Plot CE0 and PL9 Families

Imports

```
import seaborn as sns
import pandas as pd
import numpy as np
```

Create data frames

incsv contains protein sequence ID and whether they are in CE0 or PL9.

infile contains the output of DIAMOND Fast. Caculation for BSR is done.

```
incsv = f"../Data/CE0_PL9/CE0_PL9_accessions.csv"
# read in CE0 and PL9 accessions/ sequence names.
dffam = pd.read_csv(incsv) # read csv into a pandas dataframe.

infile = f"../Results/CE0_PL9/CE0_PL9rundiamondfast.tsv" # Set diamond
input.

df = pd.read_table(infile, header=None) # Create a dataframe of
Diamond input.
df.columns = ["qseqid", "sseqid", "qlen", "qstart", "qend", "pident",
"bitscore"]
# Name the columnes in the dataframe.
df["normalisedbitscore"]=df["bitscore"]/df["qlen"]
# Caculate the normalised bitscore.
df["qcov"] = (df["qend"]-df["qstart"])/df["qlen"] # Calculate query
coverage.
```

Create dataframe for BSR then plot clustermap

The culstermap is plotted with a large figure size to ensure all the xtick and ytick lables can be read.

```
widedfx = pd.pivot(
    df,
    index="qseqid",
    columns= "sseqid",
    values="normalisedbitscore"
) # Turn into a wide dataframe.
widedf = widedfx.fillna(0) # Remove any values NaN and replace with 0.

famqseqid = []
#create empty lists for the families of the query and subject sequence
IDs.
famsseqid = []
```

```
for qseqid in widedf: # going through the row names in df.
    fil = dffam[dffam['genbank_accession'] == qseqid] # filter through
accessions
    if len(fil) > 1:
        family = 'CE0+PL9' # identify and annotate multi-domain
CAZymes
    else:
        family = fil.iloc[0]['family']
    famqseqid.append(family)
for sseqid in widedf.columns: # same as before but for columns not
rows.
    fil = dffam[dffam['genbank_accession'] == sseqid]
    if len(fil) > 1:
        family = 'CE0+PL9'
    else:
        family = fil.iloc[0]['family']
    famsseqid.append(family)

widedf['Family'] = famqseqid # Add family annotations to BSR dataframe
pd_series = widedf.pop('Family')
lut = dict(zip(set(famqseqid), sns.color_palette("Set1",
n_colors=len(set(famqseqid)))))
row_colours = pd_series.map(lut)

def plotdiamond(fast): # Function is called plotdiamond.
    """Function takes the output matrix calculated by diamond and
plots a clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'. """
    sns.set(font_scale=0.5)
    figure=sns.clustermap(# Plot clustermap of the data frame created.
        widedf,
        cmap="Blues",
        figsize=(450, 450),
        row_colors=row_colours,
        col_colors=row_colours,
        yticklabels=1,
        xticklabels=1
    );
    for label in list(lut.keys()):
        figure.ax_row_dendrogram.bar(0, 0, color=lut[label],
label=label, linewidth=0)

    l3 = figure.ax_row_dendrogram.legend(
        title='Legend',
        loc='upper right',
        ncol=1,
        fontsize=400
    )

    figure.ax_heatmap.set_xlabel("Subject Sequence ID",fontsize=300,
```

```
labelpad=15)
    figure.ax_heatmap.set_ylabel("Query Sequence ID",fontsize=300,
labelpad=15)
    figure.ax_heatmap.set_title(
        f'CE0 and PL9 CAZymes Normalised Bitscore Calculated by
Diamond Fast',
        fontsize=400,
        pad=80
    )
    figure.savefig(f'../Results/CE0_PL9/CE0_PL9_BSR_hugeREAD.png')
    # Save in results folder.
    return figure

plotBSR = plotdiamond('fast') # Run function for 100 sequences at fast

help(plotdiamond) # Call functions doc string to explain what the
function does
```

```
/home/cjohns/.local/lib/python3.6/site-packages/seaborn/matrix.py:654:
UserWarning: Clustering large matrix with scipy. Installing
`fastcluster` may give better performance.
  warnings.warn(msg)

Help on function plotdiamond in module __main__:

plotdiamond(fast)
    Function takes the output matrix calculated by diamond and plots a
clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'.
```

Build CSV file of the order the query and subject sequences appear in the BSR cluster map

```
columnorder = list(plotBSR.__dict__['data2d'].keys())
# set column order to order calculated for BSR clustermap.
roworder = list(plotBSR.__dict__['data2d'].index)
# set row order to order calculated for BSR clustermap.

dfBSR = widedf[columnorder]
dfBSR = dfBSR.reindex(roworder) # reordered dataframe.

dfBSR.to_csv('../Results/CE0_PL9/CE0_PL9_BSR.csv') # Save results to
CSV file.
```

Plot of BSR a 2nd time with known order

```
famqseqid = []
#create empty lists for the families of the query and subject sequence
```

```
IDs.
famsseqid = []

for qseqid in dfBSR: # going through the row names in df.
    fil = dffam[dffam['genbank_accession'] == qseqid] # filter through
accessions
    if len(fil) > 1:
        family = 'CE0+PL9' # identify and annotate multi-domain
CAZymes
    else:
        family = fil.iloc[0]['family']
    famqseqid.append(family)
for sseqid in dfBSR.columns: # going through the column names in df.
    fil = dffam[dffam['genbank_accession'] == sseqid]
    # same as before but for columns not rows.
    if len(fil) > 1:
        family = 'CE0+PL9'
    else:
        family = fil.iloc[0]['family']
    famsseqid.append(family)

dfBSR['Family'] = famqseqid # Add family annotations to BSR dataframe
pd_series = dfBSR.pop('Family')
lut = dict(zip(set(famqseqid), sns.color_palette("Set1",
n_colors=len(set(famqseqid)))))
row_colours = pd_series.map(lut)

def plotdiamond(fast): # Function is called plotdiamond.
    """Function takes the output matrix calculated by diamond and
plots a clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'. """
    sns.set(font_scale=0.5)
    figure=sns.clustermap(
        dfBSR,
        cmap="Blues",
        figsize=(450, 450),
        row_colors=row_colours,
        col_colors=row_colours,
        yticklabels=1, xticklabels=1,
        row_cluster=False,
        col_cluster=False
    ); # Plot clustermap of the data frame created.

    for label in list(lut.keys()):
        figure.ax_row_dendrogram.bar(0, 0, color=lut[label],
label=label, linewidth=0)

    l3 = figure.ax_row_dendrogram.legend(
        title='Legend',
        loc='upper right',
```

```
        ncol=1,
        fontsize=400
    )

    figure.ax_heatmap.set_xlabel("Subject Sequence ID",fontsize=300,
labelpad=15)
    figure.ax_heatmap.set_ylabel("Query Sequence ID",fontsize=300,
labelpad=15)
    figure.ax_heatmap.set_title(
        f'CE0 and PL9 CAZymes Normalised Bitscore Calculated by
Diamond Fast',
        fontsize=400,
        pad=80
    )
    figure.savefig(f'../Results/CE0_PL9/CE0_PL9_BSR_huge.png') # Save
in results folder.
    return figure

plotBSR = plotdiamond('fast') # Run function for 100 sequences at fast

help(plotdiamond) # Call functions doc string to explain what the
function does

Help on function plotdiamond in module __main__:

plotdiamond(fast)
    Function takes the output matrix calculated by diamond and plots a
clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'.
```

Find interesting proteins then sub set dataframe.

Write out protein with both CE0 and PL9 domains to a CSV file.

Proteins of interest are those which have a BSR > 1 in common with a protein

contained in both CE0 and PL9 families.

```
cooccurring = pd_series.loc[pd_series == 'CE0+PL9']
# write multi-domain CAZymes to a list.
cooccurring.to_csv('../Results/CE0_PL9/Cooccuring.csv') # save the
list.

pro = ['AEI43346.1', 'AFH63317.1', 'AFK65394.1', 'QYM77803.1'] #
multi-domain CAZymes list.
threshold = 1 # Set BSR threshold to 1.
interest = {'AEI43346.1', 'AFH63317.1', 'AFK65394.1', 'QYM77803.1'}
# dictionary called interest.
```

```
for sseqid in pro:
    col = list(dfBSR[sseqid])
    for i in range(len(col)):
        if col[i] >= threshold:
            interest.add(dfBSR.iloc[i].name)
            # Add any sequences in the same column as a CE0-PL9
protein with a BSR>1 to interest.
    row = list(dfBSR.loc[sseqid])
    for i in range(len(row)):
        if row[i] >= threshold:
            print(i, row[i])
            interest.add(dfBSR.columns[i])
            # Add any sequences in the same row as a CE0-PL9 protein
with a BSR>1 to interest.
```

```
4233 2.002014098690836
4234 1.5387713997985901
4235 1.539778449144008
4233 1.9665379665379665
4234 2.0167310167310166
4235 2.0167310167310166
4233 1.9540816326530612
4234 2.0
4235 2.0191326530612246
3215 1.8465753424657534
```

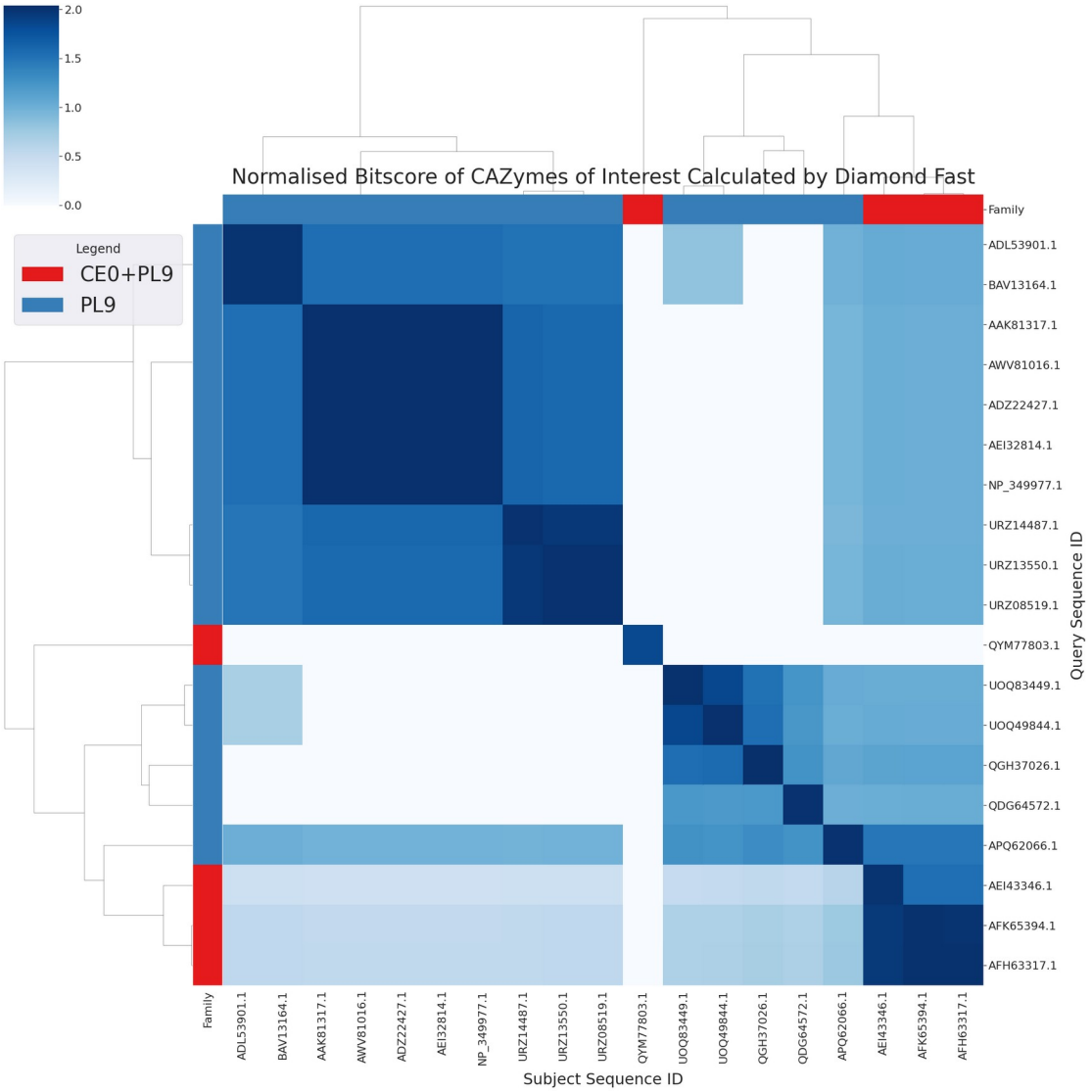
```
dfnew = dfBSR[interest]
dfsmol2 = dfnew.loc[interest] # subset dataframe
```

```
famqseqid = [] #create empty lists for the families of the query and
subject sequence IDs.
famsseqid = []

for qseqid in dfsmol2: # going through the row names in df.
    fil = dffam[dffam['genbank_accession'] == qseqid] # filter through
accessions
    if len(fil) > 1:
        family = 'CE0+PL9' # identify and annotate multi-domain
CAZymes
    else:
        family = fil.iloc[0]['family']
    famqseqid.append(family)
for sseqid in dfsmol2.columns:
    # going through the column names in df same as before but for
columns not rows.
    fil = dffam[dffam['genbank_accession'] == sseqid]
    if len(fil) > 1:
        family = 'CE0+PL9'
    else:
        family = fil.iloc[0]['family']
    famsseqid.append(family)
```

```
dfsmol2['Family'] = famqseqid # Add family annotations to BSR
dataframe
pd_series = dfsmol2.pop('Family')
lut = dict(zip(set(famqseqid), sns.color_palette("Set1",
n_colors=len(set(famqseqid)))))
row_colours = pd_series.map(lut)

def plotdiamond(fast): # Function is called plotdiamond.
    """Function takes the output matrix calculated by diamond and
plots a clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'. """
    sns.set(font_scale=2)
    figure=sns.clustermap(
        dfsmol2,
        cmap="Blues",
        figsize=(30, 30),
        row_colors=row_colours,
        col_colors=row_colours,
        yticklabels=1,
        xticklabels=1
    ); # Plot clustermap of the data frame created.
    for label in list(lut.keys()):
        figure.ax_row_dendrogram.bar(0, 0, color=lut[label],
label=label, linewidth=0)

    l3 = figure.ax_row_dendrogram.legend(
        title='Legend',
        loc='upper right',
        ncol=1,
        fontsize=40
    )

    figure.ax_heatmap.set_xlabel("Subject Sequence ID",fontsize=30,
labelpad=15)
    figure.ax_heatmap.set_ylabel("Query Sequence ID",fontsize=30,
labelpad=15)
    figure.ax_heatmap.set_title(
        f'Normalised Bitscore of CAZymes of Interest Calculated by
Diamond Fast',
        fontsize=40,
        pad=80
    )
    figure.savefig(f'../Results/CE0_PL9/CE0_PL9_BSRZoom.png') # Save
in results folder.
    return figure

plotBSRZoom = plotdiamond('fast') # Run function for 100 sequences at
fast
```

```
help(plotdiamond) # Call functions doc string to explain what the
function does
```

```
Help on function plotdiamond in module __main__:

plotdiamond(fast)
    Function takes the output matrix calculated by diamond and plots a
clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'.
```



Get order of the zoomed in Clusterplot and print to CSV file

```
corder = list(plotBSRZoom.__dict__['data2d'].keys())
# Get column order from zoomed in BSR clustermap for query coverage
map.
rorder = list(plotBSRZoom.__dict__['data2d'].index) # get row order.
```

```
dfprint = dfsmol2[corder]
dfprint = dfprint.reindex(rorder) # reorder dataframe

dfprint.to_csv('../Results/CE0_PL9/Zoom.csv')
# Save copy of zoomed in dataframe to a CSV file.
```

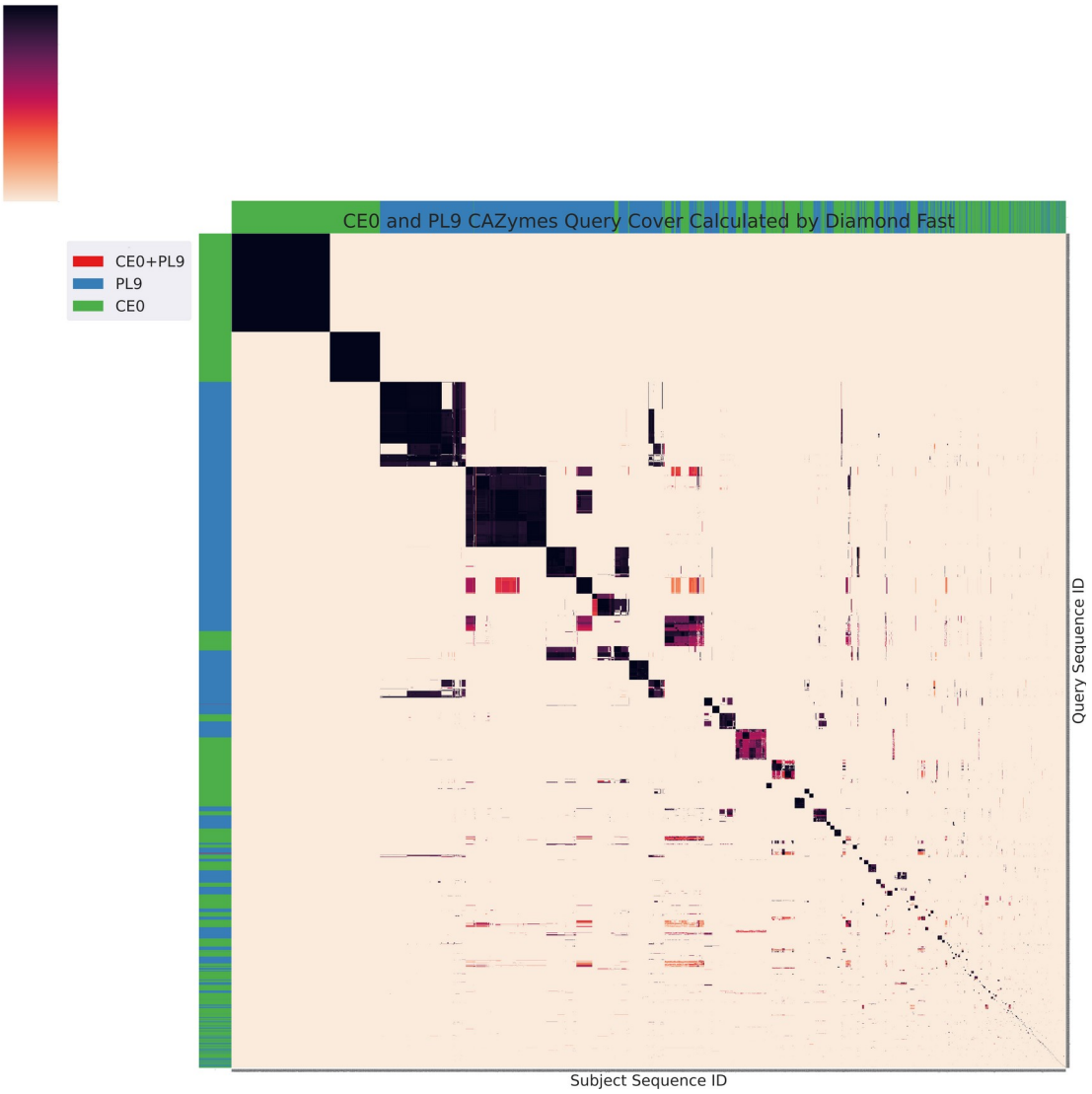
Create Dataframe for Query Cover, ensuring the sequences appear

in the same order as for BSR matrix and plot clustermap

```
widedfxq = pd.pivot(df, index="qseqid", columns= "sseqid",
values="qcov")
# Turn Long dataframe into a wide dataframe.
widedfq = widedfxq.fillna(0) # Remove any values NaN and replace with
0.

# Reordering dtaframe to be same as BSR,  and print it.
dfqcov = widedfq[columnorder]
dfqcov = dfqcov.reindex(roworder)

dfqcov.to_csv('../Results/CE0_PL9/CE0_PL9_qcov.csv')
# Save a copy of query coverage matrix to a CSV file.

famqseqid = [] #create empty lists for the families of the query and
subject sequence IDs.
famsseqid = []

for qseqid in dfqcov: # going through the row names in df.
    fil = dffam[dffam['genbank_accession'] == qseqid] # filter through
accessions
    if len(fil) > 1:
        family = 'CE0+PL9' # identify and annotate multi-domain
CAZymes
    else:
        family = fil.iloc[0]['family']
    famqseqid.append(family)

for sseqid in dfqcov.columns:
    # going through the column names in df same as before but for
columns not rows.
    fil = dffam[dffam['genbank_accession'] == sseqid]
    if len(fil) > 1:
        family = 'CE0+PL9'
    else:
        family = fil.iloc[0]['family']
    famsseqid.append(family)

dfqcov['Family'] = famqseqid # Add family annotations to BSR dataframe
pd_series = dfqcov.pop('Family')
lut = dict(zip(set(famqseqid), sns.color_palette("Set1",
```

```
n_colors=len(set(famqseqid)))))
row_colours = pd_series.map(lut)

def plotdiamond(fast): # Function is called plotdiamond.
    """Function takes the output matrix calculated by diamond and
plots a clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'. """
    sns.set(font_scale=0.6)
    figure=sns.clustermap(
        dfqcov,
        cmap="rocket_r",
        figsize=(200, 200),
        row_colors=row_colours,
        col_colors=row_colours,
        yticklabels=1,
        xticklabels=1,
        row_cluster=False,
        col_cluster=False,
    ); # Plot clustermap of the data frame created.
    for label in list(lut.keys()):
        figure.ax_row_dendrogram.bar(0, 0, color=lut[label],
label=label, linewidth=0)

    l3 = figure.ax_row_dendrogram.legend(
        title='Legend',
        loc='upper right',
        ncol=1,
        fontsize=200
    )

    figure.ax_heatmap.set_xlabel("Subject Sequence ID",fontsize=200,
labelpad=15)
    figure.ax_heatmap.set_ylabel("Query Sequence ID",fontsize=200,
labelpad=15)
    figure.ax_heatmap.set_title(
        f'CE0 and PL9 CAZymes Query Cover Calculated by Diamond Fast',
        fontsize=250,
        pad=80
    )
    figure.savefig(f'../Results/CE0_PL9/CE0_PL9_qcov.png') # Save in
results folder.
    return figure

plotqcov = plotdiamond('fast') # Run function for 100 sequences at
fast

help(plotdiamond) # Call functions doc string to explain what the
function does
```

```
Help on function plotdiamond in module __main__:

plotdiamond(fast)
    Function takes the output matrix calculated by diamond and plots a
clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'.
```



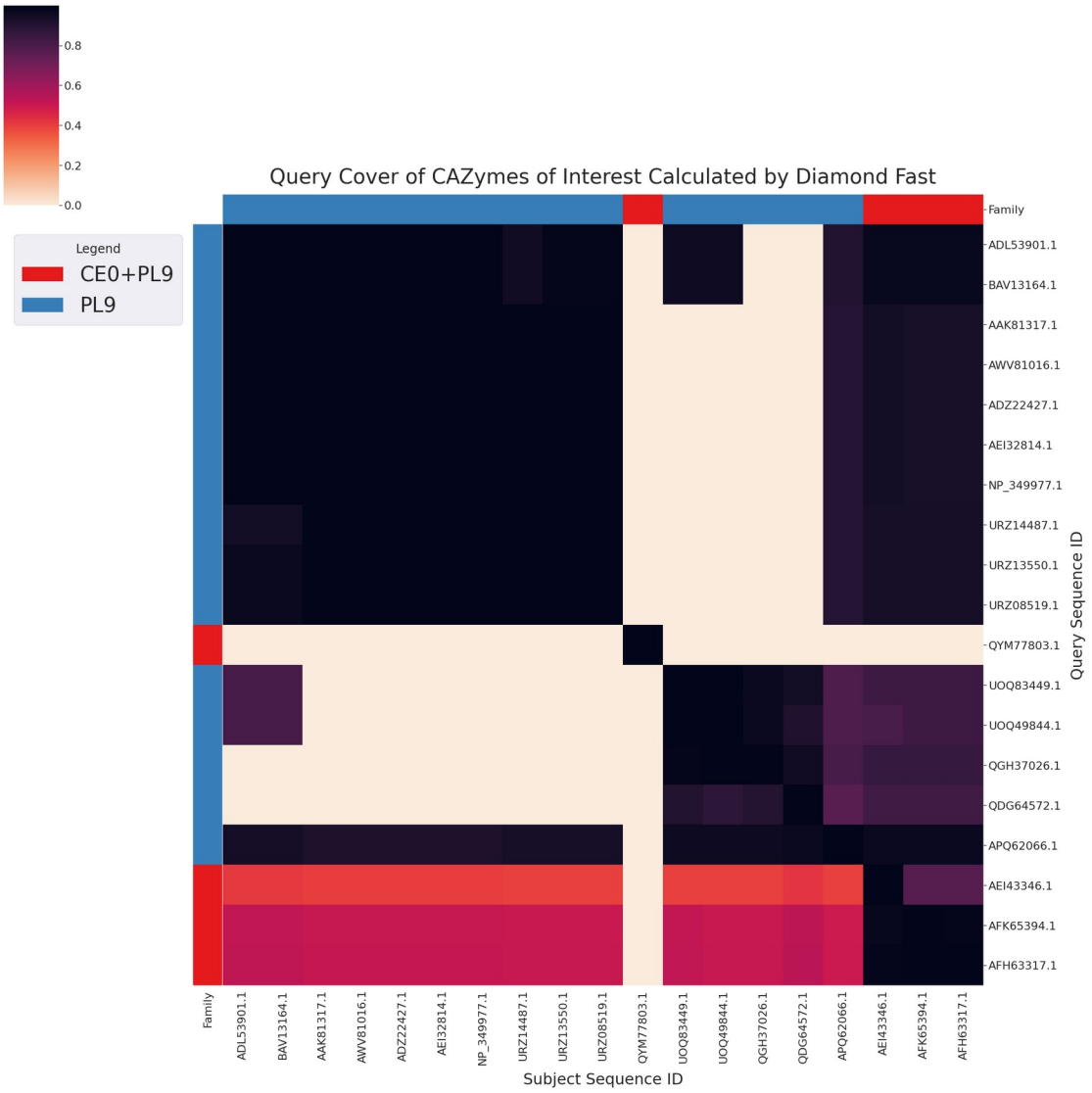
Plot interesting Proteins for Query Cover

```
dfnewq = dfqcov[interest]
# subset query cover data frame to only contain proteins of interest
stored in the 'interest' list.
dfsmolq = dfnewq.loc[interest]

dforderq = dfsmolq[corder]
# reorder dataframe based off the order of the subsetted BSR
```

```
clustermap.
dfqcov = dforderq.reindex(rorder)

famqseqid = [] #create empty lists for the families of the query and
subject sequence IDs.
famsseqid = []

for qseqid in dfsmolq: # going through the row names in df.
    fil = dffam[dffam['genbank_accession'] == qseqid] # filter through
accessions
    if len(fil) > 1:
        family = 'CE0+PL9' # identify and annotate multi-domain
CAZymes
    else:
        family = fil.iloc[0]['family']
    famqseqid.append(family)
for sseqid in dfsmolq.columns:
    # going through the column names in df same as before but for
columns not rows.
    fil = dffam[dffam['genbank_accession'] == sseqid]
    if len(fil) > 1:
        family = 'CE0+PL9'
    else:
        family = fil.iloc[0]['family']
    famsseqid.append(family)

dfsmolq['Family'] = famqseqid # Add family annotations to BSR
dataframe
pd_series = dfsmolq.pop('Family')
lut = dict(zip(set(famqseqid), sns.color_palette("Set1",
n_colors=len(set(famqseqid)))))
row_colours = pd_series.map(lut)

def plotdiamond(fast): # Function is called plotdiamond.
    """Function takes the output matrix calculated by diamond and
plots a clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'. """
    sns.set(font_scale=2)
    figure=sns.clustermap(
        dfqcov,
        cmap="rocket_r",
        figsize=(30, 30),
        row_colors=row_colours,
        col_colors=row_colours,
        yticklabels=1,
        xticklabels=1,
        row_cluster=False,
        col_cluster=False
    ); # Plot clustermap of the data frame created.
    for label in list(lut.keys()):
```

```
        figure.ax_row_dendrogram.bar(0, 0, color=lut[label],
label=label, linewidth=0)

    l3 = figure.ax_row_dendrogram.legend(
        title='Legend',
        loc='upper right',
        ncol=1,
        fontsize=40
    )

    figure.ax_heatmap.set_xlabel("Subject Sequence ID",fontsize=30,
labelpad=15)
    figure.ax_heatmap.set_ylabel("Query Sequence ID",fontsize=30,
labelpad=15)
    figure.ax_heatmap.set_title(
        f'Query Cover of CAZymes of Interest Calculated by Diamond
Fast',
        fontsize=40,
        pad=80
    )
    figure.savefig(f'../Results/CE0_PL9/CE0_PL9_QcovZoom.png') # Save
in results folder.
    return figure

plotBSRZoom = plotdiamond('fast') # Run function for 100 sequences at
fast

help(plotdiamond) # Call functions doc string to explain what the
function does
```

```
Help on function plotdiamond in module __main__:

plotdiamond(fast)
    Function takes the output matrix calculated by diamond and plots a
clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'.
```



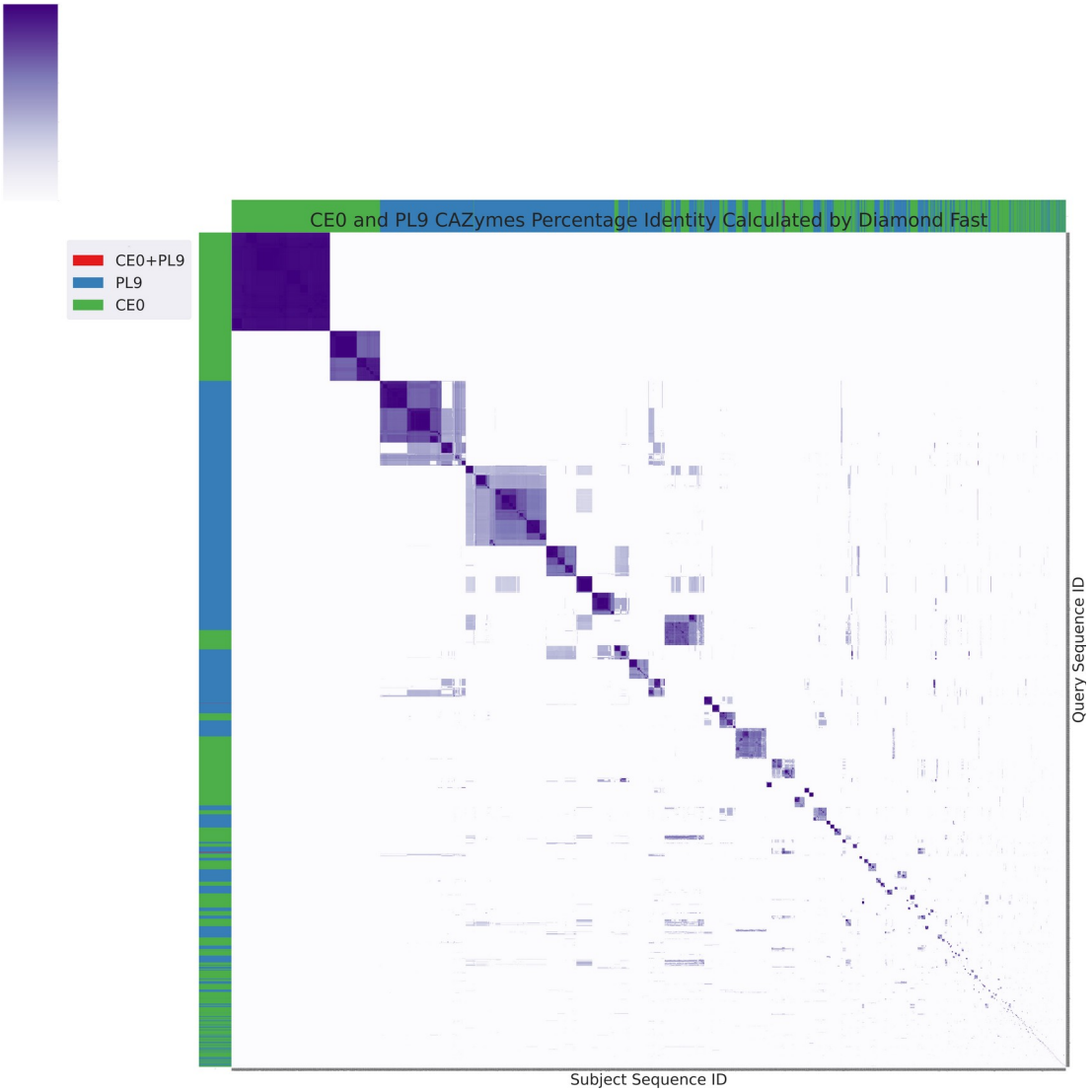
Create Dataframe for percentage identity, ensuring the sequences

appear in the same order as BSR and plot clustrmap

```
widedfxi = pd.pivot(df, index="qseqid", columns= "sseqid",
values="pident")
# Turn Long dataframe into a wide dataframe.
widedfi = widedfxi.fillna(0) # Remove any values NaN and replace with
0.

# Reordering dtaframe to be same as BSR.
dfpident = widedfi[columnorder]
dfpident= dfpident.reindex(roworder)

famqseqid = [] #create empty lists for the families of the query and
subject sequence IDs.
famsseqid = []
```

```
for qseqid in dfpident: # going through the row names in df.
    fil = dffam[dffam['genbank_accession'] == qseqid] # filter through
accessions
    if len(fil) > 1:
        family = 'CE0+PL9' # identify and annotate multi-domain
CAZymes
    else:
        family = fil.iloc[0]['family']
    famqseqid.append(family)

for sseqid in dfpident.columns:
    # going through the column names in df same as before but for
columns not rows.
    fil = dffam[dffam['genbank_accession'] == sseqid]
    if len(fil) > 1:
        family = 'CE0+PL9'
    else:
        family = fil.iloc[0]['family']
    famsseqid.append(family)

dfpident['Family'] = famqseqid # Add family annotations to BSR
dataframe
pd_series = dfpident.pop('Family')
lut = dict(zip(set(famqseqid), sns.color_palette("Set1",
n_colors=len(set(famqseqid)))))
row_colours = pd_series.map(lut)

def plotdiamond(fast): # Function is called plotdiamond.
    """Function takes the output matrix calculated by diamond and
plots a clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'. """
    sns.set(font_scale=0.6)
    figure=sns.clustermap(
        dfpident,
        cmap="Purples",
        figsize=(200, 200),
        row_colors=row_colours,
        col_colors=row_colours,
        yticklabels=1,
        xticklabels=1,
        row_cluster=False,
        col_cluster=False
    ); # Plot clustermap of the data frame created.
    for label in list(lut.keys()):
        figure.ax_row_dendrogram.bar(0, 0, color=lut[label],
label=label, linewidth=0)

    l3 = figure.ax_row_dendrogram.legend(
        title='Legend',
```

```
        loc='upper right',
        ncol=1,
        fontsize=200
    )

    figure.ax_heatmap.set_xlabel("Subject Sequence ID",fontsize=200,
labelpad=15)
    figure.ax_heatmap.set_ylabel("Query Sequence ID",fontsize=200,
labelpad=15)
    figure.ax_heatmap.set_title(
        f'CE0 and PL9 CAZymes Percentage Identity Calculated by
Diamond Fast',
        fontsize=250,
        pad=80
    )
    figure.savefig(f'../Results/CE0_PL9/CE0_PL9_pident.png') # Save in
results folder.
    return figure

plotqcov = plotdiamond('fast') # Run function for 100 sequences at
fast

help(plotdiamond) # Call functions doc string to explain what the
function does

Help on function plotdiamond in module __main__:

plotdiamond(fast)
    Function takes the output matrix calculated by diamond and plots a
clustermap with
    the argument as DIAMOND sensitvity, eg) 'Fast'.
```


CE0 and PL9 CAZymes Percentage Identity Calculated by Diamond Fast
CE0+PL9
PL9
CE0
Query Sequence ID
Subject Sequence ID