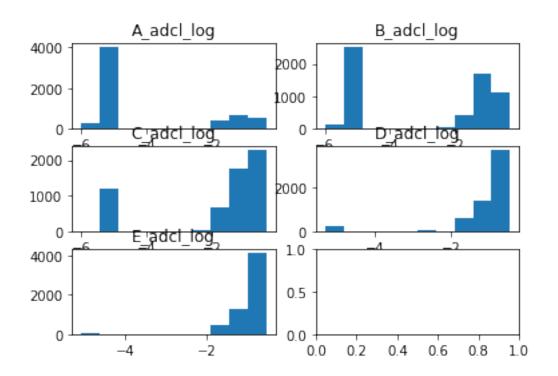
## all\_data

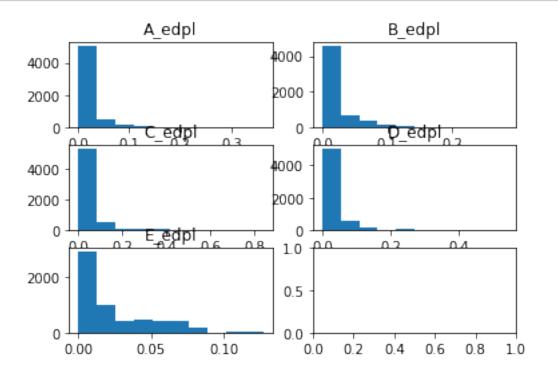
#### February 26, 2020

```
[1]: import os
   from IPython.display import display, Image
   import pandas as pd
   import numpy as np
   import seaborn as sns
   %matplotlib inline
   import matplotlib.pyplot as plt
   from matplotlib import colors
   from matplotlib.ticker import PercentFormatter
   from scipy.stats import linregress
   import math
   from functools import reduce
   import matplotlib
   import argparse
   from Bio import SeqIO, Entrez, pairwise2
   Entrez.email = 'hongyingsun1101@gmail.com'
   from Bio.SeqRecord import SeqRecord
   import re, time
   import os, sys, glob
   import random
   import uuid
   # from skbio.tree import TreeNode
   # from skbio import read
   # from skbio.stats.distance import DistanceMatrix
   # from skbio.stats.distance import DissimilarityMatrix
   from scipy import stats
   from ast import literal_eval
   import sqlite3
   # roc curve and auc score
   from sklearn.datasets import make_classification
   from sklearn.neighbors import KNeighborsClassifier
   from sklearn.ensemble import RandomForestClassifier
   from sklearn.model_selection import train_test_split
   from sklearn.metrics import roc_curve
   from sklearn.metrics import roc_auc_score
   import warnings
```

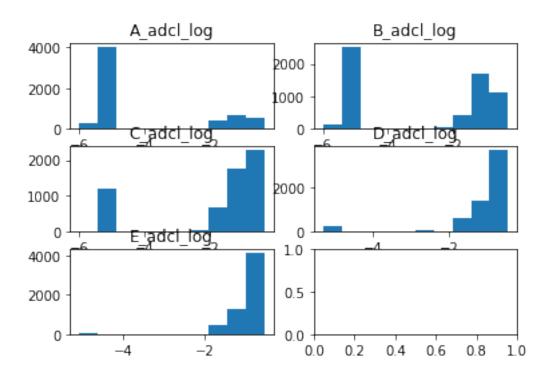
```
warnings.filterwarnings("ignore")
 [2]: df = pd.read_csv("all_data.csv", index_col=0)
     score= pd.read_csv("score_merged.csv", index_col=0)
 [3]: reference ={'A':"RDP_10398", 'B':'RDP_5224', 'C':"RDP_1017", 'D':'RDP_92', 'E':
      → 'RDP 12'}
 [4]: \#pplacer\_ref\_list = ['A', 'B', 'C', \sqcup]
      \hookrightarrow 'D', 'E'], pplacer\_stats\_list=['\_adcl\_log', '\_edpl', \sqcup]
      →'_prichness'],community_list=['0','1','2','3','4'],cutoff_list=['mean','min','25%','50%','7
 [5]: def is_float(string):
       try:
         return float(string) and '.' in string # True if string is a number_
      \rightarrow contains a dot
       except ValueError: # String is not a number
         return False
 [6]: reference
 [6]: {'A': 'RDP_10398',
      'B': 'RDP_5224',
      'C': 'RDP_1017',
      'D': 'RDP_92',
      'E': 'RDP 12'}
 [7]: columnList=list(df.columns)
 [8]: communityList = df.community
[9]: # df.describe()
[10]: def plot_pplacer(variable):
         fig, axes = plt.subplots(nrows=3, ncols=2)
         ax0, ax1, ax2, ax3, ax4, ax5 = axes.flatten()
         ax0.hist(df['A'+variable])
         ax0.set_title('A'+variable)
         ax1.hist(df['B'+variable])
         ax1.set_title('B'+variable)
         ax2.hist(df['C'+variable])
         ax2.set_title('C'+variable)
         ax3.hist(df['D'+variable])
         ax3.set_title('D'+variable)
         ax4.hist(df['E'+variable])
         ax4.set_title('E'+variable)
[11]: plot_pplacer('_adcl_log')
```



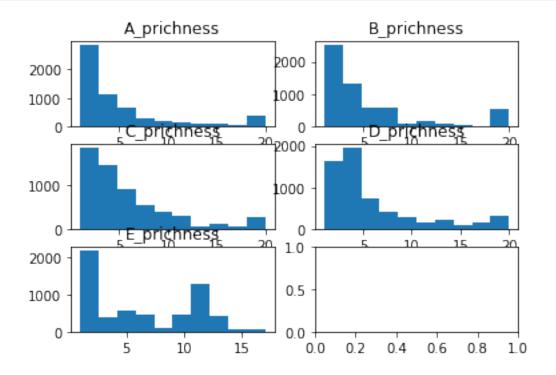
### [12]: plot\_pplacer('\_edpl')



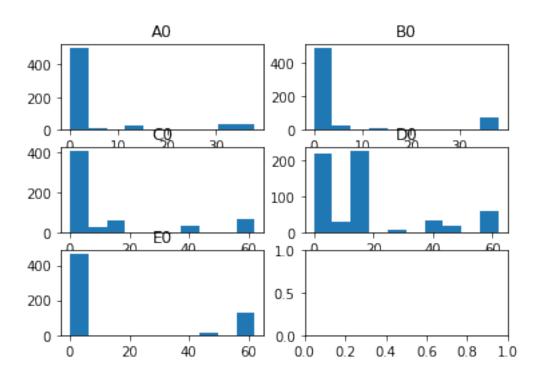
[13]: plot\_pplacer('\_adcl\_log')



### [14]: plot\_pplacer('\_prichness')



[15]: plot\_pplacer('0');



```
[16]: def plotScatter(reference,community):
    fig, axes = plt.subplots(nrows=2, ncols=2)
    ax0, ax1, ax2, ax3 = axes.flatten()

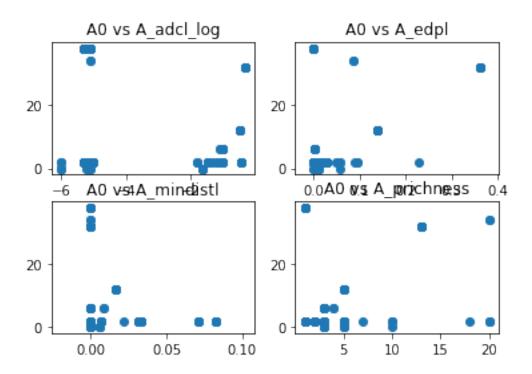
ax0.scatter(df[reference+'_adcl_log'], df[reference+community])
    ax0.set_title(reference+community+' vs '+ reference + '_adcl_log')

ax1.scatter(df[reference+'_edpl'], df[reference+community])
    ax1.set_title(reference+community+' vs '+ reference + '_edpl')

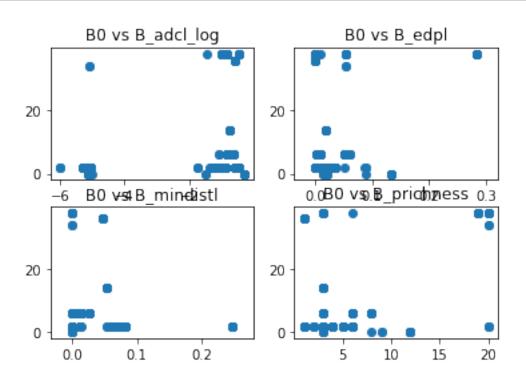
ax2.scatter(df[reference+'_mindistl'], df[reference+community])
    ax2.set_title(reference+community+' vs '+ reference + '_mindistl')

ax3.scatter(df[reference+'_prichness'], df[reference+community])
    ax3.set_title(reference+community+' vs '+ reference + '_prichness')

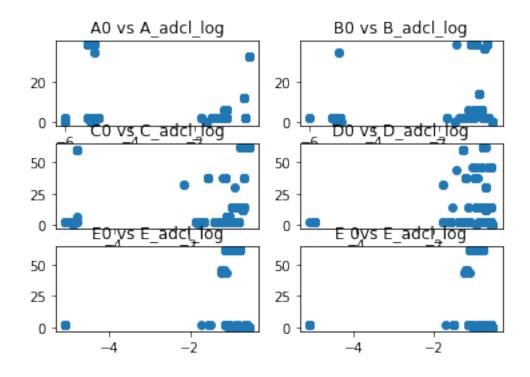
[17]: plotScatter('A','0')
```



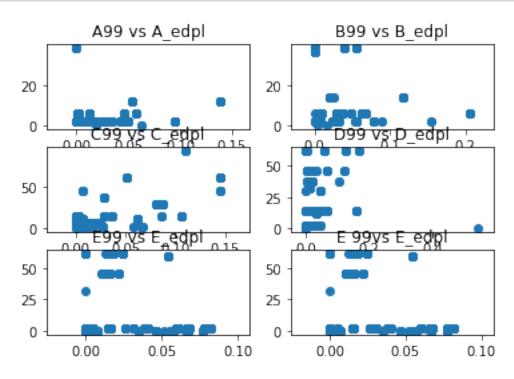
#### [18]: plotScatter('B','0')



```
[19]: def plotScatterRef(variable, community):
         fig, axes = plt.subplots(nrows=3, ncols=2)
         ax0, ax1, ax2, ax3, ax4, ax5 = axes.flatten()
         ax0.scatter(df['A'+variable], df['A'+community])
         ax0.set_title('A' + community +' vs A' + variable)
         ax1.scatter(df['B'+variable], df['B'+community])
         ax1.set_title('B' + community +' vs B' + variable)
         ax2.scatter(df['C'+variable], df['C'+community])
         ax2.set_title('C' + community +' vs C' + variable)
         ax3.scatter(df['D'+variable], df['D'+community])
         ax3.set_title('D' + community +' vs D' + variable)
         ax4.scatter(df['E'+variable], df['E'+community])
         ax4.set_title('E' + community +' vs E' + variable)
         ax5.scatter(df['E'+variable], df['E'+community])
         ax5.set_title('E' + community +'vs E' + variable)
    plotScatterRef('_adcl_log','0');
```



```
[20]:
plotScatterRef('_edpl','99');
```



```
[21]: cols=df.columns.tolist()
      # cols[:20]
[164]: def plot_roc_curve(fpr, tpr):
          plt.plot(fpr, tpr, color='orange', label='ROC')
          plt.plot([0, 1], [0, 1], color='darkblue', linestyle='--')
          plt.xlabel('False Positive Rate')
          plt.ylabel('True Positive Rate')
          plt.title('Receiver Operating Characteristic (ROC) Curve')
          plt.legend()
          plt.show()
[169]: def plot_roc(data_X, class_label):
          trainX, testX, trainy, testy = train_test_split(data_X, class_label,_
       →test_size=0.3, random_state=1)
          model = RandomForestClassifier()
          model.fit(trainX, trainy)
          probs = model.predict_proba(testX)
          probs = probs[:, 1]
          auc = roc_auc_score(testy, probs)
          fpr, tpr, thresholds = roc_curve(testy, probs)
          optimal_idx = np.argmax(tpr - fpr)
```

```
optimal_threshold = thresholds[optimal_idx]
          print('optimal_threshold: %.2f' % optimal_threshold)
          print('AUC: %.2f' % auc)
          print( thresholds)
           print( thresholds)
      #
           print('Model: ')
            print(model)
          plot_roc_curve(fpr, tpr)
[170]: def makeTable(headerRow,columnizedData,columnSpacing=2):
          """Creates a technical paper style, left justified table"""
          from numpy import array,max,vectorize
          cols = array(columnizedData,dtype=str)
          colSizes = [max(vectorize(len)(col)) for col in cols]
          header = ''
          rows = ['' for i in cols[0]]
          for i in range(0,len(headerRow)):
              if len(headerRow[i]) > colSizes[i]: colSizes[i]=len(headerRow[i])
              headerRow[i]+=' '*(colSizes[i]-len(headerRow[i]))
              header+=headerRow[i]
              if not i == len(headerRow)-1: header+=' '*columnSpacing
              for j in range(0,len(cols[i])):
                  if len(cols[i][j]) < colSizes[i]:</pre>
                      cols[i][j]+=' '*(colSizes[i]-len(cols[i][j])+columnSpacing)
                  rows[j]+=cols[i][j]
                  if not i == len(headerRow)-1: rows[j]+=' '*columnSpacing
          line = '-'*len(header)
          print(line)
          print(header)
          print(line)
          for row in rows: print(row)
          print(line)
      header = ['AUROC','Categoroy']
      cutoffs = ['0.9-1.0', '0.8-0.9', '0.7-0.8', '0.6-0.7', '0.5-0.6']
      evalualtion = ['Very good', 'Good', 'Fair', 'Poor', 'Fail']
      makeTable(header,[cutoffs,evalualtion])
```

```
AUROC Categoroy
-----
0.9-1.0 Very good
0.8-0.9 Good
0.7-0.8 Fair
```

```
0.6-0.7 Poor
0.5-0.6 Fail
```

```
[171]: def plot_roc_microbiome(data_X, class_label, x, y, data_test=False):
          if(not data_test):
                print("data_set is False")
              trainX, testX, trainy, testy = train_test_split(data_X, class_label,_
       →test_size=0.3, random_state=1)
              model = RandomForestClassifier()
              model.fit(trainX, trainy)
              probs = model.predict_proba(testX)
              probs = probs[:, 1]
              auc = roc_auc_score(testy, probs)
              fpr, tpr, thresholds = roc_curve(testy, probs)
              optimal_idx = np.argmax(tpr - fpr)
              optimal_threshold = thresholds[optimal_idx]
              print('optimal_threshold: %.2f' % optimal_threshold)
              print('AUC: %.2f' % auc)
              print('thresholds: ' + thresholds)
              plot_roc_curve(fpr, tpr)
          else:
              print("data set is True")
              trainX, testX, trainy, testy = train_test_split(data_X, class_label,_
       →test_size=0.3, random_state=1)
              model = RandomForestClassifier()
              model.fit(trainX, trainy)
              probs1 = model.predict_proba(testX)
              probs1 = probs1[:, 1]
              auc1 = roc_auc_score(testy, probs1)
              fpr1, tpr1, thresholds1 = roc_curve(testy, probs1)
              optimal_idx1 = np.argmax(tpr1 - fpr1)
              optimal_threshold1 = thresholds1[optimal_idx1]
              print('AUC1: %.2f' % auc1)
              print('optimal_threshold1: %.2f' % optimal_threshold1)
              print(thresholds1)
              plot_roc_curve(fpr1, tpr1)
              probs2 = model.predict_proba(x)
              probs2 = probs2[:, 1]
              auc2 = roc_auc_score(y, probs2)
              fpr2, tpr2, thresholds2 = roc_curve(y, probs2)
              optimal_idx2 = np.argmax(tpr2 - fpr2)
              optimal_threshold2 = thresholds2[optimal_idx2]
              print('AUC2: %.2f' % auc2)
```

```
print('optimal_threshold2: %.2f' % optimal_threshold2)
              print( thresholds2)
              plot_roc_curve(fpr2, tpr2)
[172]: def plot_roc_curve_microbiome(pplacer_ref_list, pplacer_stats_list,__
       →community_list, cutoff_list, scoreOption=True):
          for (refIndex,pplacer ref) in enumerate(pplacer ref list):
            for refIndex in range(len(pplacer_ref_list)):
      #
                pplacer_ref = pplacer_ref_list[refIndex]
              for (statsIndex,pplacer_stats) in enumerate(pplacer_stats_list):
                for statsIndex in range(len(pplacer_stats_list)):
                    pplacer_stats = pplacer_stats_list[statsIndex]
                  for (communityIndex,community) in enumerate(community_list):
                    for communityIndex in range(len(community_list)):
                        community = community_list[communityIndex]
                      for (i, cutoff) in enumerate(cutoff_list):
                        for i in range(len(cutoff_list)):
                             cutoff=cutoff_list[i]
                          if(is_float(cutoff)):
                              cutoff_binary=float(cutoff)
                          else:
                              if(scoreOption):
                                   cutoff_binary=float(df[pplacer_ref+community].
       →describe().loc[[cutoff]])
                              else:
                                   cutoff_binary = float(df[pplacer_ref+pplacer_stats].
       →describe().loc[[cutoff]])
                          if(scoreOption):
                              mask = df[pplacer_ref+community] <= cutoff_binary</pre>
                              df.loc[mask, pplacer_ref+community+'_binary'] = 1
                              mask = df[pplacer_ref+community] >cutoff_binary
                              df.loc[mask, pplacer_ref+community+'_binary'] = 0
                              df_binary = df[[pplacer_ref+pplacer_stats,__
       →pplacer_ref+community+'_binary']].dropna()
                              data_stats = df_binary[pplacer_ref+pplacer_stats].
       \rightarrowto_numpy().reshape(-1,1)
                              binary_label = _

→df_binary[pplacer_ref+community+'_binary'].to_numpy()

                              print(' The score cutoff '+ cutoff +' for Reference ' +
       →pplacer_ref +' community ' + community + ' with pplacer_stats '+□
       →pplacer_stats[1:] + ': %.2f' % cutoff_binary )
                              plot_roc(data_stats,binary_label)
                          else:
                              mask = df[pplacer_ref+pplacer_stats] <= cutoff_binary</pre>
                              df.loc[mask, pplacer_ref+pplacer_stats+'_binary'] = 1
                              mask = df[pplacer_ref+pplacer_stats] >cutoff_binary
```

1 different reference same pplacer stats same community to test different cutoffs and different references for score

```
[173]: # plot_roc_curve_microbiome(pplacer_ref_list =_
       \rightarrow ['A', 'B', 'C', 'D', 'E'], pplacer\_stats\_list=['\_adcl\_log'], community\_list=['A'], cutoff\_list=['mm]
       → 'min', '25%', '50%', '75%'], scoreOption=False)
[174]: df['E0'].describe()
[174]: count
                605.000000
      mean
                 14.601653
      std
                 25.354082
      min
                 0.000000
      25%
                  0.000000
      50%
                  2.000000
      75%
                  2.000000
                 62.000000
      max
      Name: EO, dtype: float64
```

- 2 Different reference same pplacer stats same community to test different cutoffs and different references for adcl\_log
- 3 Fitting on large reference and test on small reference datasets

```
[175]: def plot_roc_curve_microbiome_test2(pplacer_ref_list, pplacer_stats_list, u → community_list, cutoff_list, test_data_list, scoreOption=True, u → testOption=False):

for refIndex in range(len(pplacer_ref_list)):

    pplacer_ref = pplacer_ref_list[refIndex]

    for statsIndex in range(len(pplacer_stats_list)):

        pplacer_stats = pplacer_stats_list[statsIndex]
```

```
for communityIndex in range(len(community_list)):
               community = community_list[communityIndex]
               for i in range(len(cutoff_list)):
                   cutoff=cutoff_list[i]
                   if(is_float(cutoff)):
                       cutoff_binary=float(cutoff)
                   else:
                       if(scoreOption):
                            cutoff binary=float(df[pplacer ref+community].
→describe().loc[[cutoff]])
                       else:
                           cutoff_binary = float(df[pplacer_ref+pplacer_stats].
→describe().loc[[cutoff]])
                   # no test situation, which is the default option
                   if (not testOption):
                       if(scoreOption):
                            mask = df[pplacer_ref+community] <= cutoff_binary</pre>
                           df.loc[mask, pplacer_ref+community+'_binary'] = 1
                           mask = df[pplacer_ref+community] >cutoff_binary
                           df.loc[mask, pplacer_ref+community+'_binary'] = 0
                           df_binary = df[[pplacer_ref+pplacer_stats,__
→pplacer_ref+community+'_binary']].dropna()
                           data_stats = df_binary[pplacer_ref+pplacer_stats].
\rightarrowto_numpy().reshape(-1,1)
                           binary_label = _

→df_binary[pplacer_ref+community+'_binary'].to_numpy()

                           print(' The score cutoff '+ cutoff +' for Reference⊔
→' + pplacer_ref +' community ' + community + ' with pplacer_stats '+⊔
→pplacer_stats[1:] + ': %.2f' % cutoff_binary )
                            # plot_roc(data_stats,binary_label)
⇒plot_roc_microbiome(data_stats,binary_label,x=None,y=None,data_test=False)
                       else:
                           mask = df[pplacer ref+pplacer stats] <= ___</pre>
df.loc[mask, pplacer_ref+pplacer_stats+'_binary'] =__
\hookrightarrow 1
                           mask = df[pplacer_ref+pplacer_stats] >cutoff_binary
                           df.loc[mask, pplacer_ref+pplacer_stats+'_binary'] =__
→0
                           df_binary = df[[pplacer_ref+community,__
→pplacer_ref+pplacer_stats+'_binary']].dropna()
                           data stats = df binary[pplacer ref+community].
\rightarrowto_numpy().reshape(-1,1)
```

```
binary_label = _
→df_binary[pplacer_ref+pplacer_stats+'_binary'].to_numpy()
                           print(' The pplacer_stats_cutoff '+ cutoff +' for_
→Reference ' + pplacer_ref +' community ' + community + ' pplacer_stats ' +⊔
→pplacer_stats[1:] + ': %.2f' % cutoff_binary )
                           # plot roc(data stats, binary label)
→plot_roc_microbiome(data_stats,binary_label,x=None,y=None,data_test=False)
                   # if there is test
                   else:
                       for j in range(len(test_data_list)):
                           test=test_data_list[j]
                           if(scoreOption):
                               mask = df[pplacer_ref+community] <= __</pre>
df.loc[mask, pplacer_ref+community+'_binary'] =__
→1
                               mask = df[pplacer_ref+community] >cutoff_binary
                               df.loc[mask, pplacer_ref+community+'_binary'] =
⇔0
                               df_binary = df[[pplacer_ref+pplacer_stats,__
→pplacer_ref+community+'_binary']].dropna()
                               data_stats =

→df_binary[pplacer_ref+pplacer_stats].to_numpy().reshape(-1,1)

                               binary_label = _

→df_binary[pplacer_ref+community+'_binary'].to_numpy()

                               mask_test = df[test+community] <= cutoff_binary</pre>
                               df.loc[mask_test, test+community+'_binary'] = 1
                               mask_test = df[test+community] >cutoff_binary
                               df.loc[mask_test, test+community+'_binary'] = 0
                               df_binary = df[[test+pplacer_stats,__
→test+community+'_binary']].dropna()
                               x = df binary[test+pplacer stats].to numpy().
\rightarrowreshape(-1,1)
                               y = df_binary[test+community+'_binary'].
→to_numpy()
                               print(' The score cutoff '+ cutoff +' for⊔
→Reference ' + pplacer_ref +' community ' + community + ' with_
→pplacer_stats '+ pplacer_stats[1:] + ' compared with test ' + test +': %.2f'
→% cutoff_binary )
→plot_roc_microbiome(data_stats,binary_label,x,y,data_test=True)
```

```
mask = df[pplacer_ref+pplacer_stats] <= __</pre>
df.loc[mask,
→pplacer_ref+pplacer_stats+'_binary'] = 1
                               mask = df[pplacer_ref+pplacer_stats]__
→>cutoff_binary
                               df.loc[mask,__
→pplacer_ref+pplacer_stats+'_binary'] = 0
                               df_binary = df[[pplacer_ref+community,__
→pplacer_ref+pplacer_stats+'_binary']].dropna()
                               data_stats = df_binary[pplacer_ref+community].
\rightarrowto_numpy().reshape(-1,1)
                               binary_label = _

→df_binary[pplacer_ref+pplacer_stats+'_binary'].to_numpy()
                               mask_test = df[test+pplacer_stats] <= __</pre>
→cutoff_binary
                               df.loc[mask_test, test+pplacer_stats+'_binary']__
→= 1
                               mask_test = df[test+pplacer_stats]__
→>cutoff binary
                               df.loc[mask_test, test+pplacer_stats+'_binary']__
→= 0
                               df_binary = df[[test+community,__
→test+pplacer_stats+'_binary']].dropna()
                               x = df_binary[test+community].to_numpy().
\rightarrowreshape(-1,1)
                               y = df_binary[test+pplacer_stats+'_binary'].
→to_numpy()
                               print(' The pplacer_stats_cutoff '+ cutoff +'__
→for Reference ' + pplacer_ref +' community ' + community + ' pplacer_stats '⊔
→ + pplacer_stats[1:] + ' compared with test ' + test + ': %.2f' % ∪
→cutoff_binary )
→plot_roc_microbiome(data_stats,binary_label,x,y,data_test=True)
```

# 3.1 Model from larger reference sets to fit data used small reference set. Could be worse on both directions

The score cutoff 10.00 for Reference A community 0 with pplacer\_stats adcl\_log

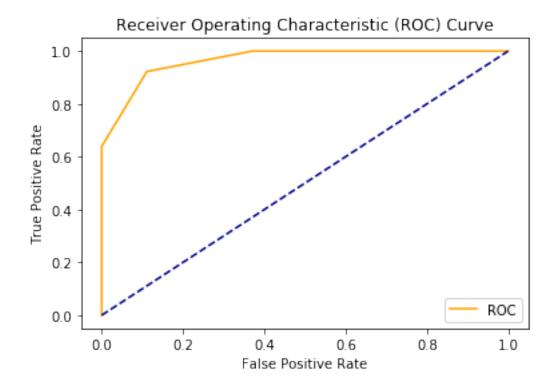
compared with test B: 10.00

data\_set is True

AUC1: 0.97

optimal\_threshold1: 0.84

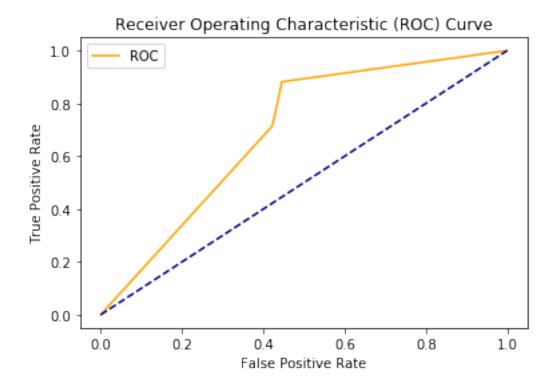
[2. 1. 0.84006066 0.59846994 0. ]



AUC2: 0.69

optimal\_threshold2: 0.60

[2. 1. 0.84006066 0.59846994 0. ]



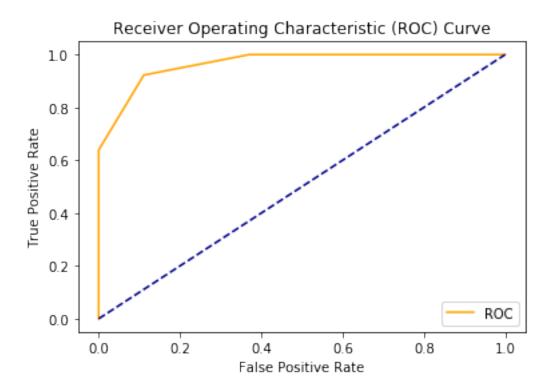
The score cutoff 10.00 for Reference A community 0 with pplacer\_stats adcl\_log compared with test  $C:\ 10.00$ 

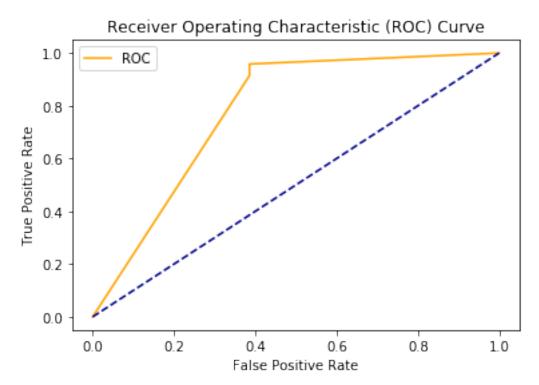
data\_set is True

AUC1: 0.97

optimal\_threshold1: 0.84

[2. 1. 0.83861265 0.6011308 0. ]





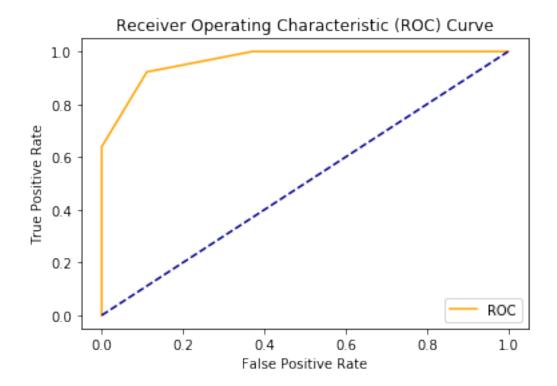
The score cutoff 10.00 for Reference A community 0 with pplacer\_stats adcl\_log compared with test  $D:\ 10.00$ 

data\_set is True

AUC1: 0.97

optimal\_threshold1: 0.84

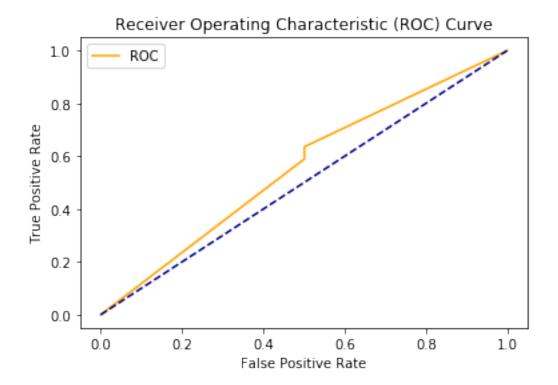
[2. 1. 0.83522539 0.58105212 0. ]



AUC2: 0.56

optimal\_threshold2: 0.84

[2. 1. 0.83522539 0. ]



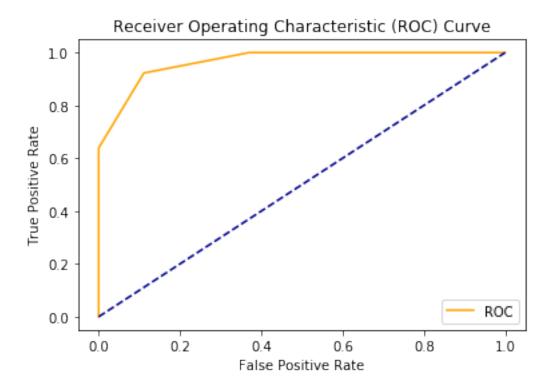
The score cutoff 10.00 for Reference A community 0 with pplacer\_stats adcl\_log compared with test  $E\colon 10.00$ 

data\_set is True

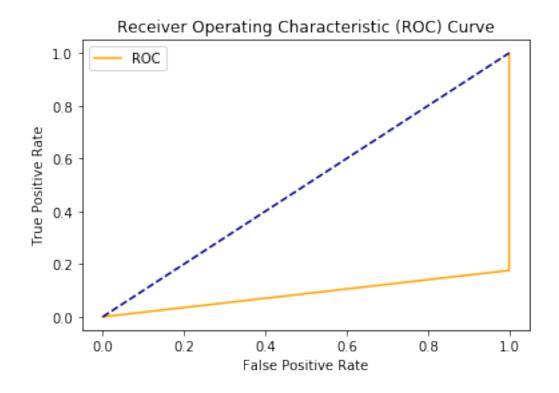
AUC1: 0.97

optimal\_threshold1: 0.86

[2. 1. 0.85596766 0.60895695 0. ]



AUC2: 0.09 optimal\_threshold2: 2.00 [2. 1. 0.85596766 0.



]

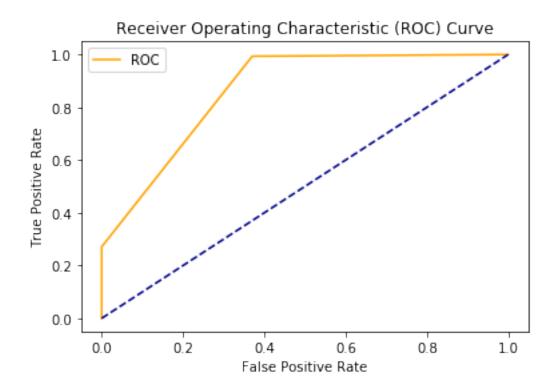
The score cutoff 10.00 for Reference A community 0 with pplacer\_stats edpl compared with test  $B\colon 10.00$ 

data\_set is True

AUC1: 0.86

optimal\_threshold1: 0.90

[2. 1. 0.9018491 0. ]

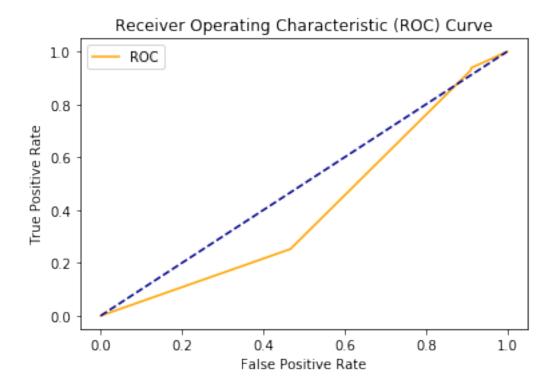


AUC2: 0.41

optimal\_threshold2: 0.20

[2. 1. 0.9018491 0.2

0. ]



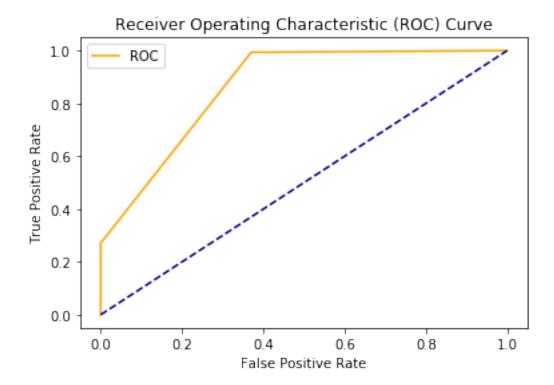
The score cutoff 10.00 for Reference A community 0 with pplacer\_stats edpl compared with test  $C:\ 10.00$ 

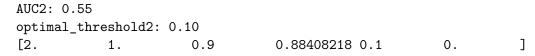
data\_set is True

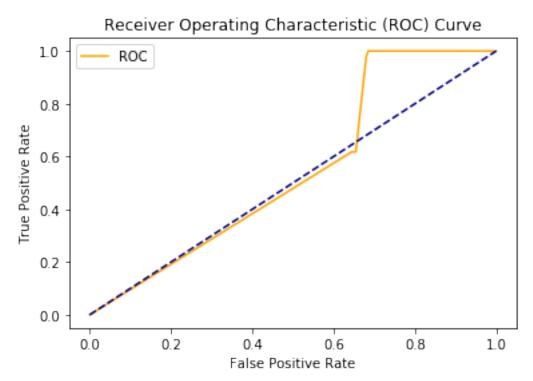
AUC1: 0.86

optimal\_threshold1: 0.88

[2. 1. 0.88408218 0. ]







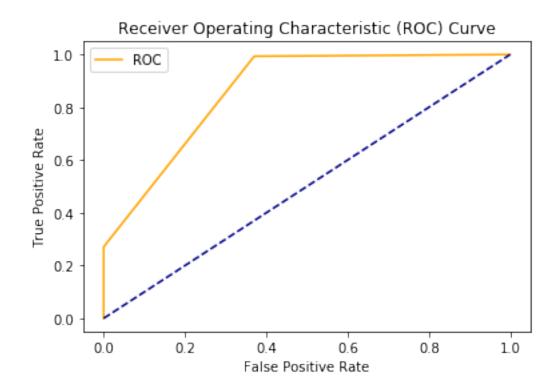
The score cutoff 10.00 for Reference A community 0 with pplacer\_stats edpl compared with test  $D\colon 10.00$ 

data\_set is True

AUC1: 0.86

optimal\_threshold1: 0.87

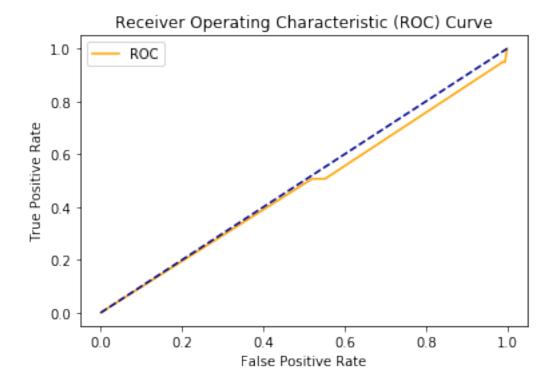
[2. 1. 0.87262189 0. ]



AUC2: 0.48

optimal\_threshold2: 2.00

[2. 1. 0.9 0.87262189 0.1 0. ]



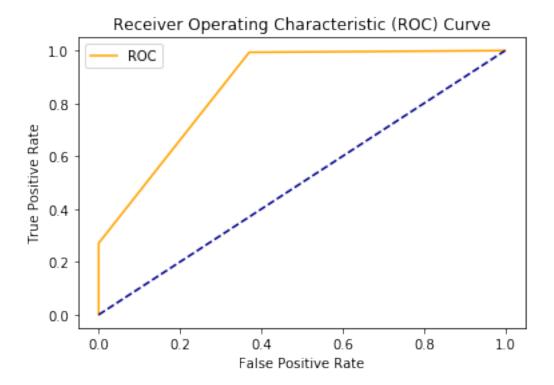
The score cutoff 10.00 for Reference A community 0 with pplacer\_stats edpl compared with test  $E\colon 10.00$ 

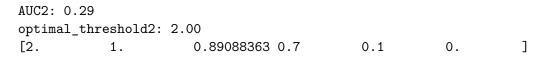
data\_set is True

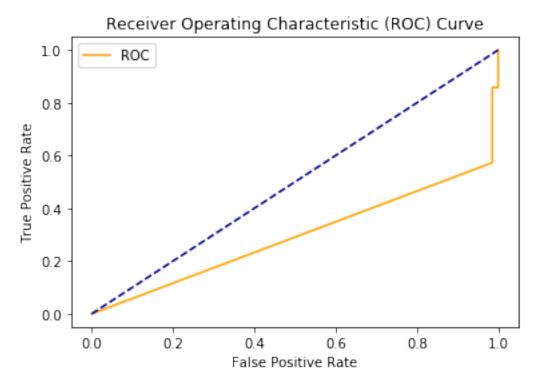
AUC1: 0.86

optimal\_threshold1: 0.89

[2. 1. 0.98710937 0.89088363 0. ]

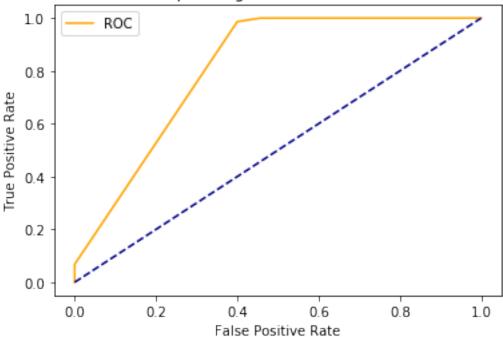




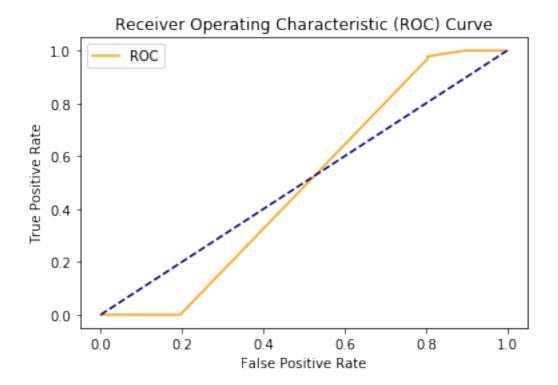


```
[177]: plot_roc_curve_microbiome_test2(pplacer_ref_list = □ → ['A'], pplacer_stats_list=['_adcl_log'], community_list=['0'], cutoff_list=['-4. → 00'], test_data_list=['B','C','D','E'], testOption=True, scoreOption=False)
```





AUC2: 0.49 optimal\_threshold2: 0.90 [2. 1. 0.92196452 0.9 0.75654762 0. ]

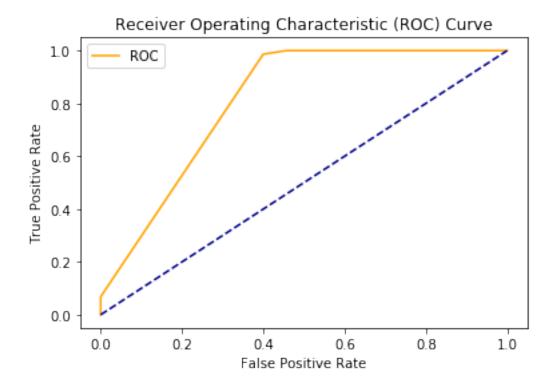


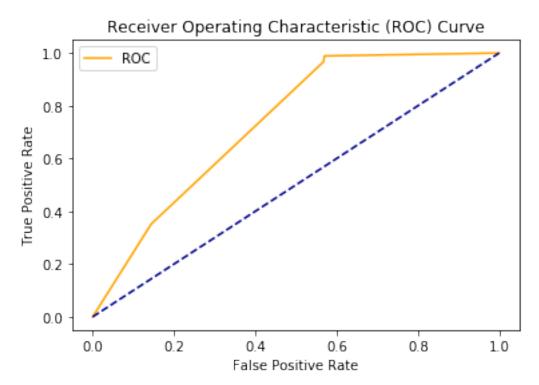
The pplacer\_stats\_cutoff -4.00 for Reference A community O pplacer\_stats adcl\_log compared with test C: -4.00 data\_set is True

AUC1: 0.81

optimal\_threshold1: 0.92

[2. 1. 0.92433893 0.6797619 0. ]





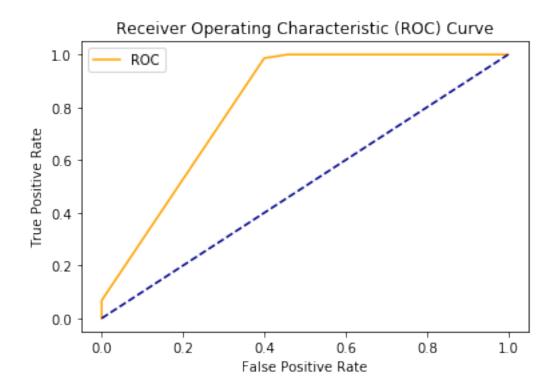
The pplacer\_stats\_cutoff -4.00 for Reference A community O pplacer\_stats adcl\_log compared with test D: -4.00  $\,$ 

data\_set is True

AUC1: 0.81

optimal\_threshold1: 0.92

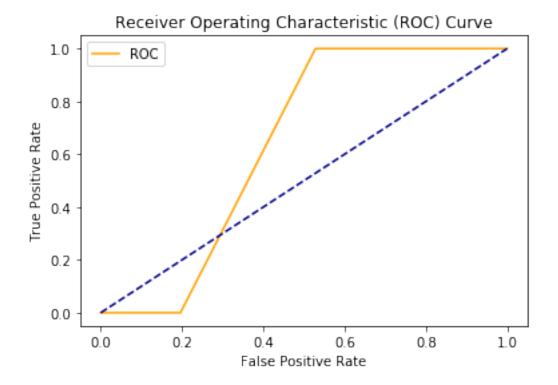
[2. 1. 0.91710262 0.5984632 0. ]



AUC2: 0.64

optimal\_threshold2: 0.92

[2. 1. 0.91710262 0.5984632 0. ]

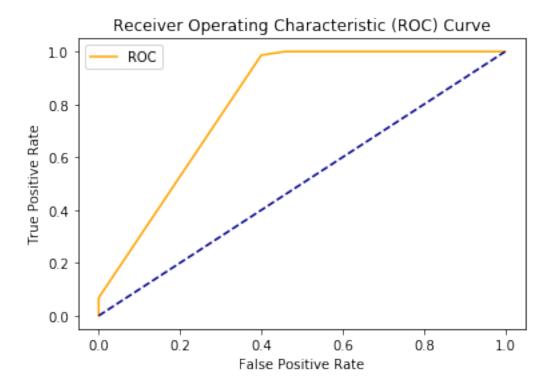


The pplacer\_stats\_cutoff -4.00 for Reference A community O pplacer\_stats adcl\_log compared with test E: -4.00 data\_set is True

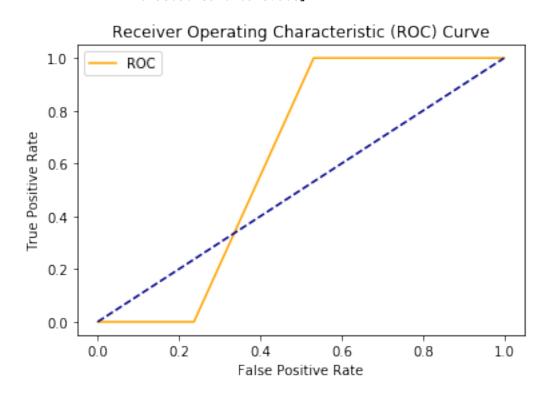
AUC1: 0.81

optimal\_threshold1: 0.93

0.93096139 0.69437908 0. ] [2. 1.



AUC2: 0.62 optimal\_threshold2: 0.93 [2. 1. 0.93096139 0.69437908]



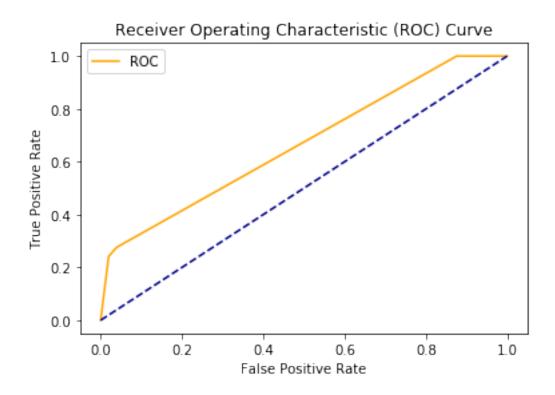
```
[136]: plot\_roc\_curve\_microbiome\_test2(pplacer\_ref\_list = \_ Glassical curve\_microbiome\_test2(pplacer\_ref\_list = _ Glassical curve\_microbiome\_test2(pplacer
```

The pplacer\_stats\_cutoff 25% for Reference A community O pplacer\_stats adcl\_log compared with test B: -5.22

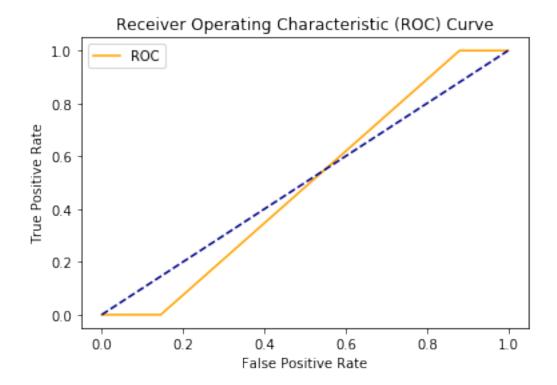
data\_set is True

AUC1: 0.67

optimal\_threshold1: 0.46



AUC2: 0.49 optimal\_threshold2: 0.15

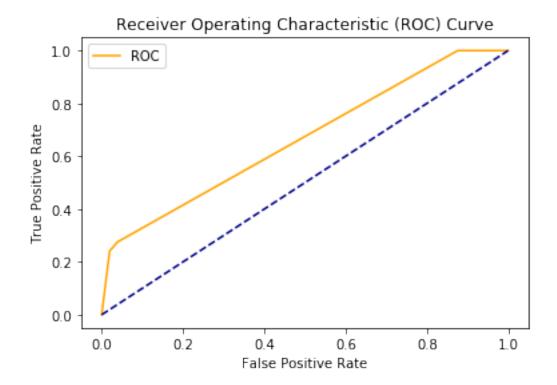


The pplacer\_stats\_cutoff 25% for Reference A community O pplacer\_stats adcl\_log compared with test C: -5.22

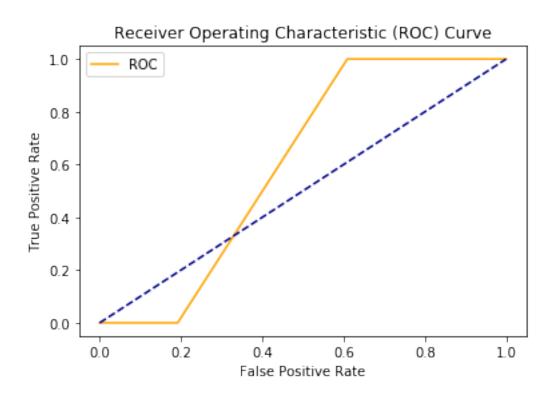
data\_set is True

AUC1: 0.67

optimal\_threshold1: 0.42



AUC2: 0.60 optimal\_threshold2: 0.14



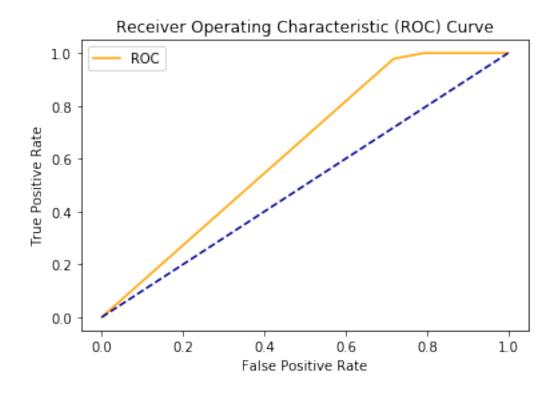
```
[128]: plot\_roc\_curve\_microbiome\_test2(pplacer\_ref\_list = \_ Gradel_log'], community\_list=['0'], cutoff\_list=['25%'], _ Gradel_log'], community\_list=['0'], cutoff\_list=['25%'], _ Gradel_log'], _ Gradel_log
```

The pplacer\_stats\_cutoff 25% for Reference B community O pplacer\_stats adcl\_log compared with test A: -5.15

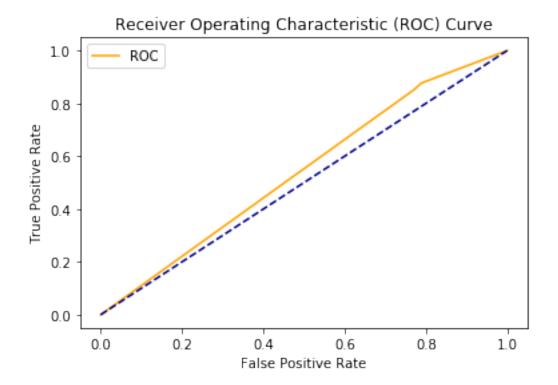
data\_set is True

AUC1: 0.63

optimal\_threshold1: 0.23



AUC2: 0.54 optimal\_threshold2: 0.11

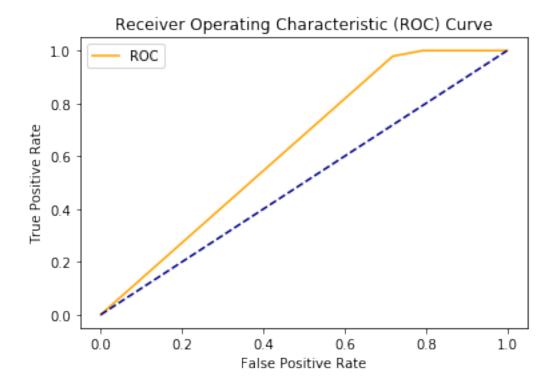


The pplacer\_stats\_cutoff 25% for Reference B community O pplacer\_stats adcl\_log compared with test C: -5.15

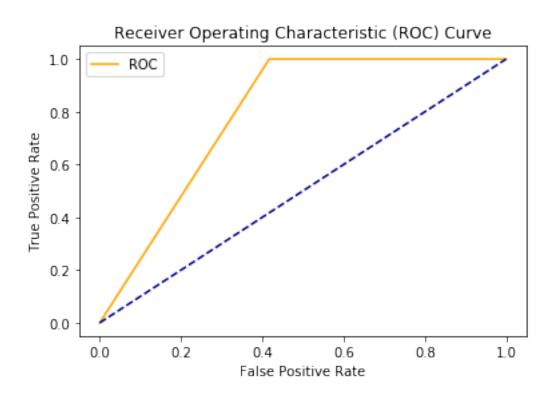
data\_set is True

AUC1: 0.63

optimal\_threshold1: 0.23



AUC2: 0.79 optimal\_threshold2: 0.23



```
[96]: # print("the head for df is {}".format(df.head)+ " the columns of the df is {}".
      \rightarrow format(df.columns))
     #
[33]: # df['A0'].describe(), df['B0'].describe(), df['C0'].describe(), df['D0'].
      →describe(), df['E0'].describe()
[34]: # for community in ['A', 'B', 'C', 'D', 'E']:
           for i in range(10):
                    print(df[community+str(i)].describe())
[35]: df_0 = df
[36]: # plot_pplacer('90')
[37]: # plotScatter('B','0')
[38]: # plotScatterRef('_adcl_log', '0')
[39]: # plot_pplacer('_adcl_log')
[40]: df['A_adcl_log'].describe()
[40]: count
              5974.000000
     mean
                 -4.083366
     std
                 1.837510
     min
                -5.995679
     25%
                -5.221126
     50%
                -5.096367
     75%
                -1.706947
                -0.344675
     Name: A_adcl_log, dtype: float64
[41]: # plot_pplacer('0')
[42]: df['A0'].describe()
[42]: count
              605.000000
     mean
                6.390083
     std
               10.778008
     min
                0.000000
     25%
                2.000000
     50%
                2.000000
     75%
                2,000000
     max
               38.000000
     Name: AO, dtype: float64
[43]: df1 = df[(df['A0']>10)]
[44]: df1['A0'].describe()
```

```
[44]: count
                                            99.000000
                                            28.626263
               mean
               std
                                            10.791707
               min
                                            12.000000
               25%
                                            12.000000
               50%
                                            32.000000
               75%
                                            38.000000
               max
                                            38.000000
               Name: AO, dtype: float64
[45]: 99/605
[45]: 0.16363636363636364
[46]: df1['B0'].describe()
[46]: count
                                            99.000000
               mean
                                            25.070707
               std
                                            17.438670
                                               0.000000
               min
               25%
                                               0.000000
               50%
                                            36.000000
               75%
                                            38.000000
                                            38.000000
               max
               Name: BO, dtype: float64
[47]: df2=df[['seqID','A0','B0', 'C0','D0','E0']].dropna()
[48]: df3 = df2[(df2['A0']>10) & (df2['B0']>10) & (df2['C0']>10) & (df2['D0']>10) & (df2[

    df2['E0']>10)]
[49]: # df2.describe(), df3.describe()
[50]: df3
[50]:
                                                                                                                                                                                     ΑO
                                                                                                                                                                                                        B0
                                                                                                                                                                                                                            CO
                                                                                                                                                                                                                                               DO
                                                                                                                                                                                                                                                                  ΕO
                                                                                                                                                         seqID
                                 CC11CM5SCR137ef78188b94db7b59504dc64363aa3
                                                                                                                                                                                                                                        32.0 44.0
                                                                                                                                                                               34.0
                                                                                                                                                                                                  34.0
                                                                                                                                                                                                                  32.0
               5314
                                 CC11CMOSCR35529da454f0497fa16e04841e8e1639
                                                                                                                                                                               34.0
                                                                                                                                                                                                34.0
                                                                                                                                                                                                                    32.0
                                                                                                                                                                                                                                       32.0 44.0
[51]: 2/605
[51]: 0.003305785123966942
[52]: |dfc90| = df[(df['A90']>10) \& (df['B90']>10) \& (df['C90']>10) \& (df['D90']>10)_{\square}
                   →& (df['E90']>10)]
[53]: dfc90['B0'].describe()
[53]: count
                                            0.0
                                            NaN
               mean
               std
                                            NaN
                                            NaN
               min
               25%
                                            NaN
               50%
                                            NaN
```

```
75% NaN max NaN
```

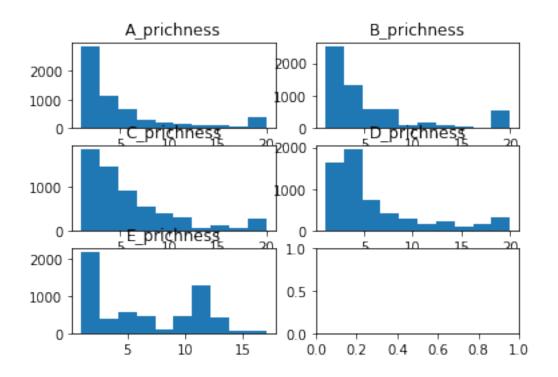
Name: BO, dtype: float64

```
[54]: df[(df.community=='CC11CMO')]['C_adcl_log'].dropna().describe()
```

[54]: count 55.000000 -1.885119 mean std 1.762885 -5.300162 min 25% -1.773077 50% -1.040954 75% -0.682030 -0.373058 max

Name: C\_adcl\_log, dtype: float64

## [55]: plot\_pplacer('\_prichness')

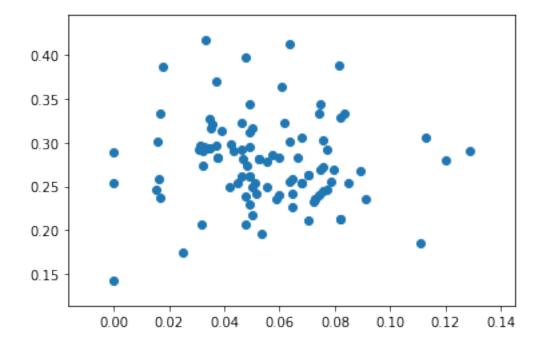


## [56]: df['A\_prichness'].describe()

[56]:	count	5974.000000
	mean	4.727653
	std	5.465596
	min	1.000000
	25%	1.000000
	50%	3.000000
	75%	5.000000

```
20.000000
     max
     Name: A_prichness, dtype: float64
[57]: df [df.A0>10].A0.count()
[57]: 99
[58]: df [df.A0>10].A0.count()/df.A0.count()
[58]: 0.16363636363636364
[59]: # df.head()
[60]: df.A_adcl.count()
[60]: 5974
[61]: d={"a":1, "b":2}
[62]: d
[62]: {'a': 1, 'b': 2}
[63]: dd = pd.Series(d, name='score')
[64]: dd.index.name="community"
[65]: dd.reset_index()
[65]:
       community
                  score
               а
                       1
                       2
     1
               b
[66]: "CC11CM"+str(0)
[66]: 'CC11CMO'
[67]: c0=df['A0'][df['community']=='CC11CM0']
[68]: per=c0[c0>10].count()/c0.count()
[69]: def generateScore(stats, referenceID, scorecutoff, statscutoff):
         d1={}
         d2={}
         for i in range(100):
             values = df[referenceID+str(i)][df.community=='CC11CM'+str(i)]
             statsvalues = df[stats][df['community']=='CC11CM'+str(i)]
             d1['CC11CM'+str(i)] = values[values>scorecutoff].count()/values.count()
             d2['CC11CM'+str(i)] =statsvalues[statsvalues>statscutoff].count()/
      ⇒statsvalues.count()
         d1=pd.Series(d1, name=referenceID)
         d1.index.name='community'
         d1=d1.reset_index()
         d2=pd.Series(d2, name=stats)
         d2.index.name='community'
         d2=d2.reset_index()
```

[71]: <matplotlib.collections.PathCollection at 0x1efb8cd0>



```
[72]: t=[]
     for referenceID in ['A','B','C','D','E']:
         t.append(generateScore('A_adcl', referenceID, 10, 0.001))
[73]: t[0].head()
[73]:
      community
                         A community
                                        A_adcl
         CC11CMO
                 0.090909
                             CC11CMO 0.236364
     1
        CC11CM1 0.082192
                             CC11CM1 0.328767
     2
        CC11CM2 0.025000
                             CC11CM2 0.175000
        CC11CM3 0.050847
                             CC11CM3 0.254237
     3
     4
        CC11CM4 0.000000
                             CC11CM4 0.288462
[74]: tt = pd.concat([t[0],t[1],t[2],t[3],t[4]], axis=1)
[75]: def generateScoreu(stats, referenceID,scorecutoff,statscutoff):
         d1=\{\}
         d2={}
         for i in range(100):
             values = df[referenceID+str(i)][df.community=='CC11CM'+str(i)]
```

```
statsvalues = df[referenceID+stats][df['community']=='CC11CM'+str(i)]
    d1['CC11CM'+str(i)] = values[values>scorecutoff].count()/values.count()
    d2['CC11CM'+str(i)] = statsvalues[statsvalues>statscutoff].count()/

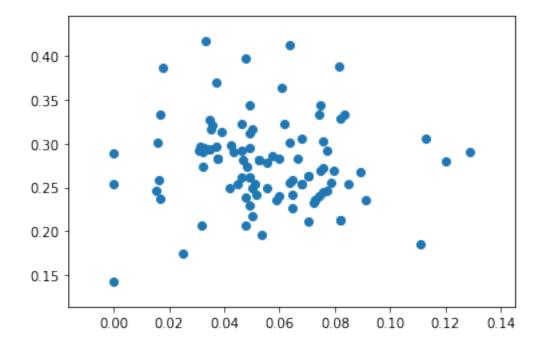
    statsvalues.count()

    d1=pd.Series(d1, name=referenceID)
    d1.index.name='community'
    d1=d1.reset_index()
    d2=pd.Series(d2, name=referenceID+stats)
    d2.index.name='community'
    d2=d2.reset_index()
    dt = pd.concat([d1,d2], axis=1)
    dt=dt.loc[:, ~dt.columns.duplicated()]
    dt=dt.set_index('community')
    return (dt)

[76]: dtu=generateScoreu('_adcl', 'A', 10, 0.001)
```

[77]: <matplotlib.collections.PathCollection at 0x1f294fd0>

[77]: plt.scatter(dtu.A, dtu.A\_adcl)



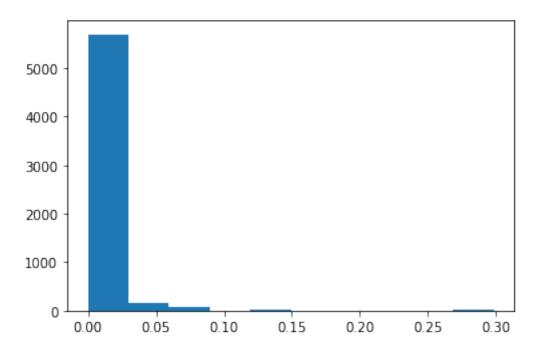
```
[]:

[78]: t=[]

statsdir= {'_adcl':0.0001, '_edpl':0,'_prichness':10,'_mindistl':0.05}

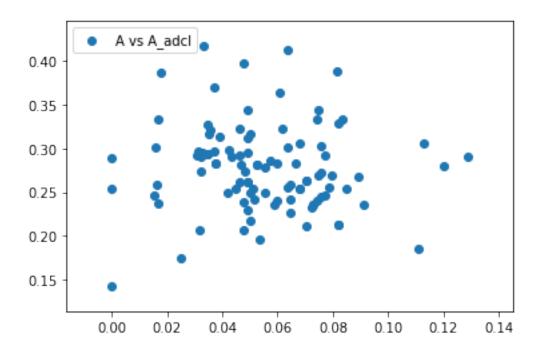
for stats in statsdir.keys():

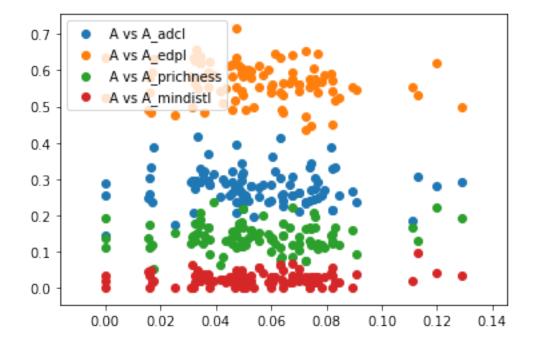
for referenceID in ['A','B','C','D','E']:
```

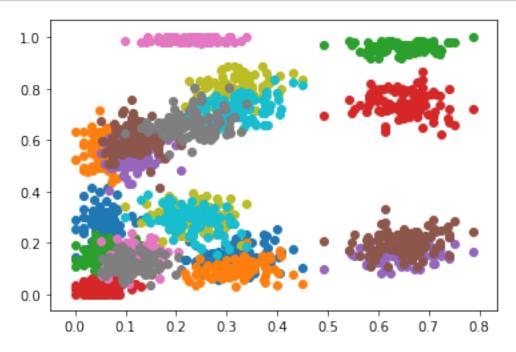


```
[83]: dp =pd.read_csv("community-based.csv", index_col=0)
[84]: dp.describe()
[84]:
                                                       B_adcl
                                                                                 C_adcl
                      Α
                             A_adcl
                                                В
                                                                         С
            100.000000
                         100.000000
                                      100.000000
                                                   100.000000
                                                                100.000000
                                                                             100.000000
     count
              0.055034
                           0.277586
                                                                               0.799584
     mean
                                        0.116043
                                                     0.557102
                                                                  0.318386
              0.024318
                           0.049060
                                        0.032415
                                                     0.054352
                                                                  0.048526
                                                                               0.044362
     std
```

```
min
              0.000000
                           0.142857
                                        0.051724
                                                     0.406780
                                                                  0.216667
                                                                               0.666667
     25%
              0.037736
                           0.246154
                                        0.095238
                                                     0.516532
                                                                  0.285119
                                                                               0.773585
     50%
              0.052178
                           0.275986
                                        0.112007
                                                     0.563333
                                                                  0.315789
                                                                               0.800000
     75%
              0.072530
                           0.301587
                                        0.136310
                                                     0.600000
                                                                   0.346392
                                                                               0.830769
              0.129032
                           0.416667
                                        0.209677
                                                     0.682540
                                                                   0.448980
                                                                               0.888889
     max
                      D
                              D adcl
                                                Ε
                                                        E_adcl
                                                                     A_prichness
                                                                       100.000000
     count
            100.000000
                         100.000000
                                      100.000000
                                                   100.000000
     mean
              0.647292
                           0.962263
                                        0.229600
                                                     0.989559
                                                                         0.140234
     std
                                                     0.008343
                                                                         0.035764
              0.051736
                           0.017520
                                        0.045910
                                                                . . .
     min
              0.491803
                           0.916667
                                        0.097222
                                                     0.975000
                                                                . . .
                                                                         0.052632
     25%
              0.612455
                           0.949788
                                        0.193768
                                                     0.983051
                                                                         0.118395
                                                                . . .
     50%
              0.649561
                           0.966667
                                        0.229508
                                                     0.984615
                                                                         0.137147
                                                                . . .
     75%
              0.682738
                           0.978723
                                        0.261943
                                                     1.000000
                                                                . . .
                                                                         0.164801
                                        0.339623
                                                     1.000000
              0.786885
                           1.000000
                                                                         0.235294
     max
                                                                . . .
            B_prichness
                          C_prichness
                                                                    A_mindistl
                                        D_prichness
                                                      E_prichness
             100.000000
                           100.000000
                                          100.000000
                                                        100.000000
                                                                     100.000000
     count
                0.147809
                              0.142149
                                            0.160060
                                                          0.304304
                                                                       0.025369
     mean
                0.041895
                                            0.034324
                                                          0.042562
     std
                              0.037576
                                                                       0.018591
     min
                0.042553
                              0.056604
                                            0.080645
                                                          0.190476
                                                                       0.000000
     25%
                0.123077
                              0.120690
                                            0.144585
                                                          0.274194
                                                                       0.015873
     50%
                0.146257
                              0.140351
                                            0.155048
                                                          0.306452
                                                                       0.020221
     75%
                0.179410
                              0.157540
                                            0.180082
                                                          0.338524
                                                                       0.034044
                0.240741
                              0.254545
                                            0.244898
                                                          0.393443
                                                                       0.096774
     max
            B mindistl
                         C_mindistl
                                      D mindistl
                                                  E mindistl
            100.000000
                         100.000000
                                      100.000000
                                                   100.000000
     count
     mean
              0.114361
                           0.097589
                                        0.198869
                                                     0.290481
                                        0.042808
     std
              0.030794
                           0.030017
                                                     0.047167
     min
              0.037037
                           0.033333
                                        0.109091
                                                     0.156863
     25%
              0.095013
                           0.079132
                                        0.172414
                                                     0.265789
     50%
              0.111111
                           0.096774
                                        0.196400
                                                     0.298507
     75%
              0.134615
                           0.114754
                                        0.229823
                                                     0.323077
              0.187500
                           0.203390
                                        0.333333
                                                     0.387755
     max
     [8 rows x 25 columns]
[85]: for score in ['A','B','C','D','E'][0:1]:
         for stats in ['_adcl', '_edpl','_prichness','_mindistl'][0:1]:
             plt.scatter(dp[score], dp[score+stats], label=score + ' vs '+_
      →score+stats)
             plt.legend(loc='upper left')
             plt.show
```







3]: dp.de	scribe()						
3]:	A	A_adcl	В	B_adcl	С	C_adcl	\
count	100.000000	100.000000	100.000000	100.000000	100.000000	100.000000	
mean	0.055034	0.277586	0.116043	0.557102	0.318386	0.799584	
std	0.024318	0.049060	0.032415	0.054352	0.048526	0.044362	
min	0.000000	0.142857	0.051724	0.406780	0.216667	0.666667	
25%	0.037736	0.246154	0.095238	0.516532	0.285119	0.773585	
50%	0.052178	0.275986	0.112007	0.563333	0.315789	0.800000	
75%	0.072530	0.301587	0.136310	0.600000	0.346392	0.830769	
max	0.129032	0.416667	0.209677	0.682540	0.448980	0.888889	
	D	D_adcl	E	E_adcl	A_pric	hness \	
count	100.000000	100.000000	100.000000	100.000000	100.0	100.000000	
mean	0.647292	0.962263	0.229600	0.989559	0.1	0.140234	
std	0.051736	0.017520	0.045910	0.008343	0.0	35764	
min	0.491803	0.916667	0.097222	0.975000	0.0	52632	
25%	0.612455	0.949788	0.193768	0.983051	0.1	18395	

```
50%
         0.649561
                      0.966667
                                   0.229508
                                                0.984615
                                                                    0.137147
75%
         0.682738
                      0.978723
                                   0.261943
                                                1.000000
                                                                    0.164801
max
         0.786885
                       1.000000
                                   0.339623
                                                 1.000000
                                                                    0.235294
       B_prichness
                     C_prichness
                                                 E_prichness
                                   D_prichness
                                                               A_mindistl
        100.000000
                      100.000000
                                     100.000000
                                                   100.000000
                                                                100.000000
count
           0.147809
                         0.142149
                                       0.160060
                                                     0.304304
                                                                  0.025369
mean
std
           0.041895
                         0.037576
                                       0.034324
                                                     0.042562
                                                                  0.018591
min
           0.042553
                         0.056604
                                       0.080645
                                                     0.190476
                                                                  0.000000
25%
           0.123077
                         0.120690
                                       0.144585
                                                     0.274194
                                                                  0.015873
50%
           0.146257
                         0.140351
                                       0.155048
                                                     0.306452
                                                                  0.020221
75%
           0.179410
                         0.157540
                                       0.180082
                                                     0.338524
                                                                  0.034044
                                                     0.393443
max
           0.240741
                         0.254545
                                       0.244898
                                                                  0.096774
       B_{mindistl}
                    C_{mindistl}
                                 D_{mindistl}
                                              E_{mindistl}
       100.000000
                    100.000000
                                 100.000000
                                              100.000000
count
         0.114361
                      0.097589
                                   0.198869
                                                0.290481
mean
std
         0.030794
                      0.030017
                                   0.042808
                                                0.047167
min
         0.037037
                      0.033333
                                   0.109091
                                                0.156863
25%
         0.095013
                      0.079132
                                   0.172414
                                                0.265789
50%
         0.111111
                      0.096774
                                   0.196400
                                                0.298507
                                   0.229823
75%
         0.134615
                      0.114754
                                                0.323077
         0.187500
                      0.203390
                                   0.333333
max
                                                0.387755
```

[8 rows x 25 columns]

[]: