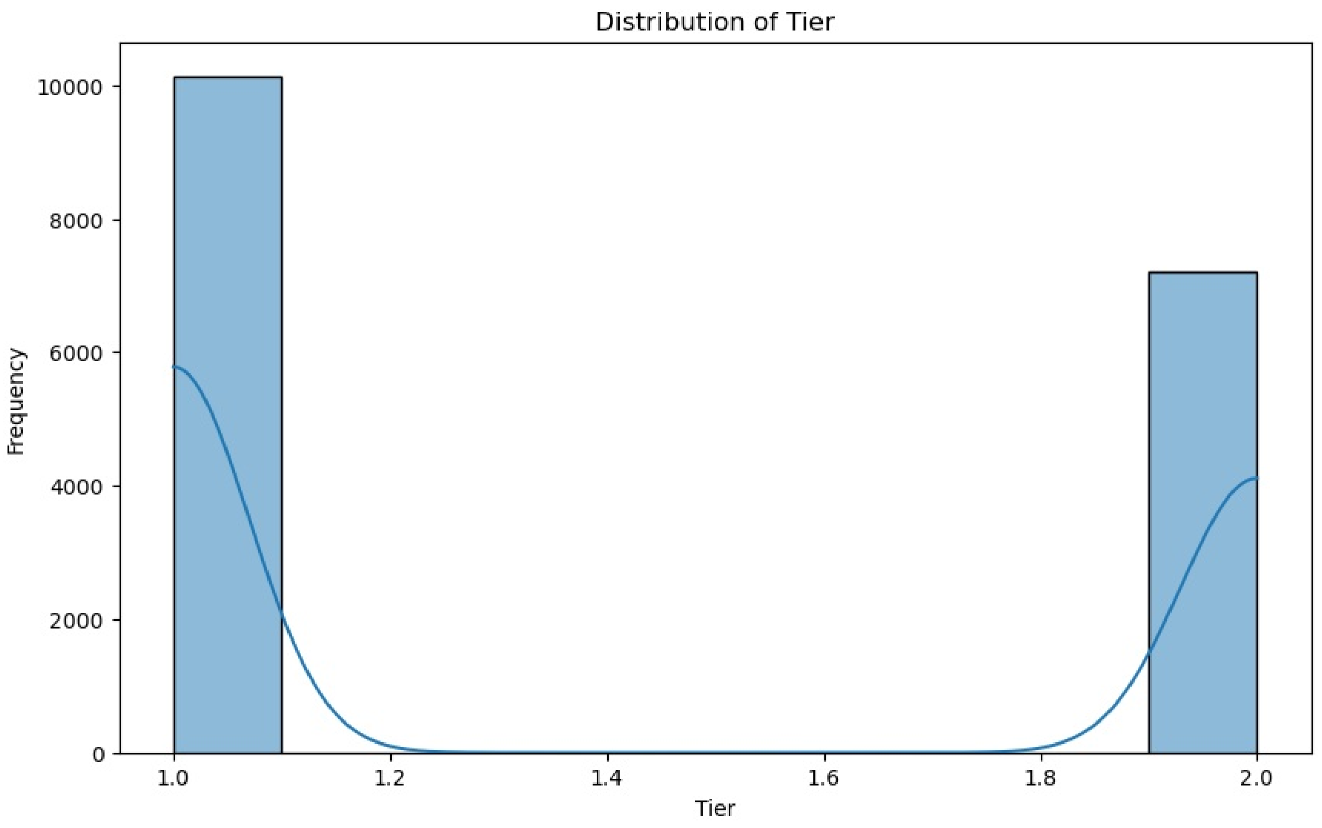
```
Out[11]: Drug                              15
         Common Variant                 13449
         INITIAL CONFIDENCE GRADING         6
         FINAL CONFIDENCE GRADING           6
         dtype: int64
```

```
In [17]: numeric_columns = ['Tier', 'Present_SOLO_R', 'Present_SOLO_SR', 'Present_S', 'Absent_S',
                            'Present_R', 'Absent_R']
```

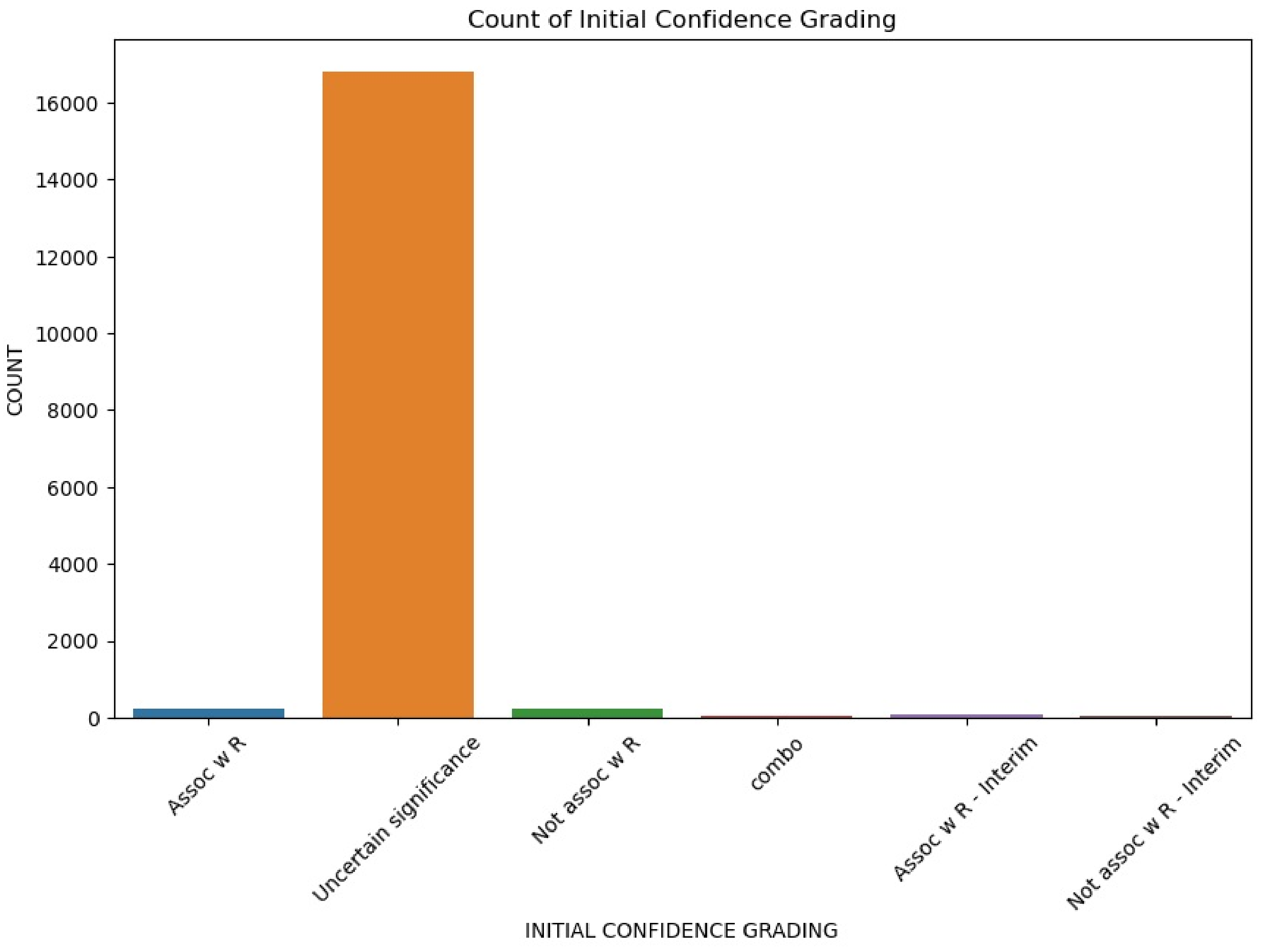
```
In [18]: sns.pairplot(df[numeric_columns])
         plt.show()
```



```
In [15]: plt.figure(figsize=(10, 6))
         sns.histplot(data=df, x='Tier', bins=10, kde=True)
         plt.xlabel('Tier')
         plt.ylabel('Frequency')
         plt.title('Distribution of Tier')
         plt.show()
```

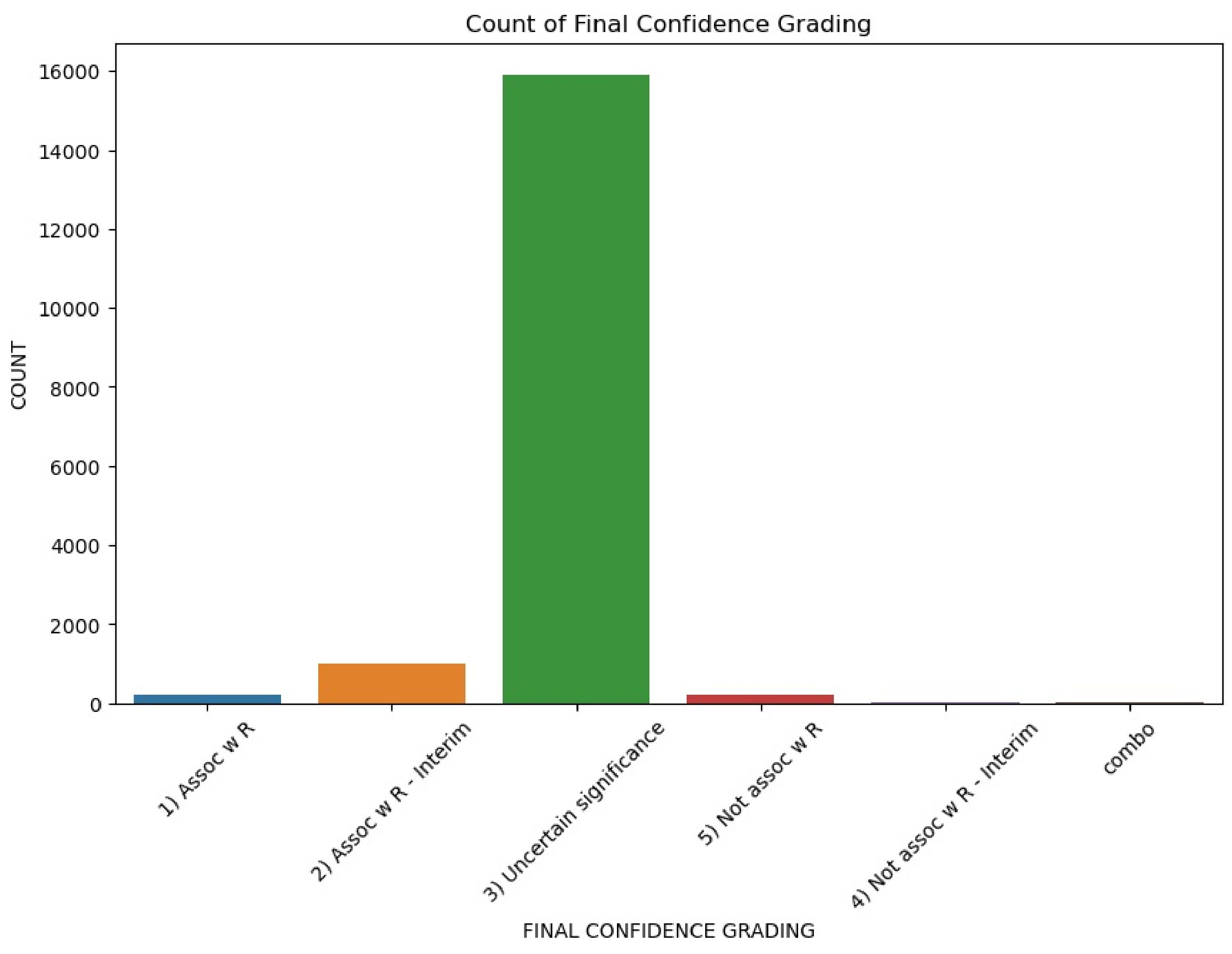


In [21]:
```
plt.figure(figsize=(10, 6))
sns.countplot(data=df, x='INITIAL CONFIDENCE GRADING')
plt.xticks(rotation=45)
plt.xlabel('INITIAL CONFIDENCE GRADING')
plt.ylabel('COUNT')
plt.title('Count of Initial Confidence Grading')
plt.show()
```

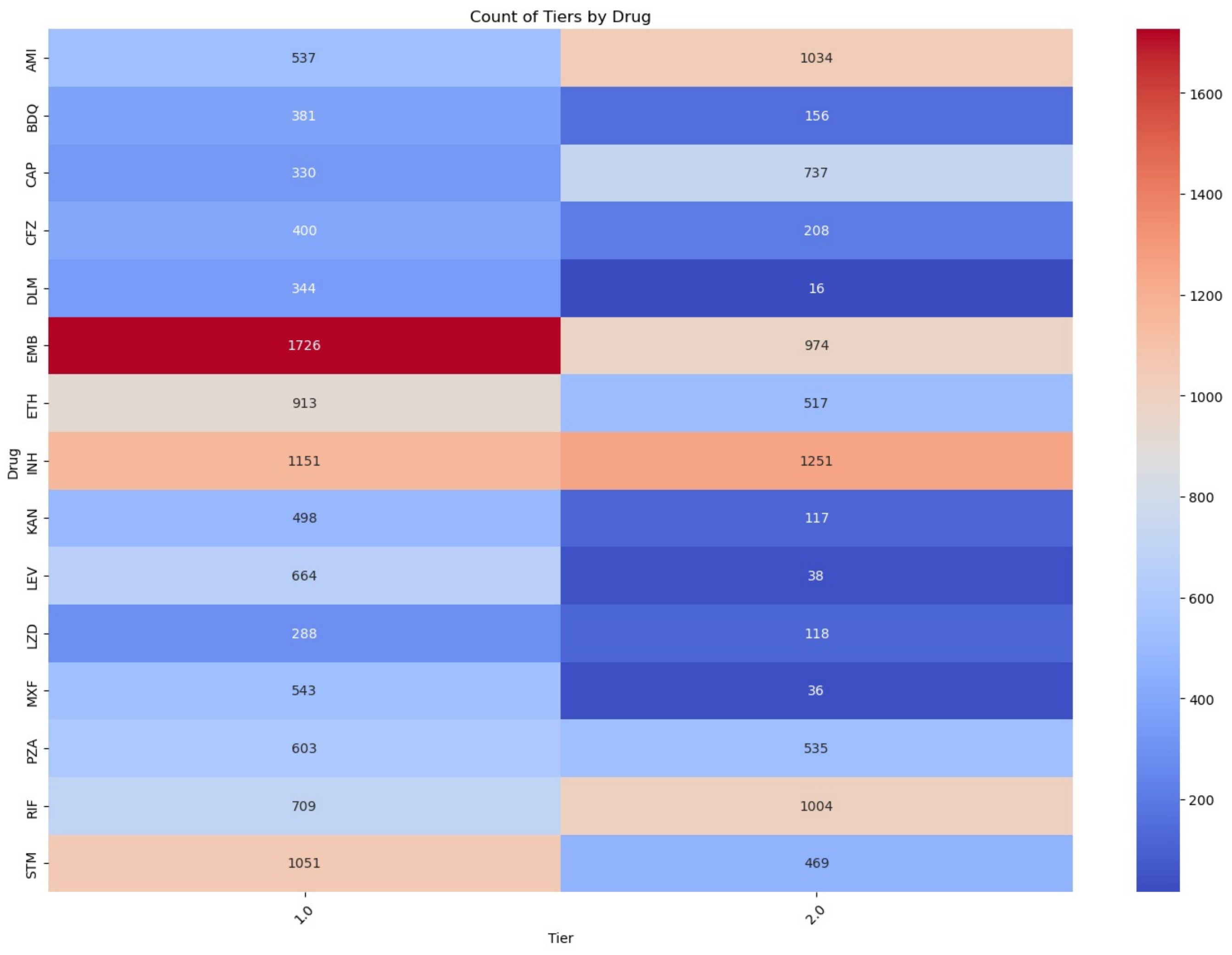


In [22]:
```
plt.figure(figsize=(10, 6))
sns.countplot(data=df, x='FINAL CONFIDENCE GRADING')
plt.xticks(rotation=45)
```

```python
plt.xlabel('FINAL CONFIDENCE GRADING')
plt.ylabel('COUNT')
plt.title('Count of Final Confidence Grading')
plt.show()
```

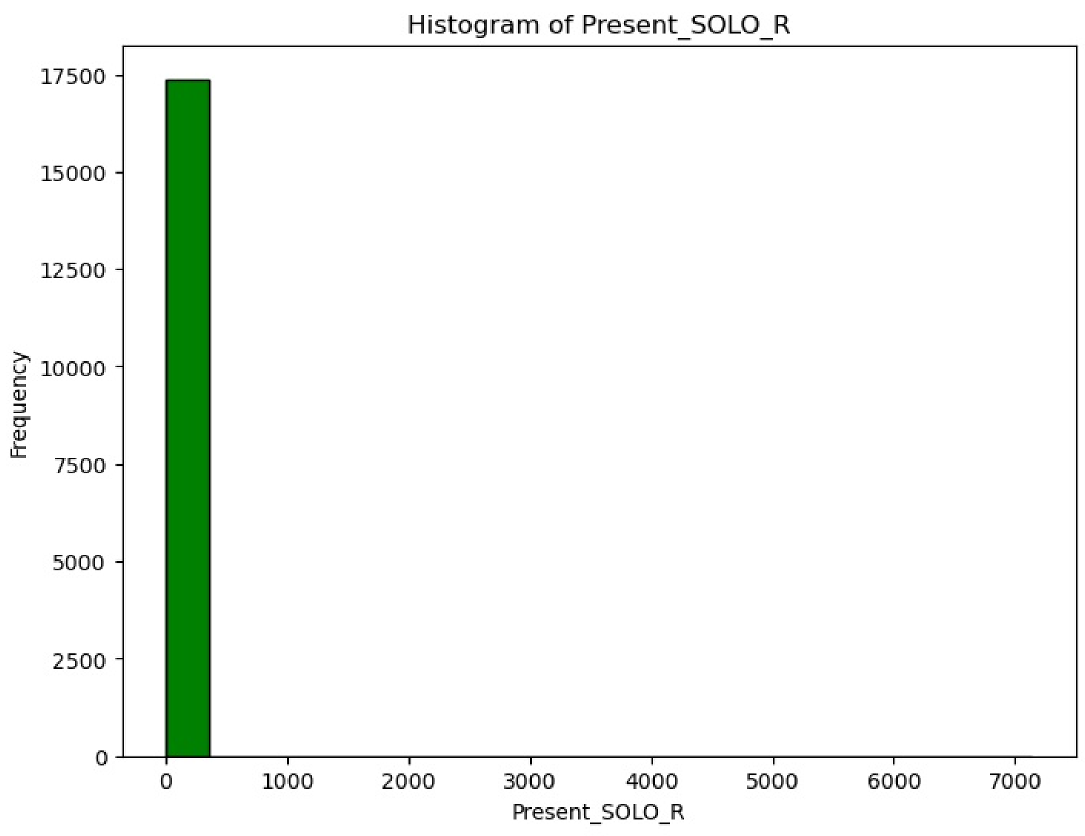


In [23]:
```python
pivot_table = df.pivot_table(index='Drug', columns='Tier', aggfunc='size', fill_value=0)

# Plot heatmap
plt.figure(figsize=(14, 10))
sns.heatmap(pivot_table, cmap='coolwarm', annot=True, fmt='d')
plt.title('Count of Tiers by Drug')
plt.xlabel('Tier')
plt.ylabel('Drug')
plt.xticks(rotation=45)
plt.tight_layout()
plt.show()
```

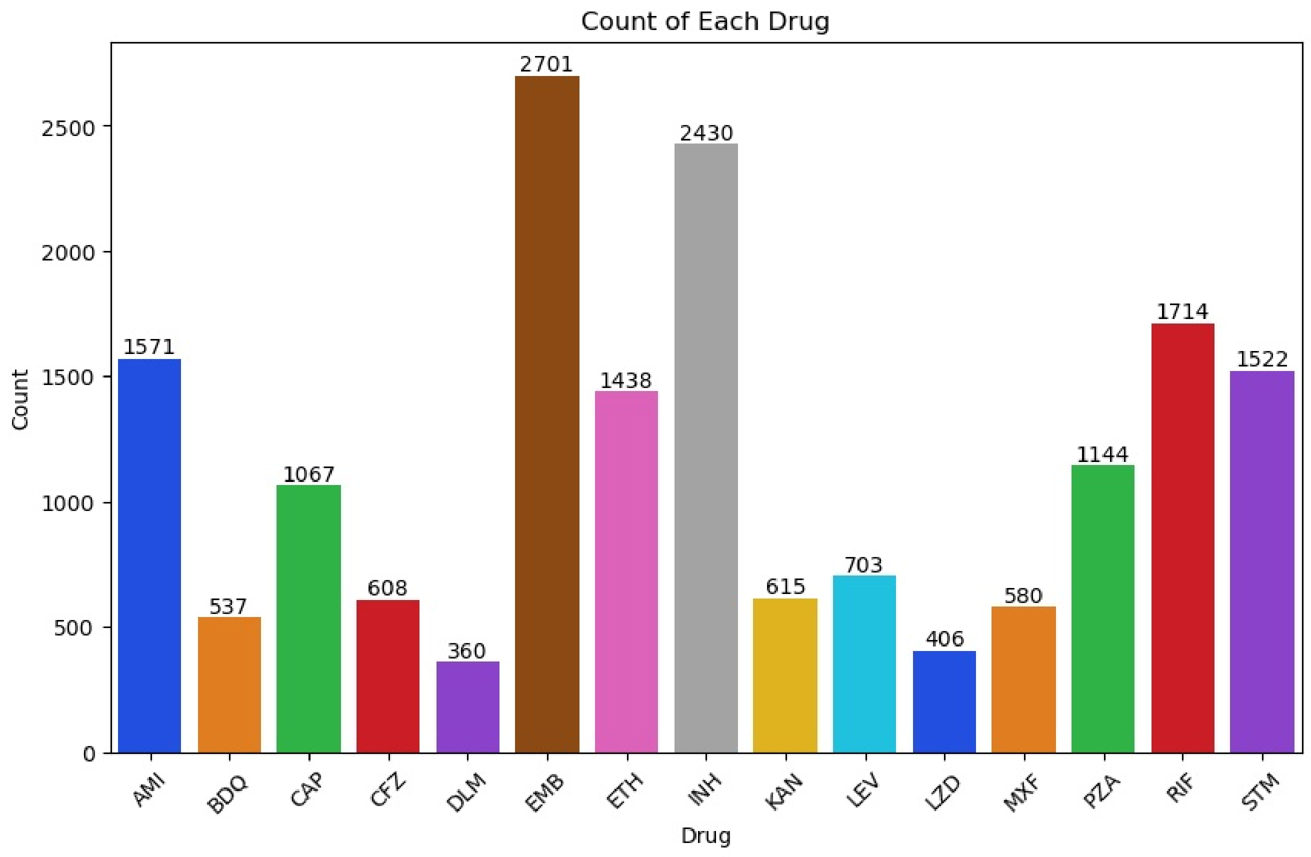


In [ ]:
```python
from sklearn.preprocessing import LabelEncoder
#categorical_cols = df.select_dtypes(include='object').columns
```

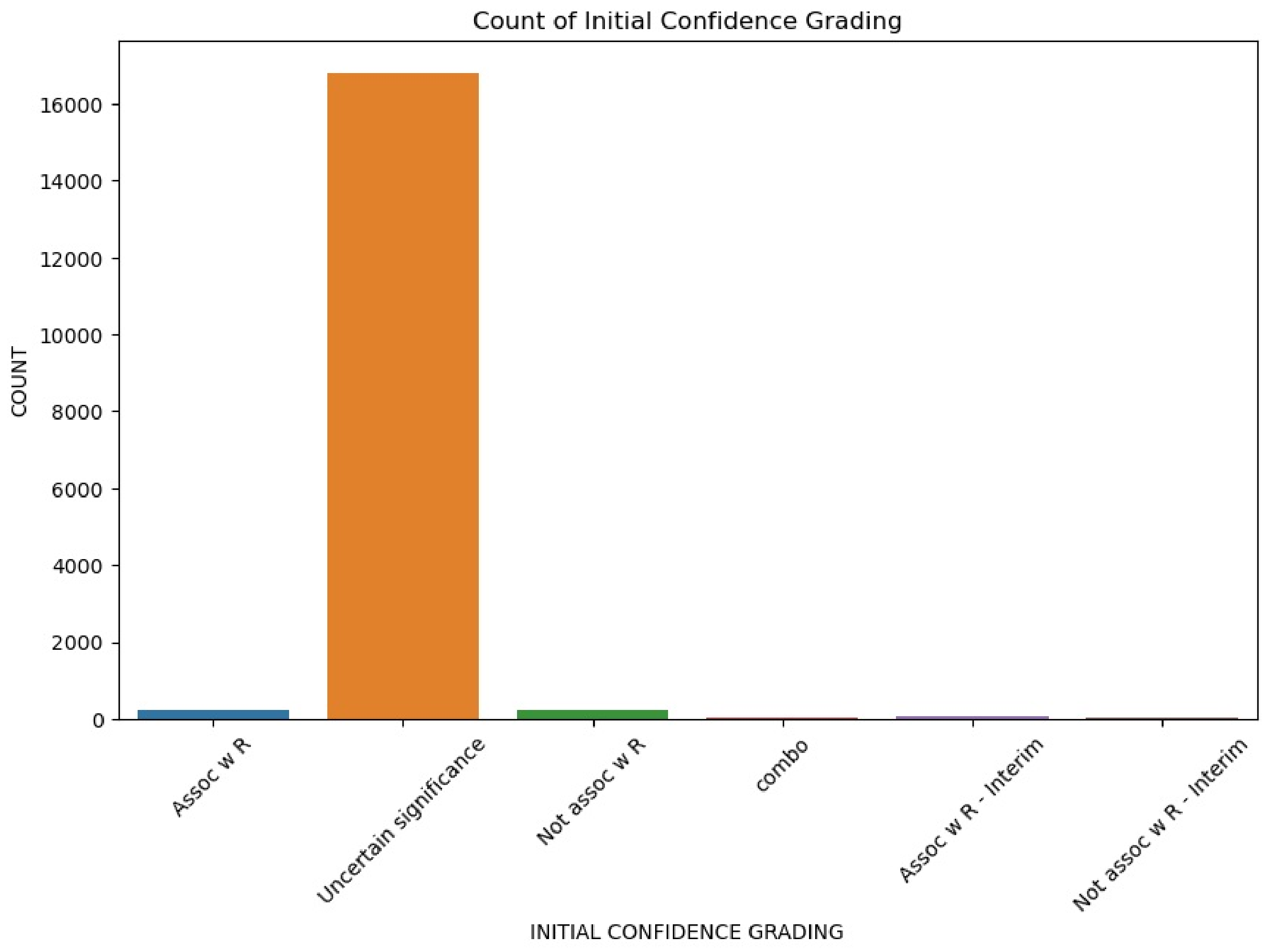
In [24]:
```python
plt.figure(figsize=(8, 6))
plt.hist(df['Present_SOLO_R'], bins=20, color='green', edgecolor='black')
plt.title('Histogram of Present_SOLO_R')
plt.xlabel('Present_SOLO_R')
plt.ylabel('Frequency')
plt.grid(False)
plt.show()
```



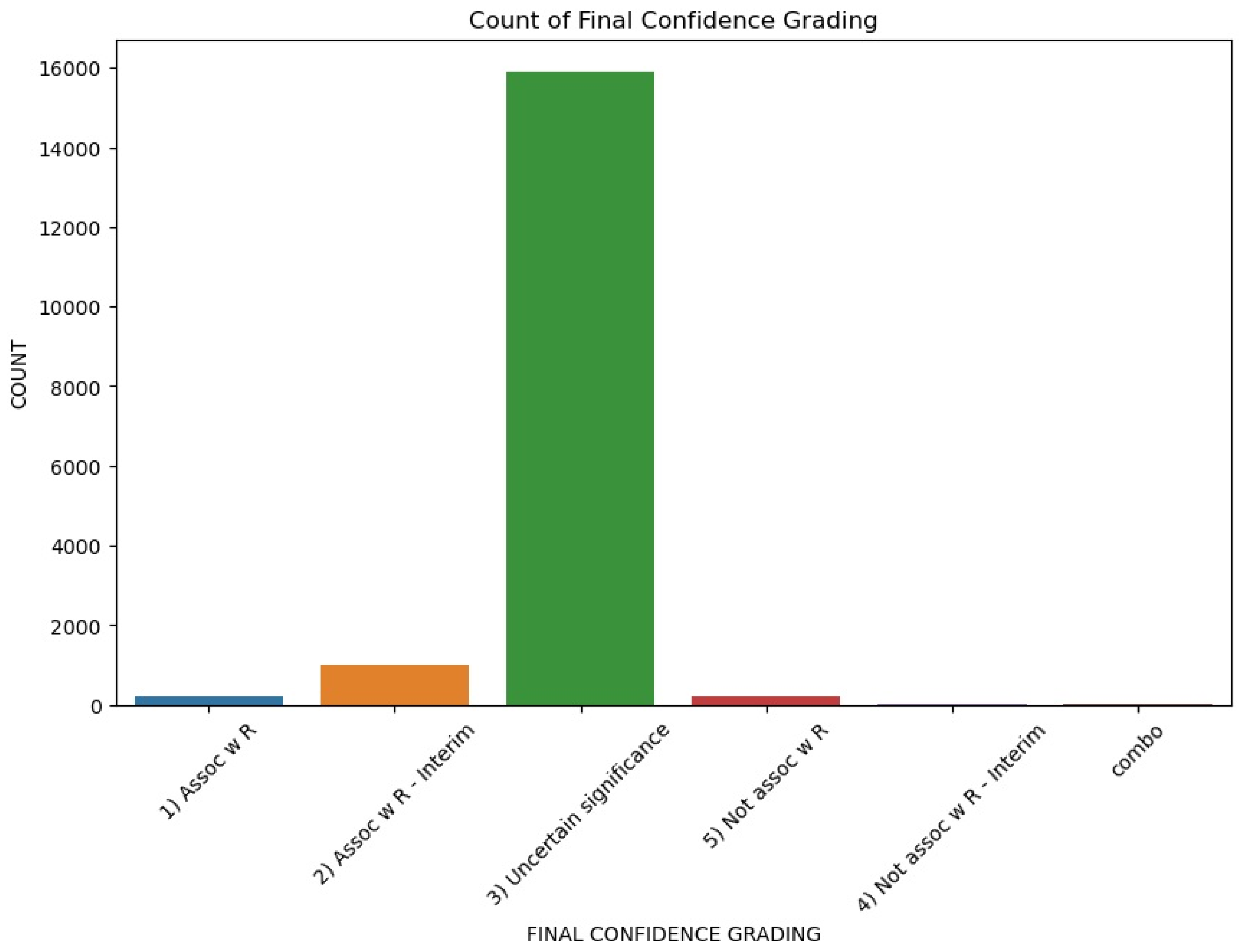
In [25]:
```
plt.figure(figsize=(10, 6))
ax = sns.countplot(data=df, x='Drug', palette='bright')

# Add text annotations to the bars
for p in ax.patches:
    ax.annotate(f'{p.get_height()}', (p.get_x() + p.get_width() / 2., p.get_height()),
                ha='center', va='center', fontsize=10, color='black', xytext=(0, 5),
                textcoords='offset points')

plt.xticks(rotation=45)
plt.xlabel('Drug')
plt.ylabel('Count')
plt.title('Count of Each Drug')
plt.show()
```



In [26]:
```
plt.figure(figsize=(10, 6))
sns.countplot(data=df, x='INITIAL CONFIDENCE GRADING')
plt.xticks(rotation=45)
plt.xlabel('INITIAL CONFIDENCE GRADING')
plt.ylabel('COUNT')
plt.title('Count of Initial Confidence Grading')
plt.show()
```

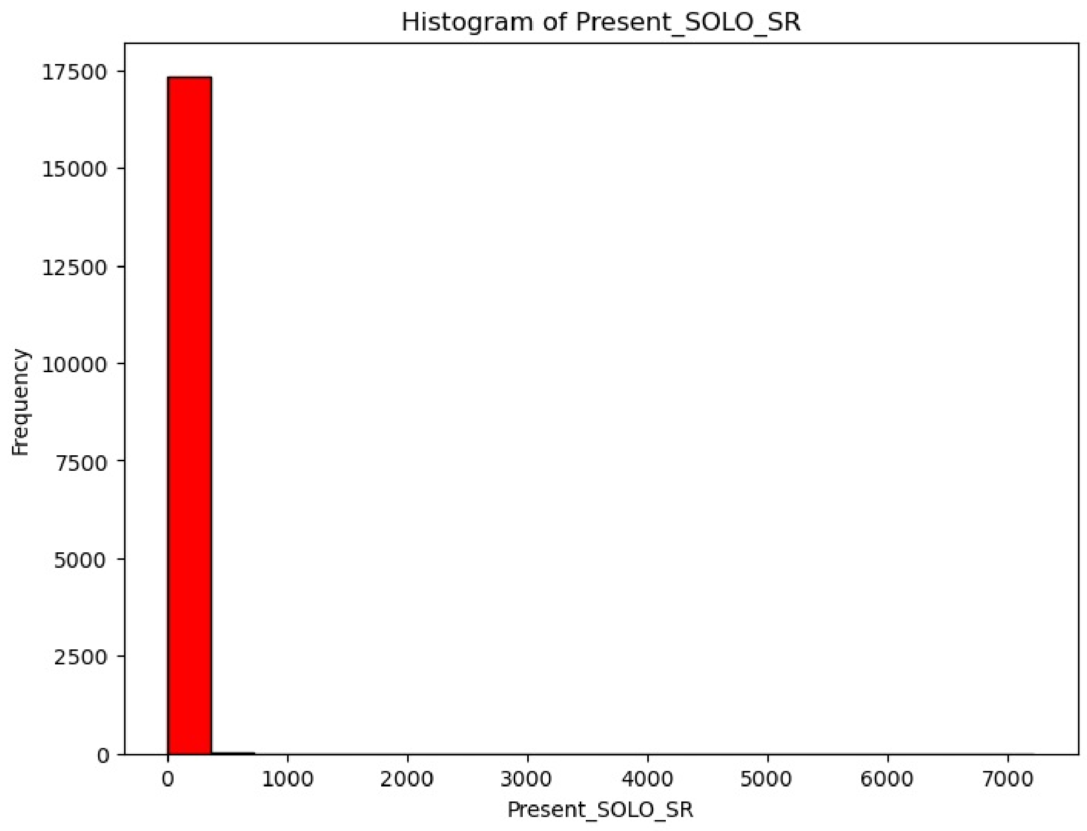


```
In [27]: plt.figure(figsize=(10, 6))
         sns.countplot(data=df, x='FINAL CONFIDENCE GRADING')
         plt.xticks(rotation=45)
         plt.xlabel('FINAL CONFIDENCE GRADING')
         plt.ylabel('COUNT')
         plt.title('Count of Final Confidence Grading')
         plt.show()
```

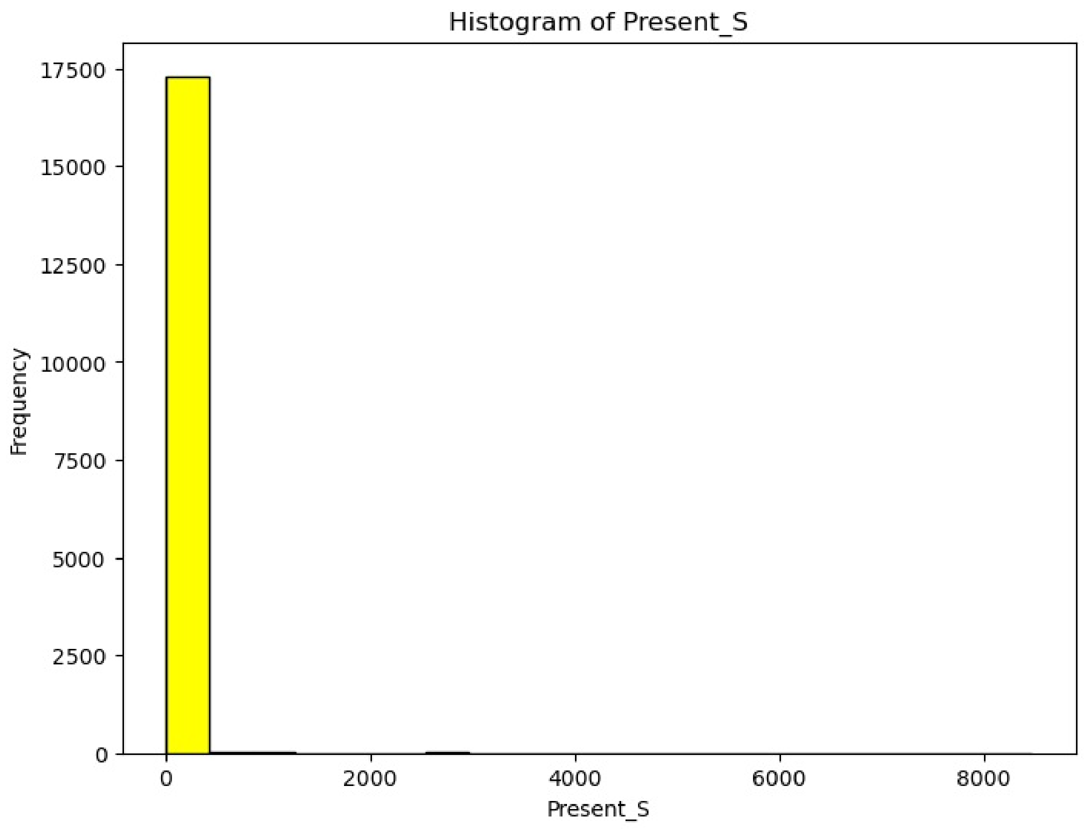


```
In [29]: from sklearn.preprocessing import LabelEncoder
         #categorical_cols = df.select_dtypes(include='object').columns
```

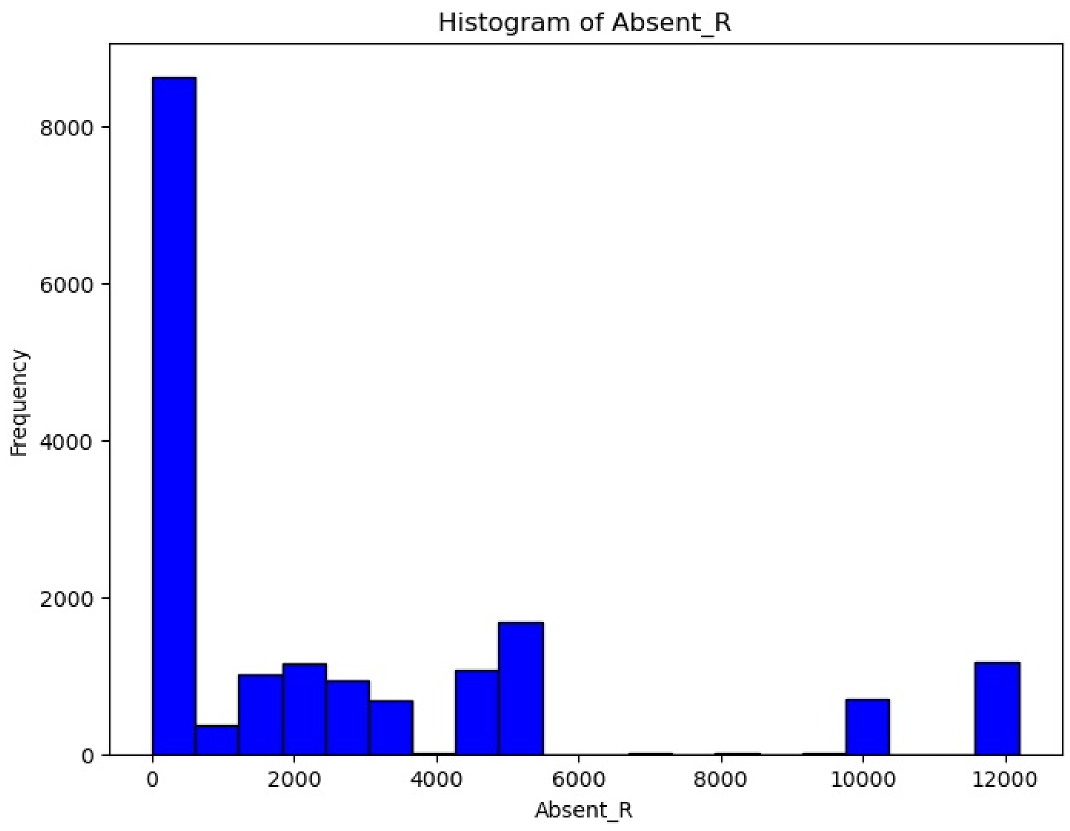
```
In [30]: plt.figure(figsize=(8, 6))
         plt.hist(df['Present_SOLO_SR'], bins=20, color='red', edgecolor='black')
         plt.title('Histogram of Present_SOLO_SR')
         plt.xlabel('Present_SOLO_SR')
         plt.ylabel('Frequency')
         plt.grid(False)
         plt.show()
```



In [31]:
```
plt.figure(figsize=(8, 6))
plt.hist(df['Present_S'], bins=20, color='yellow', edgecolor='black')
plt.title('Histogram of Present_S')
plt.xlabel('Present_S')
plt.ylabel('Frequency')
plt.grid(False)
plt.show()
```



In [32]:
```
plt.figure(figsize=(8, 6))
plt.hist(df['Absent_R'], bins=20, color='blue', edgecolor='black')
plt.title('Histogram of Absent_R')
plt.xlabel('Absent_R')
plt.ylabel('Frequency')
plt.grid(False)
plt.show()
```



In [33]:
```
#  unique values and their counts in the 'Absent_R' feature
unique_values_counts = df['Absent_R'].value_counts()
```

```
unique_values_counts
```

Out[33]:

```
4900.0      1405
480.0       1173
144.0        991
321.0        964
229.0        932
            ...
12147.0        1
12145.0        1
12142.0        1
12139.0        1
2543.0         1
Name: Absent_R, Length: 535, dtype: int64
```

In [35]:

```
import numpy as np

df.replace([np.inf, -np.inf], np.finfo(np.float64).max, inplace=True)
```

In [36]:

```
from sklearn.preprocessing import LabelEncoder

# LabelEncoder
encoder = LabelEncoder()

#Encode categorical columns
categorical_cols = ['Drug', 'Common Variant', 'INITIAL CONFIDENCE GRADING', 'FINAL CONFIDENCE GRADING']
df[categorical_cols] = df[categorical_cols].apply(encoder.fit_transform)
```

In [37]:

```
df.head()
```

Out[37]:

	Drug	Tier	Common Variant	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	Absent_R	Neutral masked	INITIAL CONFIDENCE GRADING	FI CONFIDE GRAD
0	0	1.0	11986	918.0	966.0	50.0	15640.0	939.0	349.0	0.0	0	
1	0	1.0	2333	28.0	77.0	51.0	7325.0	32.0	632.0	0.0	0	
2	0	1.0	12271	5.0	7.0	2.0	15688.0	6.0	1282.0	0.0	0	
3	0	1.0	12111	4.0	13.0	10.0	15680.0	5.0	1283.0	0.0	4	
4	0	2.0	12971	3.0	100.0	97.0	15593.0	3.0	141.0	0.0	4	

In [38]:

```
df.isnull().sum()
```

Out[38]:

```
Drug                           0
Tier                          48
Common Variant                 0
Present_SOLO_R                 8
Present_SOLO_SR                8
Present_S                      8
Absent_S                       8
Present_R                      8
Absent_R                       8
Neutral masked                 0
INITIAL CONFIDENCE GRADING     0
FINAL CONFIDENCE GRADING       0
dtype: int64
```

In [39]:

```
df.describe()
```

Out[39]:

	Drug	Tier	Common Variant	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	Absent_
count	17396.000000	17348.000000	17396.00000	17388.000000	17388.000000	17388.000000	17388.000000	17388.000000	17388.00000
mean	7.132847	1.415610	6947.03863	1.988498	6.891649	16.442202	16640.281228	4.511847	2617.12249
std	4.349835	0.492841	4133.50626	72.686258	121.648599	237.433986	6417.516064	108.337847	3464.28919
min	0.000000	1.000000	0.00000	0.000000	0.000000	0.000000	0.000000	0.000000	0.00000
25%	5.000000	1.000000	3183.75000	0.000000	0.000000	1.000000	10894.000000	0.000000	206.00000
50%	7.000000	1.000000	7145.00000	0.000000	0.000000	1.000000	15168.000000	0.000000	969.00000
75%	12.000000	2.000000	10673.25000	0.000000	1.000000	2.000000	22245.000000	0.000000	4634.00000
max	14.000000	2.000000	13448.00000	7140.000000	7221.000000	8477.000000	25808.000000	9483.000000	12195.00000

In [40]:

```
for feature in df.columns:
    median_value = df[feature].median()
    df[feature].fillna(median_value, inplace=True)
```

In [41]:

```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 17396 entries, 0 to 17395
Data columns (total 12 columns):
 #   Column                    Non-Null Count  Dtype  
---  ------                    --------------  -----  
 0   Drug                      17396 non-null  int32  
 1   Tier                      17396 non-null  float64
 2   Common Variant            17396 non-null  int32  
 3   Present_SOLO_R            17396 non-null  float64
 4   Present_SOLO_SR           17396 non-null  float64
 5   Present_S                 17396 non-null  float64
 6   Absent_S                  17396 non-null  float64
 7   Present_R                 17396 non-null  float64
 8   Absent_R                  17396 non-null  float64
 9   Neutral masked            17396 non-null  float64
 10  INITIAL CONFIDENCE GRADING  17396 non-null  int32  
 11  FINAL CONFIDENCE GRADING    17396 non-null  int32  
dtypes: float64(8), int32(4)
memory usage: 1.3 MB
```

In [42]:
```python
df.corr()
```

Out[42]:

	Drug	Tier	Common Variant	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	Absent_R	Neutr mask
Drug	1.000000	-0.093594	0.107236	0.012414	0.012896	-0.000168	0.036932	0.017281	0.231247	0.0000
Tier	-0.093594	1.000000	-0.076048	-0.021700	-0.007533	0.018833	0.100121	-0.031870	-0.569943	0.0280
Common Variant	0.107236	-0.076048	1.000000	0.010508	0.007713	0.007509	-0.179507	0.007627	0.030117	0.0074
Present_SOLO_R	0.012414	-0.021700	0.010508	1.000000	0.631376	0.020307	0.008458	0.871117	0.006031	0.0017
Present_SOLO_SR	0.012896	-0.007533	0.007713	0.631376	1.000000	0.413592	-0.022704	0.668213	-0.006268	0.2072
Present_S	-0.000168	0.018833	0.007509	0.020307	0.413592	1.000000	-0.085283	0.299541	-0.031625	0.4806
Absent_S	0.036932	0.100121	-0.179507	0.008458	-0.022704	-0.085283	1.000000	-0.008724	0.373310	-0.0847
Present_R	0.017281	-0.031870	0.007627	0.871117	0.668213	0.299541	-0.008724	1.000000	0.013122	0.1075
Absent_R	0.231247	-0.569943	0.030117	0.006031	-0.006268	-0.031625	0.373310	0.013122	1.000000	-0.0436
Neutral masked	0.000060	0.028058	0.007443	0.001739	0.207243	0.480660	-0.084763	0.107510	-0.043654	1.0000
INITIAL CONFIDENCE GRADING	-0.100572	0.089321	-0.064167	-0.175689	-0.200729	-0.197813	0.075625	-0.191941	0.005752	-0.3966
FINAL CONFIDENCE GRADING	-0.117773	0.162170	-0.048383	-0.112212	0.040371	0.265929	0.023106	-0.030491	-0.096255	0.5498

In [44]:
```python
from sklearn.preprocessing import MinMaxScaler

# numerical columns for  normalizing
numerical_columns = df.select_dtypes(include=['float64', 'int64']).columns

# Min-Max scaling (scaling features between 0 and 1)
min_max_scaler = MinMaxScaler()
df[numerical_columns] = min_max_scaler.fit_transform(df[numerical_columns])
```

In [45]:
```python
df[numerical_columns]
```

Out[45]:

	Tier	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	Absent_R	Neutral masked
0	0.0	0.128571	0.133776	0.005898	0.606014	0.099019	0.028618	0.0
1	0.0	0.003922	0.010663	0.006016	0.283827	0.003374	0.051825	0.0
2	0.0	0.000700	0.000969	0.000236	0.607874	0.000633	0.105125	0.0
3	0.0	0.000560	0.001800	0.001180	0.607564	0.000527	0.105207	0.0
4	1.0	0.000420	0.013848	0.011443	0.604192	0.000316	0.011562	0.0
...	...	...	...	...	...	...	...	...
17391	0.0	0.000280	0.036837	0.033620	0.240081	0.002109	0.208446	1.0
17392	0.0	0.000000	0.000000	0.042350	0.237213	0.002004	0.208528	1.0
17393	1.0	0.000000	0.000000	0.005898	0.249186	0.000000	0.006970	1.0
17394	1.0	0.000000	0.000000	0.007432	0.248683	0.000000	0.006970	1.0
17395	0.0	0.000000	0.000000	0.000000	0.362252	0.000844	0.379418	0.0

17396 rows × 8 columns

In [46]:
```python
# Selecting categorical columns
categorical_cols = df[['Drug', 'Common Variant', 'INITIAL CONFIDENCE GRADING', 'FINAL CONFIDENCE GRADING']]
```

```
# Selecting numerical columns
numerical_columns = df[['Tier', 'Present_SOLO_R', 'Present_SOLO_SR',
       'Present_S', 'Absent_S', 'Present_R', 'Absent_R', 'Neutral masked']]

# Concatenate along columns(axis=1) to merge them
df_merged = pd.concat([categorical_cols, numerical_columns], axis=1)

# Print the merged DataFrame
df_merged
```

Out[46]:

	Drug	Common Variant	INITIAL CONFIDENCE GRADING	FINAL CONFIDENCE GRADING	Tier	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	Absent_R
0	0	11986	0	0	0.0	0.128571	0.133776	0.005898	0.606014	0.099019	0.028618
1	0	2333	0	0	0.0	0.003922	0.010663	0.006016	0.283827	0.003374	0.051825
2	0	12271	0	1	0.0	0.000700	0.000969	0.000236	0.607874	0.000633	0.105125
3	0	12111	4	1	0.0	0.000560	0.001800	0.001180	0.607564	0.000527	0.105207
4	0	12971	4	2	1.0	0.000420	0.013848	0.011443	0.604192	0.000316	0.011562
...	...	...	...	...	...	...	...	...	...	...	...
17391	14	13290	2	4	0.0	0.000280	0.036837	0.033620	0.240081	0.002109	0.208446
17392	14	12149	2	4	0.0	0.000000	0.000000	0.042350	0.237213	0.002004	0.208528
17393	14	11603	2	4	1.0	0.000000	0.000000	0.005898	0.249186	0.000000	0.006970
17394	14	12784	2	4	1.0	0.000000	0.000000	0.007432	0.248683	0.000000	0.006970
17395	14	11566	5	5	0.0	0.000000	0.000000	0.000000	0.362252	0.000844	0.379418

17396 rows × 12 columns

In [47]:

```
# Swap the values of "final confidence" and "initial confidence" in the last row
last_index = df.index[-1]  # Get the index of the last row
final_confidence = df.at[last_index, 'FINAL CONFIDENCE GRADING']
initial_confidence = df.at[last_index, 'INITIAL CONFIDENCE GRADING']

# Swap the values
df.at[last_index, 'INITIAL CONFIDENCE GRADING'] = final_confidence
df.at[last_index, 'FINAL CONFIDENCE GRADING'] = initial_confidence

# Print the DataFrame to verify the changes
print(df)
```

```
       Drug  Tier  Common Variant  Present_SOLO_R  Present_SOLO_SR  Present_S  \
0         0   0.0           11986        0.128571         0.133776   0.005898
1         0   0.0            2333        0.003922         0.010663   0.006016
2         0   0.0           12271        0.000700         0.000969   0.000236
3         0   0.0           12111        0.000560         0.001800   0.001180
4         0   1.0           12971        0.000420         0.013848   0.011443
...     ...   ...             ...             ...              ...        ...
17391    14   0.0           13290        0.000280         0.036837   0.033620
17392    14   0.0           12149        0.000000         0.000000   0.042350
17393    14   1.0           11603        0.000000         0.000000   0.005898
17394    14   1.0           12784        0.000000         0.000000   0.007432
17395    14   0.0           11566        0.000000         0.000000   0.000000

       Absent_S  Present_R  Absent_R  Neutral masked  \
0      0.606014   0.099019  0.028618             0.0
1      0.283827   0.003374  0.051825             0.0
2      0.607874   0.000633  0.105125             0.0
3      0.607564   0.000527  0.105207             0.0
4      0.604192   0.000316  0.011562             0.0
...         ...        ...       ...             ...
17391  0.240081   0.002109  0.208446             1.0
17392  0.237213   0.002004  0.208528             1.0
17393  0.249186   0.000000  0.006970             1.0
17394  0.248683   0.000000  0.006970             1.0
17395  0.362252   0.000844  0.379418             0.0

       INITIAL CONFIDENCE GRADING  FINAL CONFIDENCE GRADING
0                               0                         0
1                               0                         0
2                               0                         1
3                               4                         1
4                               4                         2
...                           ...                       ...
17391                           2                         4
17392                           2                         4
17393                           2                         4
17394                           2                         4
17395                           5                         5

[17396 rows x 12 columns]
```

In [48]:

```
df.head()
```

In [48]:
```
df.head()
```

Out[48]:

	Drug	Tier	Common Variant	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	Absent_R	Neutral masked	INITIAL CONFIDENCE GRADING	FI CONFIDE GRAD
0	0	0.0	11986	0.128571	0.133776	0.005898	0.606014	0.099019	0.028618	0.0	0	
1	0	0.0	2333	0.003922	0.010663	0.006016	0.283827	0.003374	0.051825	0.0	0	
2	0	0.0	12271	0.000700	0.000969	0.000236	0.607874	0.000633	0.105125	0.0	0	
3	0	0.0	12111	0.000560	0.001800	0.001180	0.607564	0.000527	0.105207	0.0	4	
4	0	1.0	12971	0.000420	0.013848	0.011443	0.604192	0.000316	0.011562	0.0	4	

In [49]:
```
df.head()
```

Out[49]:

	Drug	Tier	Common Variant	Present_SOLO_R	Present_SOLO_SR	Present_S	Absent_S	Present_R	Absent_R	Neutral masked	INITIAL CONFIDENCE GRADING	FI CONFIDE GRAD
0	0	0.0	11986	0.128571	0.133776	0.005898	0.606014	0.099019	0.028618	0.0	0	
1	0	0.0	2333	0.003922	0.010663	0.006016	0.283827	0.003374	0.051825	0.0	0	
2	0	0.0	12271	0.000700	0.000969	0.000236	0.607874	0.000633	0.105125	0.0	0	
3	0	0.0	12111	0.000560	0.001800	0.001180	0.607564	0.000527	0.105207	0.0	4	
4	0	1.0	12971	0.000420	0.013848	0.011443	0.604192	0.000316	0.011562	0.0	4	

In [50]:
```
# Check for specific values in the 'Drug' column
drug_counts = df['Drug'].value_counts()
print("Counts for each drug:")
print(drug_counts)
```

```
Counts for each drug:
5      2701
7      2430
13     1714
0      1571
14     1522
6      1438
12     1144
2      1067
9       703
8       615
3       608
11      580
1       537
10      406
4       360
Name: Drug, dtype: int64
```

In [52]:
```
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score

#  Data Preprocessing
X = df.drop(columns=['FINAL CONFIDENCE GRADING'])
y = df['FINAL CONFIDENCE GRADING']
```

In [53]:
```
# Splitting the dataset into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

# Model Selection and Training
model = RandomForestClassifier()  # You can use any other classifier here
model.fit(X_train, y_train)
```

Out[53]:
```
RandomForestClassifier()
```

In [55]:
```
 #Model Evaluation
y_pred = model.predict(X_test)
accuracy = accuracy_score(y_test, y_pred)
print("Accuracy:", accuracy)
```

```
Accuracy: 0.9798850574712644
```

In [57]:
```
from sklearn.metrics import classification_report

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

```
              precision    recall  f1-score   support

           0       0.98      0.96      0.97        46
           1       0.83      0.83      0.83       203
           2       0.99      0.99      0.99      3180
           3       1.00      0.75      0.86         4
           4       1.00      1.00      1.00        40
           5       1.00      0.86      0.92         7

    accuracy                           0.98      3480
   macro avg       0.97      0.90      0.93      3480
weighted avg       0.98      0.98      0.98      3480
```

In [62]:
```python
#Prediction


# Define the new data point(s)
X_new = np.array([[6, 7, 1, 4, 8, 9, 5, 10, 12, 13, 14]])

# Use the trained model to make predictions
predictions = model.predict(X_new)

# Print the predicted values
print("Predictions:", predictions)
```

```
Predictions: [2]
```

```
C:\Users\hp\anaconda3\lib\site-packages\sklearn\base.py:450: UserWarning: X does not have valid feature names,
but RandomForestClassifier was fitted with feature names
  warnings.warn(
```

In [71]:
```python
from scipy.stats import f_oneway

# Extract numerical columns for ANOVA
numerical_columns = [col for col in df_encoded.columns if col != 'FINAL CONFIDENCE GRADING']

# Perform ANOVA
f_statistic, p_value = f_oneway(*[df_encoded[col] for col in numerical_columns])

# Print results
print("F-statistic:", f_statistic)
print("p-value:", p_value)
```

```
F-statistic: 49133.69514812919
p-value: 0.0
```

In [72]:
```python
# X_train and y_train are the training features and labels

rf_classifier = RandomForestClassifier()

# Fit the model
rf_classifier.fit(X_train, y_train)

# Get feature importances
feature_importances = rf_classifier.feature_importances_
# Match feature importances with feature names
feature_importance_dict = dict(zip(X_train.columns, feature_importances))

# Sort feature importances in descending order
sorted_feature_importances = sorted(feature_importance_dict.items(), key=lambda x: x[1], reverse=True)

# Print feature importances
for feature, importance in sorted_feature_importances:
    print(f"Feature: {feature}, Importance: {importance}")
```

```
Feature: Common Variant, Importance: 0.36323364207801706
Feature: INITIAL CONFIDENCE GRADING, Importance: 0.17870863727112804
Feature: Present_SOLO_R, Importance: 0.09191742985098356
Feature: Absent_R, Importance: 0.07381915699622639
Feature: Present_R, Importance: 0.06231854517623517
Feature: Neutral masked, Importance: 0.05717055264156813
Feature: Absent_S, Importance: 0.05480089523557505
Feature: Present_S, Importance: 0.050262684366217586
Feature: Present_SOLO_SR, Importance: 0.030618701624751925
Feature: Drug, Importance: 0.028608211386026847
Feature: Tier, Importance: 0.008541543373270323
```

In [76]:
```python
# Select the most important features identified
important_features = ['Common Variant', 'INITIAL CONFIDENCE GRADING' ,
                      'Present_SOLO_R', 'Neutral masked','Present_R','Present_S', 'Absent_R', 'Absent_S']

# Analyze the relationship between each important feature and final confidence gradings
for feature in important_features:
    # Group the data by the feature and calculate the mean final confidence grading for each group
    feature_confidence_mean = df.groupby(feature)['FINAL CONFIDENCE GRADING'].mean()

    # Print the relationship between the feature and final confidence gradings
    print(f"\nRelationship between '{feature}' and Final Confidence Gradings:\n")
    print(feature_confidence_mean)
```

```
Relationship between 'Common Variant' and Final Confidence Gradings:

Common Variant
0        2.0
1        2.0
2        2.0
3        2.0
4        2.0
        ...
13444    2.0
13445    2.0
13446    2.0
13447    2.0
13448    2.0
Name: FINAL CONFIDENCE GRADING, Length: 13449, dtype: float64

Relationship between 'INITIAL CONFIDENCE GRADING' and Final Confidence Gradings:

INITIAL CONFIDENCE GRADING
0    0.141593
1    1.000000
2    3.959459
3    3.000000
4    1.947694
5    5.000000
Name: FINAL CONFIDENCE GRADING, dtype: float64

Relationship between 'Present_SOLO_R' and Final Confidence Gradings:

Present_SOLO_R
0.000000    2.003617
0.000140    1.714411
0.000280    1.629771
0.000420    1.657895
0.000560    1.633803
              ...
0.158683    0.000000
0.216246    0.000000
0.243417    0.000000
0.746779    0.000000
1.000000    0.000000
Name: FINAL CONFIDENCE GRADING, Length: 92, dtype: float64

Relationship between 'Neutral masked' and Final Confidence Gradings:

Neutral masked
0.0    1.927099
1.0    3.959459
Name: FINAL CONFIDENCE GRADING, dtype: float64

Relationship between 'Present_R' and Final Confidence Gradings:

Present_R
0.000000    1.995467
0.000105    1.805730
0.000211    1.788214
0.000316    1.864035
0.000422    1.803922
              ...
0.236739    0.000000
0.241485    0.000000
0.540124    4.000000
0.689233    0.000000
1.000000    0.000000
Name: FINAL CONFIDENCE GRADING, Length: 152, dtype: float64

Relationship between 'Present_S' and Final Confidence Gradings:

Present_S
0.000000    1.712017
0.000118    1.967196
0.000236    1.970423
0.000354    1.954918
0.000472    1.952278
              ...
0.908104    4.000000
0.908458    4.000000
0.976997    4.000000
0.984664    4.000000
1.000000    4.000000
Name: FINAL CONFIDENCE GRADING, Length: 253, dtype: float64

Relationship between 'Absent_R' and Final Confidence Gradings:

Absent_R
0.000000    4.0
0.000082    4.0
0.000246    4.0
0.000574    4.0
```

```
0.000738    4.0
           ...
0.999508    5.0
0.999672    5.0
0.999754    5.0
0.999918    5.0
1.000000    5.0
Name: FINAL CONFIDENCE GRADING, Length: 535, dtype: float64

Relationship between 'Absent_S' and Final Confidence Gradings:

Absent_S
0.000000    4.000000
0.000116    4.000000
0.000155    4.000000
0.000271    4.000000
0.000426    4.000000
              ...
0.999845    2.000000
0.999884    1.987421
0.999923    2.000000
0.999961    2.000000
1.000000    2.021898
Name: FINAL CONFIDENCE GRADING, Length: 748, dtype: float64
```

In [63]:
```python
from sklearn.metrics import accuracy_score


# Make predictions on the testing set
y_pred = model.predict(X_test)

# Calculate accuracy on the testing set
accuracy = accuracy_score(y_test, y_pred)
print("Accuracy on testing set:", accuracy)
```

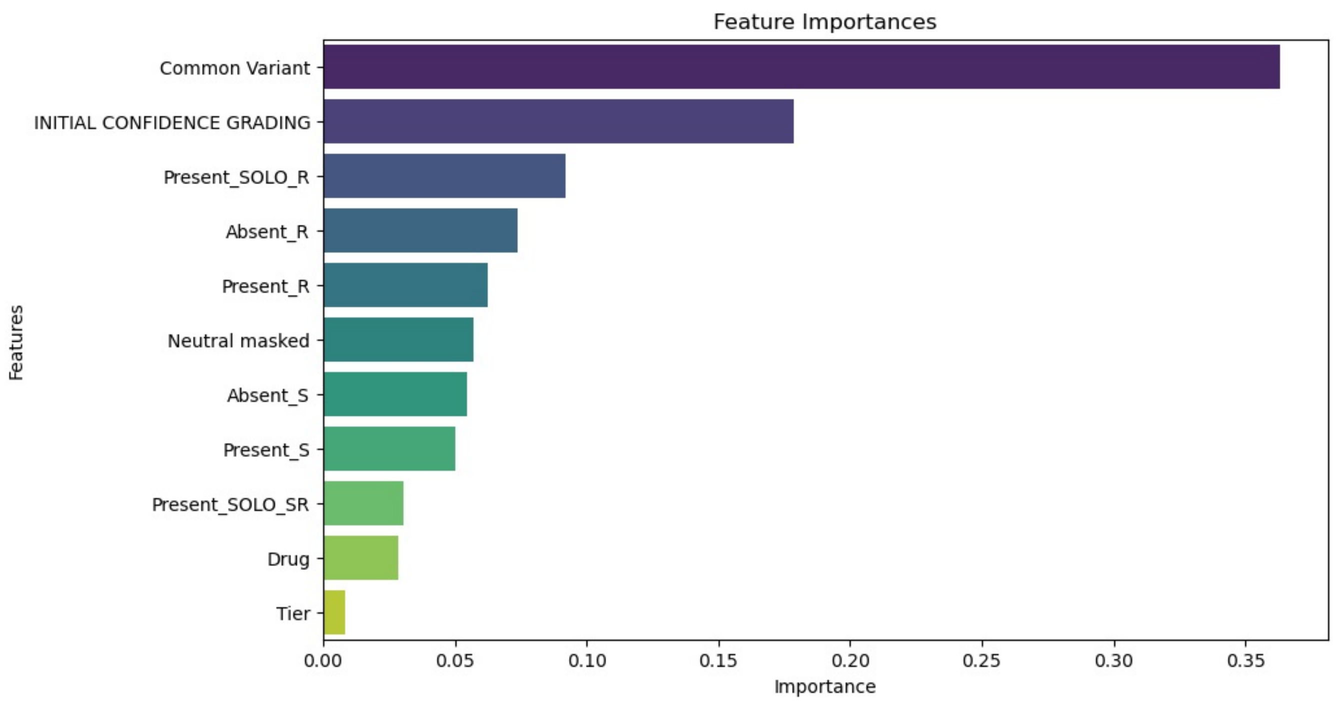
```
Accuracy on testing set: 0.9798850574712644
```

In [77]:
```python
from scipy import stats

# Select the most important features identified
important_features = ['Common Variant', 'INITIAL CONFIDENCE GRADING' ,
                      'Present_SOLO_R', 'Neutral masked','Present_R','Present_S', 'Absent_R', 'Absent_S']

# Analyze the relationship between each important feature and final confidence gradings
for feature in important_features:
    # Find pointbserialr correlation coefficient
    correlation_coefficient, p_value = stats.pointbiserialr(df[feature], df['FINAL CONFIDENCE GRADING'])

    # Print the results
    print(f"\nPoint-biserial correlation coefficient between '{feature}' and 'FINAL CONFIDENCE GRADING': {corre
    print(f"P-value: {p_value}")
```

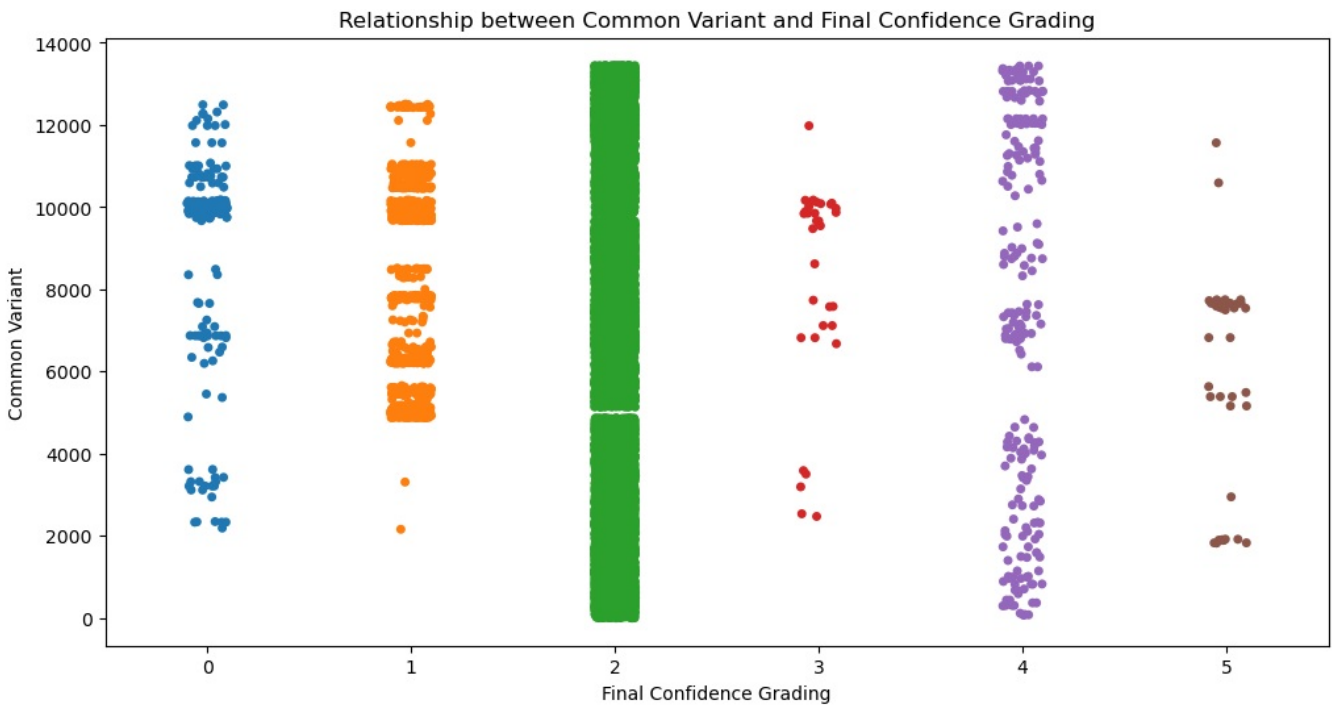
```
Point-biserial correlation coefficient between 'Common Variant' and 'FINAL CONFIDENCE GRADING': -0.048382506278
49848
P-value: 1.7180372270874056e-10

Point-biserial correlation coefficient between 'INITIAL CONFIDENCE GRADING' and 'FINAL CONFIDENCE GRADING': 0.2
797176016094426
P-value: 4.0578401675859e-310

Point-biserial correlation coefficient between 'Present_SOLO_R' and 'FINAL CONFIDENCE GRADING': -0.112212379221
96936
P-value: 7.387710645132828e-50

Point-biserial correlation coefficient between 'Neutral masked' and 'FINAL CONFIDENCE GRADING': 0.5498151025126
343
P-value: 0.0

Point-biserial correlation coefficient between 'Present_R' and 'FINAL CONFIDENCE GRADING': -0.03049148049458477
P-value: 5.763592431595842e-05

Point-biserial correlation coefficient between 'Present_S' and 'FINAL CONFIDENCE GRADING': 0.26592890781587236
P-value: 2.162312346552411e-279

Point-biserial correlation coefficient between 'Absent_R' and 'FINAL CONFIDENCE GRADING': -0.0962551796587794
P-value: 4.343903697446709e-37

Point-biserial correlation coefficient between 'Absent_S' and 'FINAL CONFIDENCE GRADING': 0.02310558389647338
P-value: 0.0023062047405744313
```

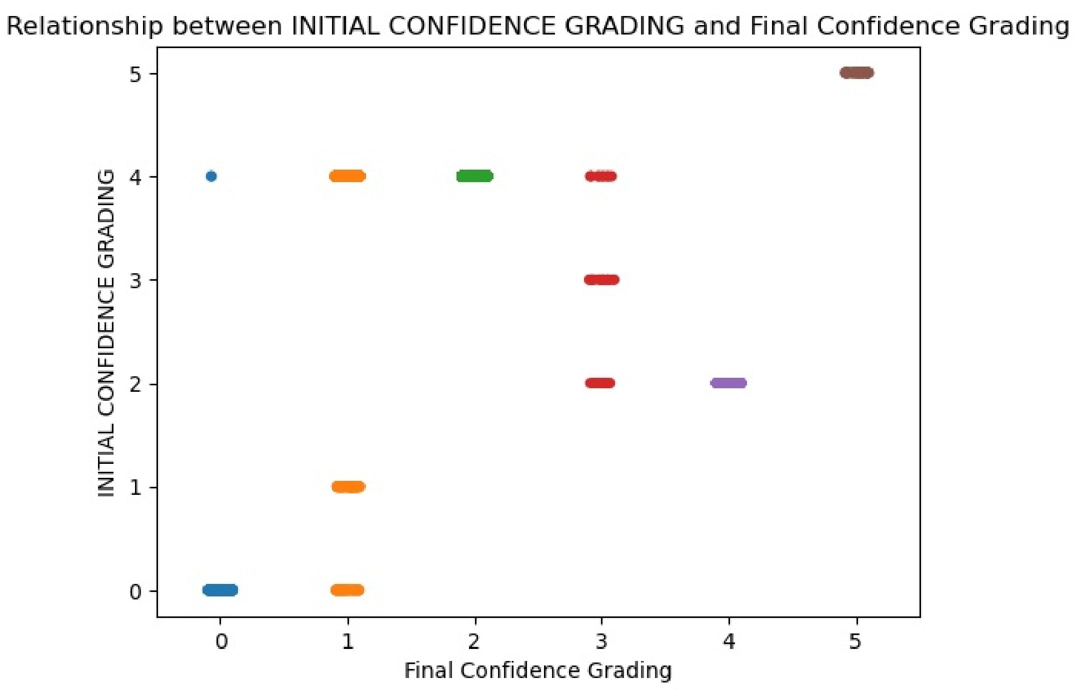
In [78]:
```python
import seaborn as sns
import matplotlib.pyplot as plt

# Convert feature importances to a DataFrame
importance_df = pd.DataFrame(sorted_feature_importances, columns=['Feature', 'Importance'])

# Plot
plt.figure(figsize=(10, 6))
sns.barplot(data=importance_df, x='Importance', y='Feature', palette='viridis')
```

```
plt.xlabel('Importance')
plt.ylabel('Features')
plt.title('Feature Importances')
plt.show()
```



In [79]:
```
# Define the features of interest
features_of_interest = ['Common Variant', 'INITIAL CONFIDENCE GRADING']

# Plot scatter plots with jittering for each feature
plt.figure(figsize=(12, 6))
for feature in features_of_interest:
    sns.stripplot(x='FINAL CONFIDENCE GRADING', y=feature, data=df, jitter=True)
    plt.title(f"Relationship between {feature} and Final Confidence Grading")
    plt.xlabel("Final Confidence Grading")
    plt.ylabel(feature)
    plt.show()
```





In [80]:
```
# Select the most important features identified
important_features = ['Common Variant', 'INITIAL CONFIDENCE GRADING' ,
                      'Present_SOLO_R', 'Neutral masked','Present_R','Present_S', 'Absent_R', 'Absent_S']

# Analyze the relationship between each important feature and final confidence gradings
for feature in important_features:
    # Group the data by the feature and calculate the mean final confidence grading for each group
    feature_confidence_mean = df.groupby(feature)['FINAL CONFIDENCE GRADING'].mean()

    # Print the relationship between the feature and final confidence gradings
    print(f"\nRelationship between '{feature}' and Final Confidence Gradings:\n")
    print(feature_confidence_mean)
```

```
Relationship between 'Common Variant' and Final Confidence Gradings:

Common Variant
0        2.0
1        2.0
2        2.0
3        2.0
4        2.0
        ...
13444    2.0
13445    2.0
13446    2.0
13447    2.0
13448    2.0
Name: FINAL CONFIDENCE GRADING, Length: 13449, dtype: float64

Relationship between 'INITIAL CONFIDENCE GRADING' and Final Confidence Gradings:

INITIAL CONFIDENCE GRADING
0    0.141593
1    1.000000
2    3.959459
3    3.000000
4    1.947694
5    5.000000
Name: FINAL CONFIDENCE GRADING, dtype: float64

Relationship between 'Present_SOLO_R' and Final Confidence Gradings:

Present_SOLO_R
0.000000    2.003617
0.000140    1.714411
0.000280    1.629771
```

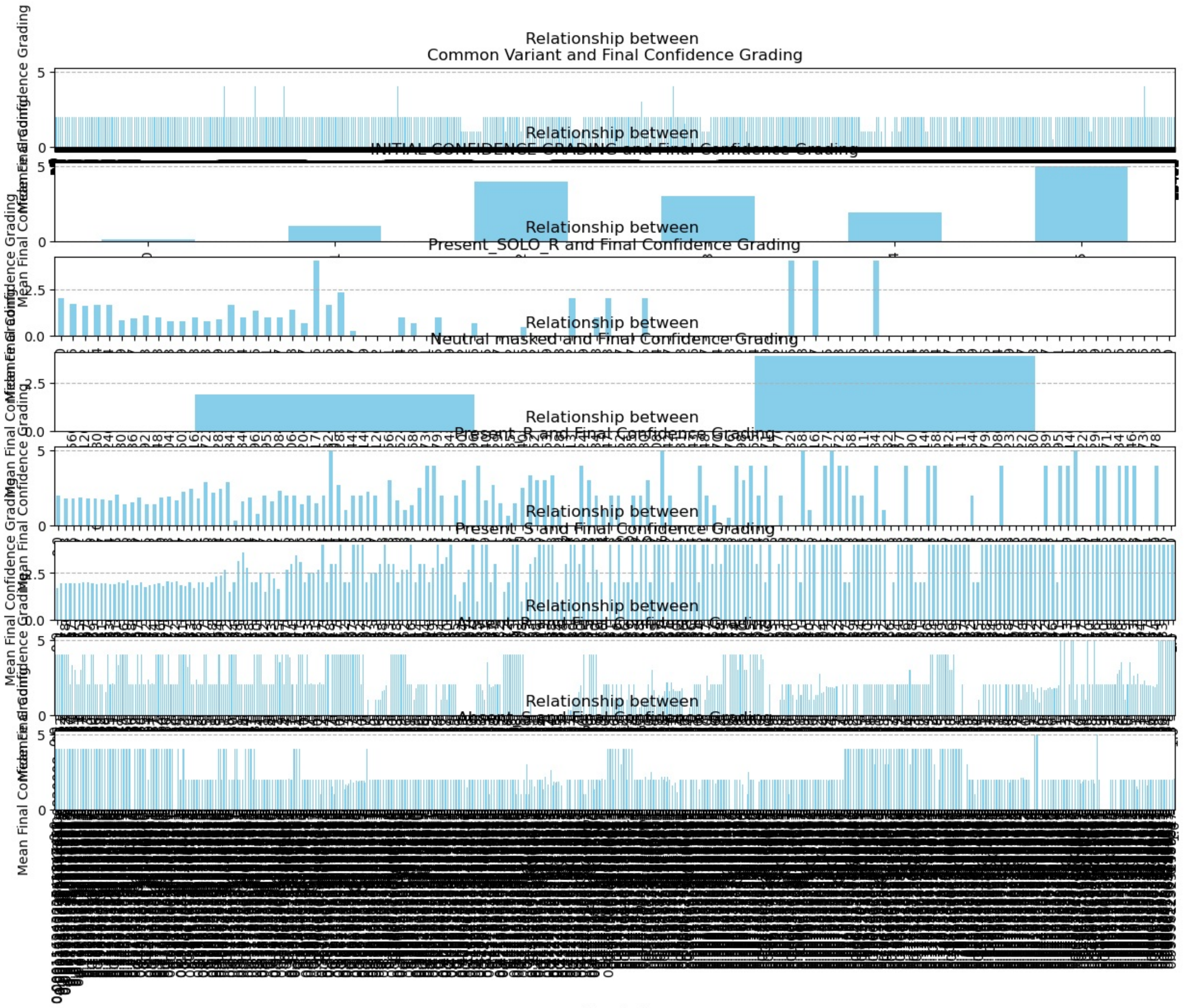
```
0.000420    1.657895
0.000560    1.633803
              ...
0.158683    0.000000
0.216246    0.000000
0.243417    0.000000
0.746779    0.000000
1.000000    0.000000
Name: FINAL CONFIDENCE GRADING, Length: 92, dtype: float64

Relationship between 'Neutral masked' and Final Confidence Gradings:

Neutral masked
0.0    1.927099
1.0    3.959459
Name: FINAL CONFIDENCE GRADING, dtype: float64

Relationship between 'Present_R' and Final Confidence Gradings:

Present_R
0.000000    1.995467
0.000105    1.805730
0.000211    1.788214
0.000316    1.864035
0.000422    1.803922
              ...
0.236739    0.000000
0.241485    0.000000
0.540124    4.000000
0.689233    0.000000
1.000000    0.000000
Name: FINAL CONFIDENCE GRADING, Length: 152, dtype: float64

Relationship between 'Present_S' and Final Confidence Gradings:

Present_S
0.000000    1.712017
0.000118    1.967196
0.000236    1.970423
0.000354    1.954918
0.000472    1.952278
              ...
0.908104    4.000000
0.908458    4.000000
0.976997    4.000000
0.984664    4.000000
1.000000    4.000000
Name: FINAL CONFIDENCE GRADING, Length: 253, dtype: float64

Relationship between 'Absent_R' and Final Confidence Gradings:

Absent_R
0.000000    4.0
0.000082    4.0
0.000246    4.0
0.000574    4.0
0.000738    4.0
           ...
0.999508    5.0
0.999672    5.0
0.999754    5.0
0.999918    5.0
1.000000    5.0
Name: FINAL CONFIDENCE GRADING, Length: 535, dtype: float64

Relationship between 'Absent_S' and Final Confidence Gradings:

Absent_S
0.000000    4.000000
0.000116    4.000000
0.000155    4.000000
0.000271    4.000000
0.000426    4.000000
              ...
0.999845    2.000000
0.999884    1.987421
0.999923    2.000000
0.999961    2.000000
1.000000    2.021898
Name: FINAL CONFIDENCE GRADING, Length: 748, dtype: float64
```

In [81]:
```
from scipy import stats

# Select the most important features identified
important_features = ['Common Variant', 'INITIAL CONFIDENCE GRADING' ,
                      'Present_SOLO_R', 'Neutral masked','Present_R','Present_S', 'Absent_R', 'Absent_S']

# Analyze the relationship between each important feature and final confidence gradings
for feature in important_features:
    # Find pointbserialr correlation coefficient
    correlation_coefficient, p_value = stats.pointbiserialr(df[feature], df['FINAL CONFIDENCE GRADING'])

    # Print the results
    print(f"\nPoint-biserial correlation coefficient between '{feature}' and 'FINAL CONFIDENCE GRADING': {corre
    print(f"P-value: {p_value}")
```

```
Point-biserial correlation coefficient between 'Common Variant' and 'FINAL CONFIDENCE GRADING': -0.048382506278
49848
P-value: 1.7180372270874056e-10

Point-biserial correlation coefficient between 'INITIAL CONFIDENCE GRADING' and 'FINAL CONFIDENCE GRADING': 0.2
797176016094426
P-value: 4.0578401675859e-310

Point-biserial correlation coefficient between 'Present_SOLO_R' and 'FINAL CONFIDENCE GRADING': -0.112212379221
96936
P-value: 7.387710645132828e-50

Point-biserial correlation coefficient between 'Neutral masked' and 'FINAL CONFIDENCE GRADING': 0.5498151025126
343
P-value: 0.0

Point-biserial correlation coefficient between 'Present_R' and 'FINAL CONFIDENCE GRADING': -0.03049148049458477
P-value: 5.763592431595842e-05

Point-biserial correlation coefficient between 'Present_S' and 'FINAL CONFIDENCE GRADING': 0.26592890781587236
P-value: 2.162312346552411e-279

Point-biserial correlation coefficient between 'Absent_R' and 'FINAL CONFIDENCE GRADING': -0.09625517965877 94
P-value: 4.343903697446709e-37

Point-biserial correlation coefficient between 'Absent_S' and 'FINAL CONFIDENCE GRADING': 0.02310558389647338
P-value: 0.0023062047405744313
```

In [82]:
```
import matplotlib.pyplot as plt

# Select the most important features identified
important_features = ['Common Variant', 'INITIAL CONFIDENCE GRADING' ,
                      'Present_SOLO_R', 'Neutral masked','Present_R','Present_S', 'Absent_R', 'Absent_S']

# Set up subplots for each feature
fig, axes = plt.subplots(nrows=len(important_features), figsize=(15, 10))

# Analyze the relationship between each important feature and final confidence gradings
for i, feature in enumerate(important_features):
    # Group the data by the feature and calculate the mean final confidence grading for each group
    feature_confidence_mean = df.groupby(feature)['FINAL CONFIDENCE GRADING'].mean()

    # Plot the bar plot
    feature_confidence_mean.plot(kind='bar', ax=axes[i], color='skyblue')
    axes[i].set_title(f'Relationship between \n{feature} and Final Confidence Grading')
    axes[i].set_ylabel('Mean Final Confidence Grading')
    axes[i].set_xlabel(feature)
    axes[i].grid(axis='y', linestyle='--', alpha=0.95)

plt.tight_layout()
plt.show()
```

```
C:\Users\hp\AppData\Local\Temp\ipykernel_20476\3042235360.py:22: UserWarning: Tight layout not applied. tight_l
ayout cannot make axes height small enough to accommodate all axes decorations.
  plt.tight_layout()
```



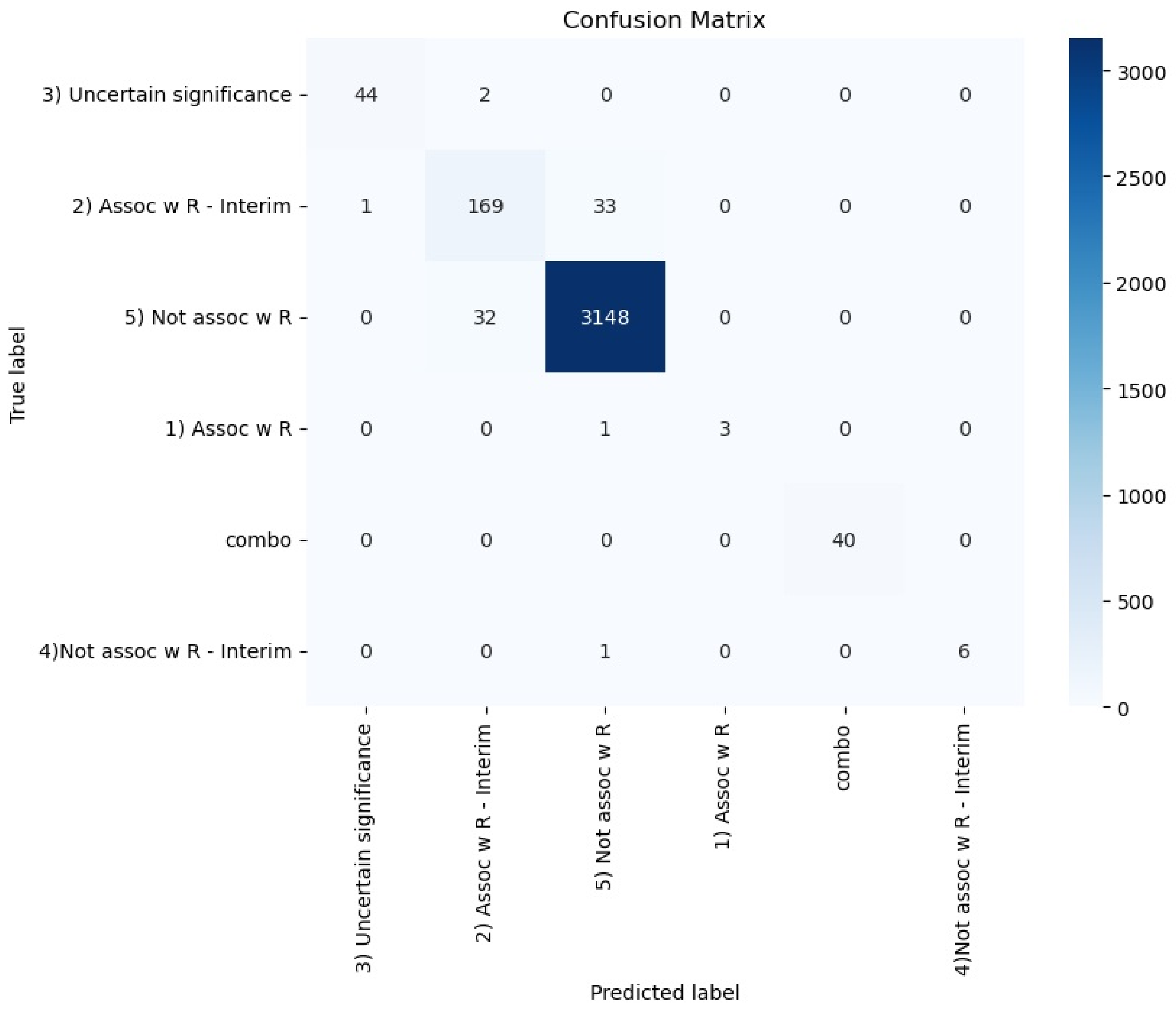
In [ ]:

In [85]:
```
from sklearn.metrics import confusion_matrix, classification_report


conf_matrix = confusion_matrix(y_test, y_pred)

# Print confusion matrix
print("Confusion Matrix:")
print(conf_matrix)

class_report = classification_report(y_test, y_pred)
```

```
print("\nClassification Report:")
print(class_report)
```

```
Confusion Matrix:
[[  44    2    0    0    0    0]
 [   1  169   33    0    0    0]
 [   0   32 3148    0    0    0]
 [   0    0    1    3    0    0]
 [   0    0    0    0   40    0]
 [   0    0    1    0    0    6]]

Classification Report:
              precision    recall  f1-score   support

           0       0.98      0.96      0.97        46
           1       0.83      0.83      0.83       203
           2       0.99      0.99      0.99      3180
           3       1.00      0.75      0.86         4
           4       1.00      1.00      1.00        40
           5       1.00      0.86      0.92         7

    accuracy                           0.98      3480
   macro avg       0.97      0.90      0.93      3480
weighted avg       0.98      0.98      0.98      3480
```

In [86]:
```
conf_matrix = confusion_matrix(y_test, y_pred)

# Create heatmap
plt.figure(figsize=(8, 6))
sns.heatmap(conf_matrix, annot=True, fmt='d', cmap='Blues',
            xticklabels=['3) Uncertain significance', '2) Assoc w R - Interim', '5) Not assoc w R', '1) Assoc w
            yticklabels=['3) Uncertain significance', '2) Assoc w R - Interim', '5) Not assoc w R', '1) Assoc w
plt.xlabel('Predicted label')
plt.ylabel('True label')
plt.title('Confusion Matrix')
plt.show()
```



In [87]:
```
import pickle

# Specify the file path where you want to save the model
file_path = "C:/Users/hp/OneDrive/Documents/Model_MDR.pkl"

# Open the file in write-binary mode
```

```python
with open(file_path, "wb") as file:
    # Use pickle to dump the trained model into the file
    pickle.dump(model, file)

print("Model saved successfully.")
```

```
Model saved successfully.
```

In [88]:
```
!pip install streamlit
```

```
Requirement already satisfied: streamlit in c:\users\hp\anaconda3\lib\site-packages (1.31.1)
Requirement already satisfied: requests<3,>=2.27 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (2
.28.1)
Requirement already satisfied: blinker<2,>=1.0.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (1
.7.0)
Requirement already satisfied: click<9,>=7.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (8.0.4
)
Requirement already satisfied: tenacity<9,>=8.1.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (
8.2.3)
Requirement already satisfied: protobuf<5,>=3.20 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (4
.23.4)
Requirement already satisfied: pydeck<1,>=0.8.0b4 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (
0.8.1b0)
Requirement already satisfied: validators<1,>=0.2 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (
0.22.0)
Requirement already satisfied: importlib-metadata<8,>=1.4 in c:\users\hp\anaconda3\lib\site-packages (from stre
amlit) (4.11.3)
Requirement already satisfied: numpy<2,>=1.19.3 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (1.
26.4)
Requirement already satisfied: python-dateutil<3,>=2.7.3 in c:\users\hp\anaconda3\lib\site-packages (from strea
mlit) (2.8.2)
Requirement already satisfied: tzlocal<6,>=1.1 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (5.2
)
Requirement already satisfied: rich<14,>=10.14.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (1
3.7.1)
Requirement already satisfied: packaging<24,>=16.8 in c:\users\hp\anaconda3\lib\site-packages (from streamlit)
(21.3)
Requirement already satisfied: pyarrow>=7.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (15.0.0
)
Requirement already satisfied: cachetools<6,>=4.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (
5.3.2)
Requirement already satisfied: gitpython!=3.1.19,<4,>=3.0.7 in c:\users\hp\anaconda3\lib\site-packages (from st
reamlit) (3.1.42)
Requirement already satisfied: typing-extensions<5,>=4.3.0 in c:\users\hp\anaconda3\lib\site-packages (from str
eamlit) (4.3.0)
Requirement already satisfied: pandas<3,>=1.3.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (1.
4.4)
Requirement already satisfied: altair<6,>=4.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (5.2.
0)
Requirement already satisfied: watchdog>=2.1.5 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (2.1
.6)
Requirement already satisfied: toml<2,>=0.10.1 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (0.1
0.2)
Requirement already satisfied: pillow<11,>=7.1.0 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (9
.2.0)
Requirement already satisfied: tornado<7,>=6.0.3 in c:\users\hp\anaconda3\lib\site-packages (from streamlit) (6
.1)
Requirement already satisfied: toolz in c:\users\hp\anaconda3\lib\site-packages (from altair<6,>=4.0->streamlit
) (0.11.2)
Requirement already satisfied: jsonschema>=3.0 in c:\users\hp\anaconda3\lib\site-packages (from altair<6,>=4.0-
>streamlit) (4.16.0)
Requirement already satisfied: jinja2 in c:\users\hp\anaconda3\lib\site-packages (from altair<6,>=4.0->streamli
t) (2.11.3)
Requirement already satisfied: colorama in c:\users\hp\anaconda3\lib\site-packages (from click<9,>=7.0->streaml
it) (0.4.5)
Requirement already satisfied: gitdb<5,>=4.0.1 in c:\users\hp\anaconda3\lib\site-packages (from gitpython!=3.1.
19,<4,>=3.0.7->streamlit) (4.0.11)
Requirement already satisfied: zipp>=0.5 in c:\users\hp\anaconda3\lib\site-packages (from importlib-metadata<8,
>=1.4->streamlit) (3.8.0)
Requirement already satisfied: pyparsing!=3.0.5,>=2.0.2 in c:\users\hp\anaconda3\lib\site-packages (from packag
ing<24,>=16.8->streamlit) (3.0.9)
Requirement already satisfied: pytz>=2020.1 in c:\users\hp\anaconda3\lib\site-packages (from pandas<3,>=1.3.0->
streamlit) (2022.1)
Requirement already satisfied: six>=1.5 in c:\users\hp\anaconda3\lib\site-packages (from python-dateutil<3,>=2.
7.3->streamlit) (1.16.0)
Requirement already satisfied: charset-normalizer<3,>=2 in c:\users\hp\anaconda3\lib\site-packages (from reques
ts<3,>=2.27->streamlit) (2.0.4)
Requirement already satisfied: certifi>=2017.4.17 in c:\users\hp\anaconda3\lib\site-packages (from requests<3,>
=2.27->streamlit) (2022.9.14)
Requirement already satisfied: idna<4,>=2.5 in c:\users\hp\anaconda3\lib\site-packages (from requests<3,>=2.27-
>streamlit) (3.3)
Requirement already satisfied: urllib3<1.27,>=1.21.1 in c:\users\hp\anaconda3\lib\site-packages (from requests<
3,>=2.27->streamlit) (1.26.11)
Requirement already satisfied: markdown-it-py>=2.2.0 in c:\users\hp\anaconda3\lib\site-packages (from rich<14,>
=10.14.0->streamlit) (3.0.0)
Requirement already satisfied: pygments<3.0.0,>=2.13.0 in c:\users\hp\anaconda3\lib\site-packages (from rich<14
,>=10.14.0->streamlit) (2.17.2)
Requirement already satisfied: tzdata in c:\users\hp\anaconda3\lib\site-packages (from tzlocal<6,>=1.1->streaml
it) (2024.1)
```

```
Requirement already satisfied: smmap<6,>=3.0.1 in c:\users\hp\anaconda3\lib\site-packages (from gitdb<5,>=4.0.1
->gitpython!=3.1.19,<4,>=3.0.7->streamlit) (5.0.1)
Requirement already satisfied: MarkupSafe>=0.23 in c:\users\hp\anaconda3\lib\site-packages (from jinja2->altair
<6,>=4.0->streamlit) (2.0.1)
Requirement already satisfied: pyrsistent!=0.17.0,!=0.17.1,!=0.17.2,>=0.14.0 in c:\users\hp\anaconda3\lib\site-
packages (from jsonschema>=3.0->altair<6,>=4.0->streamlit) (0.18.0)
Requirement already satisfied: attrs>=17.4.0 in c:\users\hp\anaconda3\lib\site-packages (from jsonschema>=3.0->
altair<6,>=4.0->streamlit) (21.4.0)
Requirement already satisfied: mdurl~=0.1 in c:\users\hp\anaconda3\lib\site-packages (from markdown-it-py>=2.2.
0->rich<14,>=10.14.0->streamlit) (0.1.2)
```

In [89]:

```
#Deploy the model
import streamlit as st
import joblib

# Load the trained model
model = joblib.load('trained_model.joblib')

# Define the user interface
st.title('Drug Resistance Prediction App')
st.write('Enter the features below to predict drug resistance.')

common_variant = st.number_input('Common Variant', min_value=0.0, max_value=1.0)
present_solo_r = st.number_input('Present_SOLO_R', min_value=0.0, max_value=1.0)
present_s = st.number_input('Present_S', min_value=0.0, max_value=1.0)
absent_s = st.number_input('Absent_S', min_value=0.0, max_value=1.0)
neutral_masked = st.number_input('Neutral masked', min_value=0.0, max_value=1.0)
initial_confidence_grading = st.number_input('Initial Confidence Grading', min_value=0, max_value=5)

# Make predictions
if st.button('Predict'):
    features = [[common_variant, present_solo_r, present_s, absent_s, neutral_masked, initial_confidence_gradin
    prediction = model.predict(features)
```

```
2024-03-02 03:08:17.381
  Warning: to view this Streamlit app on a browser, run it with the following
  command:

    streamlit run C:\Users\hp\anaconda3\lib\site-packages\ipykernel_launcher.py [ARGUMENTS]
```

In [ ]:

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