Comparison to BLAST

Install Blast tools

- https://blast.ncbi.nlm.nih.gov/doc/blast-help/downloadblastdata.html
- https://www.ncbi.nlm.nih.gov/books/NBK279690/

Compare our prediction with BLAST Tools

In [1]:
```
import pandas as pd
from Bio.Seq import Seq
from Bio.SeqRecord import SeqRecord
from Bio import SeqIO
import json
from tqdm import tqdm
import sklearn.metrics as metrics
from BLAST.utils import metric
```

In [2]:
```
df = pd.read_csv('./BLAST/src/testset.csv')
```

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

Out[3]:

	id	sequence	length	class
0	Thhalv10001938m -- EIL	MMMFNEMGMYGKMDFFSSTSLGEIDVCPLPQAEQDHPVVEEDYTDD...	582	EIL
1	Tp1g37880 -- EIL	MGVFFSDPDSIAEDDGYTDNELDVDELEKRIWKQEMRLRRLKEHRK...	211	EIL
2	Pbr004574.1 -- EIL	MGDVGEIGPDISSDIEEDLRCDNIAEKDVSDEEIEAEDLERRMWKD...	608	EIL
3	Sme2.5_02278.1_g00005.1 -- EIL	MNNEVVEENQEFDDEEINYDDLKRRMWKDRMMQILKGKKRDMMIE...	494	EIL
4	ONIVA11G15950.1 -- EIL	MDASKKSVMTKEEQQLSPAASPAAAVMTAEADAINEEQDKAAAATT...	466	EIL

In [4]:
```
records = []
for i, row in df.iterrows():
    record = SeqRecord(Seq(row['sequence']), id=str(i+1), description="" | '' + row['class'])
    records.append(record)

# Save to a FASTA file
output_file = "./BLAST/testset.fasta"
SeqIO.write(records, output_file, "fasta")

print(f"FASTA file saved as {output_file}")
```

```
FASTA file saved as ./BLAST/testset.fasta
```

Build reference(train) database for blast

In [5]:
```
ref_pah = "../data/mix_data/trainset"
```

In [6]:
```
gene_info_path = "../data/gene_info.json"
with open(gene_info_path, 'r') as json_file:
    gene_info = json.load(json_file)
```

In [7]:
```
records = []
for gene, info in tqdm(gene_info.items()):
    path = f"{ref_pah}/{info['file_code']}.csv"
    df_gene = pd.read_csv(path)
    df_gene = df_gene[df_gene['class'] == 1]

    # write
    for _, row in df_gene.iterrows():
        record = SeqRecord(Seq(row['sequence']), id=row['id'] + "—" + gene, description="")
        records.append(record)

# Save to a FASTA file
output_file = "./BLAST/trainset.fasta"
SeqIO.write(records, output_file, "fasta")
print(f"FASTA file saved as {output_file}")
```

```
100%|██████████| 58/58 [00:09<00:00,  6.35it/s]
FASTA file saved as ./BLAST/trainset.fasta
```

BUILD DATABASE FOR BLAST

In [8]:
```
!makeblastdb -in ./BLAST/trainset.fasta -dbtype prot -out ./BLAST/database/pygenomics_ref_db
```

```
Building a new DB, current time: 07/07/2024 09:42:23
New DB name:   /Users/genereux/Documents/UM6P/COURS-S2/S2-PROJECT/pygenomics/test/BLAST/database/pygenomics_ref_db
New DB title:  ./BLAST/trainset.fasta
Sequence type: Protein
Deleted existing Protein BLAST database named /Users/genereux/Documents/UM6P/COURS-S2/S2-PROJECT/pygenomics/test/BLAST/database/pygenomics_ref_db
Keep MBits: T
Maximum file size: 3000000000B
Adding sequences from FASTA; added 256279 sequences in 4.78068 seconds.
```

RUN BLAST SEARCH TOOL

In [16]:
```
#!blastp -query ./BLAST/testset.fasta -db ./BLAST/database/pygenomics_ref_db -out ./BLAST/blast_res
```

View Blast Analysis results

In [18]:
```
columns = [
    "query_id", "subject_id", "perc_identity", "alignment_length",
    "mismatches", "gap_opens", "q_start", "q_end", "s_start", "s_end",
    "evalue", "bit_score"
]
blast_results = pd.read_csv("./BLAST/blast_result.txt", sep="\t", names=columns)
#blast_results.to_csv("./BLAST/blast_results.csv", index=False)

# Display the first few rows of the DataFrame
blast_results.head()
```

Out[18]:

	query_id	subject_id	perc_identity	alignment_length	mismatches	gap_opens	q_start	q_end
0	1	676714038--EIL	89.696	592	49	6	1	581
1	1	XP_013629559.1--EIL	84.628	592	59	10	1	581
2	1	GSBRNA2T00066199001--EIL	83.277	592	59	10	1	581
3	1	XP_009133914.1--EIL	85.135	592	56	10	1	581
4	1	XP_009133916.1--EIL	85.135	592	56	10	1	581

Proccessing to make final inference base on threshold

In [19]:
```
voting_threshold = 50
unique_query_ids = sorted(blast_results['query_id'].unique())

predictions = ["Unknown"  for _ in range(len(df))]
for query_id in tqdm(unique_query_ids, desc="Max Voting : "):
    filtered_df = blast_results[blast_results['query_id'] == query_id]

    # Find the row with the highest perc_identity greater than voting_threshold
    best_match = filtered_df[filtered_df['perc_identity'] > voting_threshold].sort_values(by='perc_
    if not best_match.empty:
        subject_id = best_match.iloc[0]['subject_id']
        subject_id_part = subject_id.split('—')[-1]
        predictions[query_id-1] = (subject_id_part)

blast_prediction = pd.DataFrame({'prediction': predictions})
```

```
Max Voting : 100%|██████████| 64037/64037 [15:59<00:00, 66.74it/s]
```

In [20]:
```
with open("./BLAST/src/class_mapping.json", 'r') as json_file:
    class_mapping = json.load(json_file)
true_label = pd.read_csv("./BLAST/src/true_labels.csv")
```

In [21]:
```
blast_prediction["predicted_label"] = blast_prediction.prediction.map(class_mapping)
blast_prediction.head()
```

Out[21]:

	prediction	predicted_label
0	EIL	1
1	EIL	1
2	EIL	1
3	EIL	1
4	EIL	1

Display performance

In [22]:
```
metric.show_metrics(true_label, blast_prediction.predicted_label)
```

Overall Score

Accuracy	0.9686

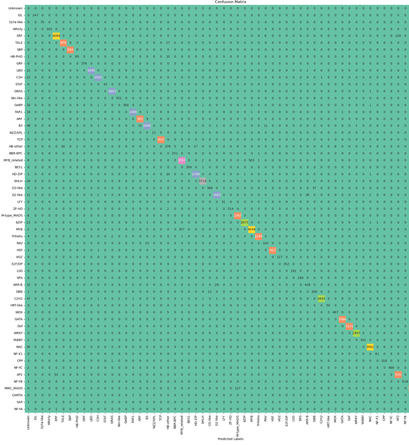
Evaluation Score	Metrics Description
Micro	Calculates metrics globally by counting the total true positives, false negatives, and false positive
Macro	Calculates metrics for each class independently and then takes the average (treating all classes equally
Weighted	Calculates metrics for each class independently and then takes the average, weighted by the number of instances of each clas

In [26]:
```
import importlib
importlib.reload(metric)
```

Out[26]:
```
<module 'BLAST.utils.metric' from '/Users/genereux/Documents/UM6P/COURS-S2/S2-PROJECT/pygenomics/test/BLAST/utils/metric.py'>
```

In [27]:
```
metric.show_confusion(true_label, blast_prediction.predicted_label, class_mapping)
```

Confusion Matrix



In [ ]: