# Additional Efforts

March 7, 2024

### 0.1 Additional Reproducibility Efforts

Importing necessary library for data analysis for .csv and .tsv files; pandas & numpy All the supplementary tables (STable\*) dowloaded from the Zenedo repository [1] of the original article [2].

- [1] A. Gavriilidou, "Compendium of specialized metabolite biosyngenomes". diversity encoded in bacterial Zenodo, Apr. 15, 2022.(https://doi.org/10.5281/zenodo.5159210).
- [2] Gavriilidou, A., Kautsar, S.A., Zaburannyi, N. et al. Compendium of specialized metabolite biosynthetic diversity encoded in bacterial genomes. Nat Microbiol 7, 726–735 (2022). (https://doi.org/10.1038/s41564-022-01110-2)

```
[1]: import numpy as np import pandas as pd
```

```
STable1: pd.DataFrame = pd.read_csv("STable1_all_genomes_info.tsv", sep="|")

STable2: pd.DataFrame = pd.read_csv("STable2_BiG-SLICE_t0.4_GCF_assignment.

csv", sep=",")

STable3: pd.DataFrame = pd.read_csv("STable3_BiG-SLICE_t0.5_GCF_assignment.

csv", sep=",")

STable4: pd.DataFrame = pd.read_csv("STable4_BiG-SLICE_t0.6_GCF_assignment.

csv", sep=",")

STable5: pd.DataFrame = pd.read_csv("STable5_BiG-SLICE_t0.7_GCF_assignment.

csv", sep=",")
```

```
[3]: # Rename the column "bgc_ids" to "bgc_id"
STable1 = STable1.rename(columns={"bgc_ids": "bgc_id"})

# Split multiple IDs in the "bgc_id" column into separate rows
STable1["bgc_id"] = STable1.bgc_id.str.split(",")
STable1 = STable1.explode("bgc_id").reset_index(drop=True)

# Convert the "bgc_id" column to integer values
STable1["bgc_id"] = STable1["bgc_id"].astype("int64")
```

For every threshold pd.merge applied. Taxonomy information is selected from taxonomy column of each dataframe. The streptomyces genus level is displayed as an output, the following question is asked:

• From the figure 1\_A the streptomyces value counts are known (see Figure\_1.ipynb), if the following filtering algorithm utilized do we get the same results?

Figure 1\_A data;

	Genus	Number of GCFs	$Threshold \ (T)$
0	Streptomyces	7294	t = 0.4
$\boldsymbol{g}$	Streptomyces	<i>5720</i>	$t{=}0.5$
18	Streptomyces	<i>4360</i>	t= $0.6$
27	Streptomyces	2889	t= $0.7$

```
[4]: def filter_and_count_streptomyces(
         stable1: pd.DataFrame,
         stable2: pd.DataFrame,
         threshold table name: str = "",
         save_to_file: bool = True,
     ) -> tuple[pd.DataFrame, pd.DataFrame, pd.Series]:
         Filters the combined DataFrame based on Streptomyces genus,
         counts GCF IDs, and returns the merged, filtered, and taxonomy DataFrames.
         Args:
             stable1 (pd.DataFrame): DataFrame containing genomic information.
             stable2 (pd.DataFrame): DataFrame containing GCF information.
              threshold_table_name (str, optional): Name prefix for the output file. \Box
      \hookrightarrow Defaults to "".
             save_to_file (bool, optional): Whether to save the results to a CSV_{\sqcup}
      ⇔file. Defaults to True.
         Returns:
              tuple[pd.DataFrame, pd.DataFrame, pd.Series]: A tuple containing:
                  - pd.DataFrame: The merged DataFrame.
                  - pd.DataFrame: The filtered DataFrame containing Streptomyces_{\sqcup}
      \hookrightarrow entries.
                  - pd. Series: Counts of GCF IDs for Streptomyces entries.
         11 11 11
         # Merge the two DataFrames based on the 'bqc_id' column
         merged_df = stable1.merge(stable2, on='bgc_id')
         # Split the 'taxonomy' column, fill missing values, and set the column name
         taxonomy = merged_df['taxonomy'].str.split(",", expand=True).fillna("")
         taxonomy.name = f"taxonomy_{threshold_table_name}"
         # Filter the DataFrame for entries where the sixth column ('taxonomy[5]')_{\sqcup}
      ⇒is "Streptomyces"
```

```
streptomyces_df = merged_df[taxonomy[5] == "Streptomyces"]

# Count occurrences of GCF IDs in the filtered DataFrame
streptomyces_gcf_count = streptomyces_df['gcf_id'].value_counts()

# Save the Series to a CSV file (optional)
if save_to_file:
    filename = f"{threshold_table_name}_streptomyces_gcf_count.csv"
    streptomyces_gcf_count.to_csv(filename)

# Return all relevant DataFrames and Series
return merged_df, taxonomy, streptomyces_gcf_count
```

[6]: len(streptomyces\_4\_count),len(streptomyces\_5\_count),len(streptomyces\_6\_count),len(streptomyces\_6\_count)

[6]: (8703, 6798, 5136, 3363)

When inspected;

Figure 1\_A data from the applied algorithm;

Original Data

Reproduced Data

	Genus	$Number\ of\ GCFs$	$Threshold \ (T)$
0	Streptomyces	7294	t = 0.4
$oldsymbol{g}$	Streptomyces	<i>5720</i>	$t{=}0.5$
18	Streptomyces	4360	t= $0.6$
27	Streptomyces	2889	t= $0.7$

	Genus	Number of GCFs	$Threshold \ (T)$
0	Streptomyces	8703	t = 0.4

	Genus	Number of GCFs	$Threshold \ (T)$
9	Streptomyces	6798	t= $0.5$
18	Streptomyces	<i>5136</i>	$t{=}0.6$
27	Streptomyces	3363	t = 0.7

[7]: len(streptomyces\_4\_count)-7294,len(streptomyces\_5\_count)-5720,len(streptomyces\_6\_count)-4360,len(streptomyces\_6\_count)-86

[7]: (1409, 1078, 776, 474)

[8]: len(streptomyces\_4\_count)-len(streptomyces\_5\_count),len(streptomyces\_5\_count)-len(streptomyces\_5\_count)

[8]: (1905, 1662, 1773)

[9]: 1409-1078, 1078-776, 776-474

[9]: (331, 302, 302)

[10]: len(STable2)-len(thresholds\_4\_gcfs),len(STable3)-len(thresholds\_5\_gcfs),len(STable4)-len(thresholds\_5\_gcfs)

[10]: (764, 37, 37, 37)

When inspected;

Figure 1\_A data from the applied algorithm;

Original Data vs Reproduced Data

 ${\bf Extra~Operations}$ 

	Genus	Number of GCFs Differ	Threshold (T)
$diff_1$	Streptomyces	1409	t = 0.4
$diff_2$	Streptomyces	1078	$t{=}0.5$
$diff_3$	Streptomyces	776	$t{=}0.6$
$diff_4$	Streptomyces	474	t= $0.7$

Operation	Values of the output
$t_{0.4} - t_{0.5}, t_{0.5} - t_{0.6}, t_{0.6} - t_{0.7}$	(1905,1662,1773)
$diff_1 - diff_2$ , $diff_2 - diff_3$ , $diff_3 - diff_3$	(331,302,302)
$\operatorname{diff}\_4\ \$$	
$Data\ Lost\ From\ INNER\ MERGE$	(764,37,37,37)
$OPERATION \ \{t=0.4, 0.5, 0.6, 0.7\}$	

## 1 Taxonomy resolution

```
[11]: def taxonomy resolution(taxonomy file: pd.DataFrame) -> pd.DataFrame:
          Calculates the number of unique taxa at each taxonomic level (phylum,\Box
       ⇔class, order, family, genus, species)
          from a given taxonomy file, and returns the results as a DataFrame.
              taxonomy_file (pd.DataFrame): DataFrame containing taxonomic_
       \hookrightarrow information,
                  have columns representing different taxonomic levels (e.g., phylum, __
       \hookrightarrow class, order, etc.).
          Returns:
              pd.DataFrame: A new DataFrame with the following columns:
                   - "phylum_taxa_name": Names of unique phyla
                   - "phylum_taxa_count": Number of occurrences for each phylum
                  - "class_taxa_name": Names of unique classes
                  - "class_taxa_count": Number of occurrences for each class
                  - "order taxa name": Names of unique orders
                  - "order_taxa_count": Number of occurrences for each order
                   - "family_taxa_name": Names of unique families
                  - "family_taxa_count": Number of occurrences for each family
                  - "genus_taxa_name": Names of unique genera
                  - "genus_taxa_count": Number of occurrences for each genus
                  - "species_taxa_name": Names of unique species
                  - "species_taxa_count": Number of occurrences for each species
          11 11 11
          # Count unique taxa at each level (phylum, class, order, family, genus, _{\sqcup}
       ⇔species)
          phylum_taxa = taxonomy_file[1].value_counts()
          class taxa = taxonomy file[2].value counts()
          order_taxa = taxonomy_file[3].value_counts()
          family_taxa = taxonomy_file[4].value_counts()
          genus_taxa = taxonomy_file[5].value_counts()
          species_taxa = taxonomy_file[6].value_counts()
          \# Determine the minimum list length to ensure equal representation across_{\sqcup}
       ⇔all levels
          max_list_number = min(len(phylum_taxa), len(class_taxa), len(order_taxa),__
       →len(family_taxa), len(genus_taxa), len(species_taxa))
          # Truncate each Series to the minimum length to maintain consistency
          phylum_taxa = phylum_taxa[:max_list_number]
          class_taxa = class_taxa[:max_list_number]
```

```
order_taxa = order_taxa[:max_list_number]
          family_taxa = family_taxa[:max_list_number]
          genus_taxa = genus_taxa[:max_list_number]
          species_taxa = species_taxa[:max_list_number]
          # Create a DataFrame from the Series data
          taxonomy_resolution = pd.DataFrame({
              "phylum_taxa_name": list(phylum_taxa.index),
              "phylum taxa count": list(phylum taxa.values),
              "class_taxa_name": list(class_taxa.index),
              "class_taxa_count": list(class_taxa.values),
              "order_taxa_name": list(order_taxa.index),
              "order_taxa_count": list(order_taxa.values),
              "family_taxa_name": list(family_taxa.index),
              "family_taxa_count": list(family_taxa.values),
              "genus_taxa_name": list(genus_taxa.index),
              "genus_taxa_count": list(genus_taxa.values),
              "species_taxa_name": list(species_taxa.index),
              "species_taxa_count": list(species_taxa.values),
          })
          # Save the DataFrame to a CSV file with a descriptive filename
          taxonomy_resolution.to_csv(f"taxonomy_resolution_{taxonomy_file.name}.csv")
          # Return the DataFrame for further use
          return taxonomy_resolution
[12]: taxonomy_resolution_4: pd.DataFrame =
       staxonomy_resolution(taxonomy_file=taxonomy_4)
      taxonomy_resolution_5: pd.DataFrame =_
       →taxonomy resolution(taxonomy file=taxonomy 5)
      taxonomy_resolution_6: pd.DataFrame =_

¬taxonomy_resolution(taxonomy_file=taxonomy_6)
      taxonomy_resolution_7: pd.DataFrame =_
       →taxonomy_resolution(taxonomy_file=taxonomy_7)
[13]: taxonomy_resolution_4.head()
[13]:
         phylum_taxa_name phylum_taxa_count
                                                  class_taxa_name class_taxa_count \
           Proteobacteria
                                      565024 Gammaproteobacteria
                                                                              507067
      1 Actinobacteriota
                                      264466
                                                                              262184
                                                   Actinobacteria
               Firmicutes
                                      229209
                                                          Bacilli
                                                                              228404
      3
             Bacteroidota
                                       32879 Alphaproteobacteria
                                                                               57906
      4
             Firmicutes_A
                                       28999
                                                      Bacteroidia
                                                                               30909
```

```
Enterobacterales
                                       202288
                                              Enterobacteriaceae
                                                                                170657
      1
          Mycobacteriales
                                       180105
                                                 Mycobacteriaceae
                                                                                164511
      2
          Pseudomonadales
                                       170045
                                                                                124741
                                                 Pseudomonadaceae
      3
          Burkholderiales
                                       100727
                                                 Burkholderiaceae
                                                                                90287
          Lactobacillales
                                        94986
                                                                                 75486
                                                 Streptococcaceae
                                                      species_taxa_name
        genus_taxa_name
                          genus_taxa_count
          Mycobacterium
      0
      1
            Pseudomonas
                                     75072
                                             Mycobacterium tuberculosis
      2
       Staphylococcus
                                     74118
                                                 Pseudomonas aeruginosa
      3
          Streptococcus
                                     74113
                                                  Staphylococcus aureus
      4
            Escherichia
                                     68537
                                               Streptococcus pneumoniae
         species_taxa_count
      0
                      115269
      1
                       93107
      2
                       74268
      3
                       63582
                       50516
[14]:
     taxonomy_resolution_5.head()
[14]:
         phylum_taxa_name phylum_taxa_count
                                                    class_taxa_name
                                                                      class_taxa_count \
      0
           Proteobacteria
                                        521947
                                                Gammaproteobacteria
                                                                                 474642
      1
        Actinobacteriota
                                        256165
                                                     Actinobacteria
                                                                                 255633
      2
               Firmicutes
                                        224467
                                                            Bacilli
                                                                                 224467
      3
             Bacteroidota
                                                                                  47278
                                         13018
                                                Alphaproteobacteria
      4
             Firmicutes_A
                                         11780
                                                        Bacteroidia
                                                                                  12755
                            order_taxa_count
                                                                    family_taxa_count \
          order_taxa_name
                                                 family_taxa_name
         Enterobacterales
                                       196062
                                               Enterobacteriaceae
                                                                                165898
          Mycobacteriales
                                       179848
                                                                                164260
      1
                                                 Mycobacteriaceae
      2
          Pseudomonadales
                                       158378
                                                 Pseudomonadaceae
                                                                                118544
      3
          Burkholderiales
                                       99779
                                                 Burkholderiaceae
                                                                                84793
          Lactobacillales
                                       93623
                                                 Streptococcaceae
                                                                                74771
                                                      species_taxa_name
        genus_taxa_name
                          genus_taxa_count
      0
          Mycobacterium
                                    104666
                                             Mycobacterium tuberculosis
      1
            Pseudomonas
                                     74864
                                                 Pseudomonas aeruginosa
      2 Staphylococcus
                                     73841
                                                  Staphylococcus aureus
      3
          Streptococcus
                                     73532
      4
            Escherichia
                                     67960
                                               Streptococcus pneumoniae
         species_taxa_count
      0
                       93094
```

order\_taxa\_name

order\_taxa\_count

family\_taxa\_count

family\_taxa\_name

```
1
                       74092
      2
                       63573
      3
                       52225
      4
                       50516
[15]:
      taxonomy_resolution_6.head()
[15]:
         phylum_taxa_name
                            phylum_taxa_count
                                                    class_taxa_name
                                                                      class_taxa_count
      0
           Proteobacteria
                                        521947
                                                Gammaproteobacteria
                                                                                 474642
      1
        Actinobacteriota
                                        256165
                                                     Actinobacteria
                                                                                 255633
      2
               Firmicutes
                                        224467
                                                             Bacilli
                                                                                 224467
      3
             Bacteroidota
                                                Alphaproteobacteria
                                         13018
                                                                                  47278
      4
             Firmicutes_A
                                         11780
                                                        Bacteroidia
                                                                                  12755
          order_taxa_name
                            order_taxa_count
                                                 family_taxa_name
                                                                    family_taxa_count
        Enterobacterales
                                       196062
                                               Enterobacteriaceae
                                                                                165898
      0
                                       179848
      1
          Mycobacteriales
                                                 Mycobacteriaceae
                                                                                164260
      2
          Pseudomonadales
                                       158378
                                                 Pseudomonadaceae
                                                                                118544
      3
          Burkholderiales
                                        99779
                                                 Burkholderiaceae
                                                                                 84793
          Lactobacillales
                                        93623
                                                 Streptococcaceae
                                                                                 74771
        genus_taxa_name
                          genus_taxa_count
                                                      species_taxa_name
                                             Mycobacterium tuberculosis
      0
          Mycobacterium
                                    104666
      1
                                     74864
                                                 Pseudomonas aeruginosa
            Pseudomonas
        Staphylococcus
                                     73841
                                                  Staphylococcus aureus
      3
          Streptococcus
                                     73532
      4
            Escherichia
                                     67960
                                               Streptococcus pneumoniae
         species_taxa_count
      0
                       93094
      1
                       74092
      2
                       63573
      3
                       52225
      4
                       50516
     taxonomy_resolution_7.head()
[16]:
         phylum_taxa_name
                            phylum_taxa_count
                                                    class_taxa_name
                                                                      class_taxa_count
      0
           Proteobacteria
                                        521947
                                                Gammaproteobacteria
                                                                                 474642
      1
         Actinobacteriota
                                        256165
                                                     Actinobacteria
                                                                                 255633
      2
               Firmicutes
                                        224467
                                                             Bacilli
                                                                                 224467
      3
             Bacteroidota
                                         13018
                                                Alphaproteobacteria
                                                                                  47278
             Firmicutes_A
                                         11780
                                                        Bacteroidia
                                                                                  12755
                            order taxa count
                                                 family_taxa_name family_taxa_count
          order taxa name
         Enterobacterales
                                       196062
                                               Enterobacteriaceae
                                                                                165898
          Mycobacteriales
                                       179848
                                                 Mycobacteriaceae
                                                                                164260
```

2	Pseudomonadale	s 15837	8 Pseudomonadaceae		118544
3	Burkholderiale	s 9977	9 Burkholderiaceae		84793
4	Lactobacillale	s 9362	3 Streptococcaceae		74771
	genus_taxa_name	genus_taxa_count	species_taxa_name	\	
0	Mycobacterium	104666	Mycobacterium tuberculosis		
1	Pseudomonas	74864	Pseudomonas aeruginosa		
2	Staphylococcus	73841	Staphylococcus aureus		
3	Streptococcus	73532			
4	Escherichia	67960	Streptococcus pneumoniae		
	species_taxa_co	unt			
0	93	094			
1	74	092			
2	63	573			
3	52	225			
4	50	516			

As it can be seen in the above outputs when dealing with MAG's it is likely to get low taxonomic resolution resolution.

The first dataset has RefSeq + MAG datasets, others have just RefSeq sequences. This influences the taxonomic resolution.

In species level resolution merged dataset has 115,269.00 missing information in the other dataset it is just 52,225.00.

```
[17]: def get_unique_gcf_count(taxonomy_file: pd.DataFrame, gcfs: pd.DataFrame) -> pd.
       →DataFrame:
          n n n
          Calculates the unique GCF count for each genus in the taxonomy file and \Box
       ⇔returns a sorted DataFrame.
          Args:
               taxonomy\_file (pd.DataFrame): DataFrame containing taxonomy information\Box
       ⇔with genus names at index 5.
               qcfs (pd.DataFrame): DataFrame containing GCF IDs in a column named _{\sqcup}
       \hookrightarrow "gcf_id".
          Returns:
              pd.DataFrame: Sorted DataFrame with columns:
                   - Genus_Taxonomy: Genus names
                   - gcf_count_unique: Number of unique GCF IDs per genus
                   - gcf_index: List of unique GCF IDs
                   - gcf_count: Corresponding counts of unique GCF IDs
          # Extract unique genus names
```

```
genus_resolution = taxonomy_file.iloc[:, 5].value_counts().index
          # Create a results DataFrame
          results_df = pd.DataFrame(
              index=genus_resolution,
              columns=["gcf_count_unique", "gcf_index", "gcf_count"],
          )
          # Iterate through each genus and fill DataFrame
          for genus in genus_resolution:
              genus_gcfs = gcfs.loc[taxonomy_file[taxonomy_file[5] == genus].index,__

y"gcf_id"]

              unique_gcfs, counts = np.unique(genus_gcfs, return_counts=True)
              results_df.loc[genus] = [len(unique_gcfs), list(unique_gcfs),_u
       ⇔list(counts)]
          # Save results to descriptively named CSV files
          results_df.to_csv(
              f"reproducibility_results_{taxonomy_file.name}.csv",
              index_label="Genus_Taxonomy",
          # Sort by unique GCF count in descending order
          results_df = results_df.sort_values("gcf_count_unique", ascending=False)
          results_df.to_csv(
              f"reproducibility results {taxonomy file.name} sorted.csv",
              index_label="Genus_Taxonomy",
          )
          return results_df
[18]: # Calculate unique GCF counts for each BiG-SLiCE threshold (4-7)
      taxonomy_4 results: pd.DataFrame = get_unique_gcf_count(taxonomy_file = __
       staxonomy_4, gcfs = thresholds_4_gcfs)
      taxonomy_5_results: pd.DataFrame = get_unique_gcf_count(taxonomy_file = __
       staxonomy_5, gcfs = thresholds_5_gcfs)
```

```
taxonomy_6_results: pd.DataFrame = get_unique_gcf_count(taxonomy_file = u
 staxonomy_6, gcfs = thresholds_6_gcfs)
taxonomy_7_results: pd.DataFrame = get_unique_gcf_count(taxonomy_file = __
 →taxonomy_7, gcfs = thresholds_7_gcfs)
```

```
[19]: print(taxonomy 4 results.head())
```

```
5
                                 10820
     Streptomyces
                                  8703
     Pseudomonas E
                                  1517
     Nocardia
                                  1421
     Micromonospora
                                  1089
                                                                gcf_index \
     5
                      [0, 1, 3, 7, 21, 24, 29, 30, 35, 37, 39, 40, 4...
                      [0, 7, 30, 41, 42, 44, 45, 46, 50, 53, 56, 57,...
     Streptomyces
                      [0, 5, 41, 44, 46, 49, 59, 79, 86, 153, 154, 1...
     Pseudomonas_E
     Nocardia
                      [0, 28, 46, 50, 76, 118, 837, 855, 883, 1061, ...
                      [0, 30, 46, 67, 75, 164, 172, 1012, 1041, 1209...
     Micromonospora
                                                                gcf_count
     5
                      [1254, 3, 2, 5, 1, 8, 29, 16, 21, 17, 4, 2, 20...
     Streptomyces
                      [186, 1, 21, 1, 4, 6, 1, 72, 10, 4, 1, 4, 1, 1...
     Pseudomonas E
                      [36, 1, 122, 3, 1, 1, 1, 10, 1, 1, 7, 1, 41, 4...
                      [25, 1, 12, 1, 1, 4, 1, 1, 2, 12, 1, 2, 1, 1, ...
     Nocardia
     Micromonospora
                      [10, 1, 4, 1, 1, 1, 1, 2, 7, 1, 1, 3, 2, 2, 1, ...]
[20]: print(taxonomy_5_results.head())
                    gcf_count_unique
     Streptomyces
                                 6798
                                 3971
     Nocardia
                                 1146
     Pseudomonas_E
                                 1101
                                  859
     Amycolatopsis
                                                               gcf_index \
     5
     Streptomyces
                     [20, 24, 25, 31, 35, 36, 38, 44, 49, 51, 60, 6...
                     [0, 7, 23, 24, 25, 28, 29, 31, 33, 34, 35, 36,...
     Nocardia
                     [22, 53, 60, 69, 106, 121, 249, 298, 561, 584,...
     Pseudomonas E
                     [24, 36, 38, 40, 47, 65, 68, 96, 106, 115, 121...
     Amycolatopsis
                     [38, 60, 77, 96, 121, 298, 411, 478, 517, 529,...
                                                               gcf_count
     Streptomyces
                     [1, 34, 4, 1, 6, 1, 7, 1, 3, 22, 1, 1, 7, 5, 5...]
                     [1, 1, 9, 14, 1, 2, 1, 24, 4, 2, 1, 46, 12, 2,...
     Nocardia
                     [1, 2, 1, 1, 2, 13, 1, 4, 8, 2, 13, 1, 2, 1, 1...
     Pseudomonas_E
                     [12, 114, 18, 1, 1, 10, 1, 6, 40, 10, 1, 2, 1,...
```

gcf\_count\_unique \

```
Amycolatopsis [1, 1, 2, 2, 3, 1, 1, 1, 2, 10, 6, 1, 10, 1, 3...
```

[21]: print(taxonomy\_6\_results.head())

### gcf\_count\_unique Streptomyces 5136 3110 Nocardia 890 Pseudomonas E 881 Amycolatopsis 700 gcf\_index \ Streptomyces [2, 3, 23, 25, 28, 30, 32, 34, 35, 36, 38, 43,... [0, 3, 4, 8, 10, 23, 25, 26, 27, 28, 30, 31, 3... Nocardia [3, 32, 40, 50, 162, 216, 323, 361, 362, 368, ... Pseudomonas\_E [28, 30, 31, 32, 35, 47, 62, 70, 78, 110, 130,... [25, 30, 32, 55, 62, 216, 263, 309, 341, 354, ... Amycolatopsis gcf\_count Streptomyces [9, 5, 1, 31, 14, 108, 93, 2, 4, 7, 28, 5, 1, ... [1, 1, 12, 1, 6, 8, 43, 4, 10, 82, 47, 20, 20,... Nocardia [1, 14, 2, 1, 10, 3, 2, 1, 1, 2, 1, 1, 12, 1, ... Pseudomonas\_E [227, 89, 3, 3, 40, 10, 23, 11, 4, 1, 5, 310, ... Amycolatopsis [10, 2, 5, 2, 2, 2, 12, 1, 5, 1, 2, 3, 1, 1, 1... [22]: print(taxonomy\_7\_results.head()) gcf\_count\_unique \ Streptomyces 3363 2253 Pseudomonas E 694 Nocardia 669 Amycolatopsis 487 gcf index \ Streptomyces [1, 2, 3, 6, 7, 10, 16, 20, 21, 23, 27, 30, 37... [0, 1, 2, 3, 4, 6, 7, 8, 9, 10, 14, 15, 16, 17... Pseudomonas\_E [1, 4, 7, 8, 10, 14, 16, 27, 31, 36, 42, 49, 5... Nocardia [1, 3, 10, 37, 46, 50, 59, 90, 98, 102, 104, 1... Amycolatopsis [1, 6, 7, 10, 46, 59, 66, 80, 98, 121, 124, 12... gcf\_count Streptomyces [166, 1, 5, 37, 125, 30, 7, 7, 1, 576, 9, 2, 9...

```
[1, 46, 12, 1, 17, 44, 54, 11, 4, 153, 31, 5, ... Pseudomonas_E [2, 1, 89, 1, 642, 11, 40, 3, 10, 55, 1, 11, 8... Nocardia [18, 1, 2, 1, 1, 1, 6, 11, 1, 3, 1, 3, 3, 1, 1... Amycolatopsis [6, 14, 3, 1, 4, 2, 1, 14, 6, 1, 1, 9, 65, 1, ...
```

### 2 END OF ADDITIONAL EFFORTS

```
[23]: # thresholds 4_qcfs: np.ndarray = np.array(STable2.qcf_id.unique())
      # thresholds 5_qcfs: np.ndarray = np.array(STable3.qcf_id.unique())
      # thresholds_6_qcfs: np.ndarray = np.array(STable4.qcf_id.unique())
      # thresholds 7 qcfs: np.ndarray = np.array(STable5.qcf_id.unique())
      # bqc_ids: DataFrame = STable1.bqc_ids.str.split(",", expand=True)
      # bgc_ids = (bgc_ids.apply(pd.to_numeric, downcast="unsigned"))
      # bqc ids[["dataset name", "AccNo", "taxonomy"]] = STable1[["dataset name", "
       → "AccNo", "taxonomy"]]
      # STable2["bgc_id"] = STable2["bgc_id"].astype(np.int64)
      # STable2.index = STable2["bqc_id"]
      # STable2["taxonomy"] = ""
      # from pandarallel import pandarallel
      # import os
      # pandarallel.initialize(nb_workers=os.cpu_count())
      # def add taxonomy to table(qcfs_array: np.ndarray, stable: DataFrame) -> None:
            # print(type(qcfs_array))
      #
            # print(qcfs array[5])
            for gcf in gcfs_array:
      #
                # print(f"gcf{gcf}\n")
                bgc_ids_of_gcf: np.ndarray = np.array(STable2[STable2.gcf_id ==_
       \hookrightarrow gcf]["bgc_id"])
                for bgc_id in bgc_ids_of_gcf:
      #
                     # print(f"bqc_id{bqc_id}\n")
      #
      #
                     # print(f"type(bqc_id{type(bqc_id)}\n")
                    bqc_tax = bqc_ids[bqc_ids.eq(bqc_id).
       \Rightarrow any (axis="columns")]["taxonomy"].iloc[0]
                     stable.loc[bqc id, "taxonomy"] = bqc tax
      #add_taxonomy_to_table = np.vectorize(add_taxonomy_to_table)
      #add taxonomy to table(qcfs array = thresholds 4 qcfs[-10:], stable = STable2)
```