

Preprocessing

Import necessary modules

```
In [39]: from Bio import SeqIO
from Bio.SeqFeature import SeqFeature, FeatureLocation
from Bio.SeqUtils.ProtParam import ProteinAnalysis
from Bio.SeqUtils import IsoelectricPoint
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from sklearn import svm
from sklearn.preprocessing import OneHotEncoder
from sklearn.multiclass import OneVsRestClassifier
from sklearn.model_selection import KFold
from sklearn.metrics import confusion_matrix
```

Read training data

```
In [2]: dataCyto=[]
for record in SeqIO.parse("cyto.fasta.txt", "fasta"):
    dataCyto.append(record)

dataMito=[]
for record in SeqIO.parse("mito.fasta.txt", "fasta"):
    dataMito.append(record)

dataNucleus=[]
for record in SeqIO.parse("nucleus.fasta.txt", "fasta"):
    dataNucleus.append(record)

dataSecreted=[]
for record in SeqIO.parse("secreted.fasta.txt", "fasta"):
    dataSecreted.append(record)

print('cyto', len(dataCyto))
print('mito', len(dataMito))
print('nucleus', len(dataNucleus))
print('secreted', len(dataSecreted))
```

```
cyto 3004
mito 1299
nucleus 3314
secreted 1605
```

```
In [3]: #example of data
print(dataCyto[0])

ID: sp|Q4JIM5|ABL2_MOUSE
Name: sp|Q4JIM5|ABL2_MOUSE
Description: sp|Q4JIM5|ABL2_MOUSE Abelson tyrosine-protein kinase
2 OS=Mus musculus GN=Abl2 PE=1 SV=1
Number of features: 0
Seq('MGQQVGRVGEAPGLQQPQPRGIRGSSAARPSGRRRDPAGRTADAGFNVFTQHDH...VQR'
, SingleLetterAlphabet())
```

Analyse the data to get features

```
In [4]: analysed=[]
for i in range(len(dataCyto)):
    analysed_seq=ProteinAnalysis(str(dataCyto[i].seq))
    analysed.append(analysed_seq)

for i in range(len(dataMito)):
    analysed_seq=ProteinAnalysis(str(dataMito[i].seq))
    analysed.append(analysed_seq)

for i in range(len(dataNucleus)):
    analysed_seq=ProteinAnalysis(str(dataNucleus[i].seq))
    analysed.append(analysed_seq)

for i in range(len(dataSecreted)):
    analysed_seq=ProteinAnalysis(str(dataSecreted[i].seq))
    analysed.append(analysed_seq)
print(len(analysed))
```

9222

```
In [5]: #example of analysed data
print('length:', analysed[0].length)
print('aminoacids', analysed[0].count_amino_acids())
print('aminoacid percent', analysed[0].amino_acids_percent)
print('molecular weight', analysed[0].molecular_weight())
```

```
length: 1182
aminoacids {'A': 97, 'C': 17, 'D': 51, 'E': 81, 'F': 35, 'G': 96,
'H': 26, 'I': 30, 'K': 72, 'L': 99, 'M': 22, 'N': 40, 'P': 96, 'Q'
: 44, 'R': 63, 'S': 118, 'T': 73, 'V': 77, 'W': 13, 'Y': 32}
aminoacid percent None
molecular weight 128194.98120000077
```

Features

```
In [6]: noOfExamples=len(dataCyto)+len(dataMito)+len(dataNucleus)+len(dataSecreted)
composition=np.zeros((noOfExamples, 20))
for i in range(len(analysed)):
    dict=analysed[i].get_amino_acids_percent()
    for pos,aa in enumerate(dict.values()):
        composition[i,pos]=aa
```

```
In [7]: length=np.zeros((noOfExamples, 1))
for i in range(len(analysed)):
    length[i,0]=analysed[i].length

iep=np.zeros((len(analysed), 1))
for i in range(len(analysed)):
    iep[i,0]=analysed[i].isoelectric_point()

noOfFeatures=22
features=np.zeros((noOfExamples,noOfFeatures))
features=np.append(np.append(composition, length,axis=1),iep, axis=1)
```

```
In [8]: d=dataCyto[1]
name='sp|P15891|ABP1_YEAST'
seq=d.seq
desc='Actin-binding protein OS=Saccharomyces cerevisiae (strain ATC
C 204508 / S288c) GN=ABP1 PE=1 SV=4'
print('Name:')
print(name)
print('Description:')
print(desc)
print('Sequence: (592 aminoacids)')
print(seq[:95])
print(seq[95:190])
print(seq[190:285])
print(seq[285:380])
print(seq[380:475])
print(seq[475:570])
print(seq[570:])
```

Name:

sp|P15891|ABP1_YEAST

Description:

Actin-binding protein OS=Saccharomyces cerevisiae (strain ATCC 204
508 / S288c) GN=ABP1 PE=1 SV=4

Sequence: (592 aminoacids)

MALEPIDYTTHSREIDA EY LKIVRGSDPD TTWLIISPNAKKEYEP ESTGSSFHDFLQLFDETKVQY
GLARVSPPGSDVEKIIIIIGWCPDSAPLKT
RASFAANFAAVANNLFKGYHVQVTARDEDDLDENELLMKISNAAGARYSIQTSSKQQGKASTPPVK
KSFTPSKSPAPVSKKEPVKTPSPAPAAKI
SSRVNDNNDDDDWNEPELKERDFDQAPLKPNQSSYKPIGKIDLQKVIAEEKAKEDPRLVQKPTAAG
SKIDPSSDIANLKNESKLKRDSEFNSFLG
TTKPPSMTESSLKNDDDKVIKGRNEKSPAQLWAERKAKQNSGNAETKAEAPKPEVPEDEPEGEPD
VKDLKSKFEGLAASEKEEEEEMENKFAPPP
KKSEPTII SPKPF SKPQEPVKAEEAEQPKTDYKKIGNPLPGMHIEADNEEEPEENDDDWDDDEDEA
AQPLPSRNVASGAPVQKEEPEQEEIAPS
LPSRNSIPAPKQEEAPEQAPEEEEIEEEAEAAAPQLPSRSSAAPPPPPRRATPEKKPKENPWATAEY
DYDAAEDNELTFVENDKIINIEFVDDDDWW
LGELEKDGSKGLFPSNYVSLGN

```
In [9]: #example of analysed data
print('length:', analysed[1].length)
print('isoelectric point:', float(np.round(iep[1],3)))
print('amino acid composition:')

amac=analysed[1].amino_acids_percent
keys=[]
values=[]
for key,value in (amac.items()):
    keys.append(key)
    values.append(value)
for i in np.arange(0,20, 3):
    if i==18:
        print(keys[i],':', np.round(values[i]*100,2),'%', keys[i+1],':', np.round(values[i+1]*100,2), '%')
    else:
        print(keys[i],':', np.round(values[i]*100,2),'%', keys[i+1],':', np.round(values[i+1]*100,2), '%', keys[i+2],':', np.round(values[i+2]*100,2), '%')

length: 592
isoelectric point: 4.589
amino acid composition:
A : 9.46 %, C : 0.17 % D : 7.94 %
E : 12.67 %, F : 2.87 % G : 3.72 %
H : 0.68 %, I : 4.73 % K : 9.97 %
L : 5.24 %, M : 0.84 % N : 5.07 %
P : 11.15 %, Q : 3.38 % R : 2.87 %
S : 8.61 %, T : 3.72 % V : 3.72 %
W : 1.35 %, Y : 1.86 %
```

Labels

```
In [10]: #labels for each dataset
labels=np.zeros(noOfExamples)

labels[0:len(dataCyto)]=1
labels[len(dataCyto):len(dataCyto)+len(dataMito)]=2
labels[len(dataCyto)+len(dataMito):len(dataCyto)+len(dataMito)+len(
dataNucleus)]=3
labels[len(dataCyto)+len(dataMito)+len(dataNucleus):]=4
```

```
In [11]: enc=OneHotEncoder(labels)
enc.categories
```

```
Out[11]: array([1., 1., 1., ..., 4., 4., 4.])
```

Model exploration

Comparing results for different models and for different datasets

```
In [12]: model2=svm.NuSVC(nu=0.5, decision_function_shape='ovo', probability
        =True)
        model2.fit(composition, enc.categories)
        print('NuSVC trained on composition, score:', model2.score(composit
        ion, enc.categories))
```

NuSVC trained on composition, score: 0.7006072435480373

```
In [13]: #grid search for best parameter:
        indexes=np.arange(0.1,0.52,0.02)
        exploreScores=np.zeros(len(indexes))
        for i,nu in enumerate(indexes):
            modelx=svm.NuSVC(nu=nu, decision_function_shape='ovo', probabilit
            y=True)
            modelx.fit(composition, enc.categories)
            exploreScores[i]=modelx.score(composition, enc.categories)
```

```
In [15]: print(exploreScores)
        print('bestScore:',np.max(exploreScores))
        print(np.argmax(exploreScores))
        best=indexes[int(np.argmax(exploreScores))]
        print('best parameter:',best)
```

```
[0.87063544 0.88928649 0.88646714 0.88874431 0.89058773 0.88147907
 0.88147907 0.87020169 0.86109304 0.84829755 0.83506831 0.81967035
 0.80676643 0.79191065 0.77792236 0.76718716 0.75287356 0.74213836
 0.7279332  0.71437866 0.70060724]
bestScore: 0.8905877250054218
4
best parameter: 0.18000000000000002
```

```
In [16]: #best nu=0.18
        model=svm.NuSVC(nu=np.round(best,2), decision_function_shape='ovo',
        probability=True)
        model.fit(composition, enc.categories)
        print('NuSVC trained on composition with best parameter, score:', m
        odel.score(composition, enc.categories))
```

NuSVC trained on composition with best parameter, score: 0.8905877250054218

```
In [17]: model11=svm.SVC(C=1.0,decision_function_shape='ovo', probability=True)
        model11.fit(composition, enc.categories)
        print('SVC trained on composition, score:', model11.score(compositi
        on, enc.categories))
```

SVC trained on composition, score: 0.6477987421383647

In [18]:

```
#grid search for best parameter:
indexesC=np.arange(1,30,2)
searchScores=np.zeros(len(indexesC))
for i,c in enumerate(indexesC):
    model=svm.SVC(C=c,decision_function_shape='ovo', probability=True)
    model.fit(composition, enc.categories)
    searchScores[i]=model.score(composition, enc.categories)
```

In [19]:

```
print(searchScores)
print('bestScore:',np.max(searchScores))
print(np.argmax(searchScores))
bestC=indexesC[int(np.argmax(searchScores))]
print('best parameter:',bestC)
```

```
[0.64779874 0.68325743 0.69963132 0.71199306 0.71969204 0.72880069
 0.73704186 0.74268055 0.74907829 0.75233138 0.75547604 0.75959662
 0.76176534 0.76534374 0.76957276]
bestScore: 0.7695727607894166
14
best parameter: 29
```

In [20]:

```
model3=svm.SVC(C=bestC,decision_function_shape='ovo', probability=True)
model3.fit(composition, enc.categories)
print('SVC trained on composition, score:', model3.score(composition, enc.categories))
```

```
SVC trained on composition, score: 0.7695727607894166
```

In [21]:

```
#best models: model and model6
print('model parameters:',)
model3.get_params()
```

```
model parameters:
```

Out[21]:

```
{'C': 29,
 'break_ties': False,
 'cache_size': 200,
 'class_weight': None,
 'coef0': 0.0,
 'decision_function_shape': 'ovo',
 'degree': 3,
 'gamma': 'scale',
 'kernel': 'rbf',
 'max_iter': -1,
 'probability': True,
 'random_state': None,
 'shrinking': True,
 'tol': 0.001,
 'verbose': False}
```

```
In [22]: model8=svm.SVC(decision_function_shape='ovo', probability=True)
model8.fit(length, enc.categories)
print('SVC trained on sequence length, score:', model8.score(length
, enc.categories))
```

SVC trained on sequence length, score: 0.43103448275862066

```
In [23]: model9=svm.SVC(decision_function_shape='ovo', probability=True)
model9.fit(iep, enc.categories)
print('SVC trained on isoelectric point, score:', model9.score(iep,
enc.categories))
```

SVC trained on isoelectric point, score: 0.405985686402082

```
In [24]: model4=svm.SVC(C=10.0,decision_function_shape='ovo', probability=True)
model4.fit(features, enc.categories)
print('SVC trained on all features, score:', model4.score(features,
enc.categories))
```

SVC trained on all features, score: 0.4308176100628931

```
In [25]: model10=svm.NuSVC(nu=0.5, decision_function_shape='ovo', probability=True)
model10.fit(length, enc.categories)
print('NuSVC trained on sequence length, score:', model10.score(length,
enc.categories))
```

NuSVC trained on sequence length, score: 0.2852960312296682

```
In [26]: model11=svm.NuSVC(nu=0.5, decision_function_shape='ovo', probability=True)
model11.fit(iep, enc.categories)
print('NuSVC trained on isoelectric point, score:', model11.score(iep,
enc.categories))
```

NuSVC trained on isoelectric point, score: 0.27521145087833443

```
In [27]: model5=svm.NuSVC(nu=0.5, decision_function_shape='ovo', probability=True)
model5.fit(features, enc.categories)
print('NuSVC trained on features, score:', model5.score(features, enc.categories))
```

NuSVC trained on features, score: 0.4097809585773151

```
In [28]: #one classifier per class
model6 = OneVsRestClassifier(model).fit(composition, enc.categories)
print('OneVsRestClassifier trained on all model1, score:', model6.score(composition, enc.categories))
```

OneVsRestClassifier trained on all model1, score: 0.773801778356105


```
In [29]: #best models: model and model6
print('model parameters:',)
model.get_params()
```

model parameters:

```
Out[29]: {'C': 29,
          'break_ties': False,
          'cache_size': 200,
          'class_weight': None,
          'coef0': 0.0,
          'decision_function_shape': 'ovo',
          'degree': 3,
          'gamma': 'scale',
          'kernel': 'rbf',
          'max_iter': -1,
          'probability': True,
          'random_state': None,
          'shrinking': True,
          'tol': 0.001,
          'verbose': False}
```

```
In [30]: print('model6 parameters:',)
model6.get_params()
```

model6 parameters:

```
Out[30]: {'estimator__C': 29,
          'estimator__break_ties': False,
          'estimator__cache_size': 200,
          'estimator__class_weight': None,
          'estimator__coef0': 0.0,
          'estimator__decision_function_shape': 'ovo',
          'estimator__degree': 3,
          'estimator__gamma': 'scale',
          'estimator__kernel': 'rbf',
          'estimator__max_iter': -1,
          'estimator__probability': True,
          'estimator__random_state': None,
          'estimator__shrinking': True,
          'estimator__tol': 0.001,
          'estimator__verbose': False,
          'estimator': SVC(C=29, break_ties=False, cache_size=200, class_weight=None, coef0=0.0,
                           decision_function_shape='ovo', degree=3, gamma='scale', kernel='rbf',
                           max_iter=-1, probability=True, random_state=None, shrinking=True, tol=0.001,
                           verbose=False),
          'n_jobs': None}
```

Cross validation

```
In [32]: predsTrain1=model.predict(composition)
corrTrain1=np.corrcoef(predsTrain1, enc.categories)
probsTrain1=model.predict_proba(composition)
predProbsTrain1=np.array(np.argmax(probsTrain1, axis=1)+1)
conf1=np.array(np.max(probsTrain1, axis=1))
print('score 1:', model.score(composition, enc.categories))
print('correlation 1:',corrTrain1[1,0])
print('average confidence 1:', np.average(conf1))

predsTrain6=model6.predict(composition)
corrTrain6=np.corrcoef(predsTrain6, enc.categories)
probsTrain6=model6.predict_proba(composition)
print('score 6:', model6.score(composition, enc.categories))
print('correlation 6:',corrTrain6[1,0])
predProbsTrain6=np.array(np.argmax(probsTrain6, axis=1)+1)
conf6=np.array(np.max(probsTrain6, axis=1))
print('average confidence 6:', np.average(conf6))
```

```
score 1: 0.7695727607894166
correlation 1: 0.6763081755747868
average confidence 1: 0.6155624635951701
score 6: 0.773801778356105
correlation 6: 0.6792502256547375
average confidence 6: 0.5973467259074295
```

```
In [33]: ## if the two models agree then great, otherwise pick the prediction with max probability

print("Compare two predictions:")
myPredsTrain=np.zeros((len(analysed), 2))

for i in range(len(analysed)):
    if predsTrain1[i]==predsTrain6[i]:
        ans=predsTrain1[i]
        ansprob=max(probsTrain1[i, int(predsTrain6[i]-1)], probsTrain6[i, int(predsTrain6[i]-1)])
        print('index:', i, 'prediction:', ans, 'with prob', ansprob)
    else:
        a=np.max(probsTrain1[i])
        b=np.max(probsTrain6[i])
        if a>b:
            ans=np.argmax(probsTrain1[i])+1
            ansprob=np.max(probsTrain1[i])
        else:
            ans=np.argmax(probsTrain6[i])+1
            ansprob=np.max(probsTrain6[i])
        print('index:',i, 'decide', ans, 'with prob', ansprob)
    myPredsTrain[i]=ans,ansprob
```

```
Compare two predictions:
index: 0 decide 3 with prob 0.4895687423690284
index: 1 prediction: 1.0 with prob 0.6658980596839909
index: 2 prediction: 1.0 with prob 0.48735582507082714
index: 3 prediction: 1.0 with prob 0.6609616427680769
index: 4 prediction: 1.0 with prob 0.616093395784446
```

index: 5 prediction: 1.0 with prob 0.5005314097674952
index: 6 prediction: 3.0 with prob 0.6529810971226947
index: 7 prediction: 1.0 with prob 0.46816227766236407
index: 8 prediction: 1.0 with prob 0.6855590518261763
index: 9 prediction: 1.0 with prob 0.6685938821615934
index: 10 prediction: 1.0 with prob 0.6953209712125541
index: 11 prediction: 1.0 with prob 0.5378936528116167
index: 12 prediction: 1.0 with prob 0.5219228726359902
index: 13 prediction: 3.0 with prob 0.5357015297293066
index: 14 prediction: 3.0 with prob 0.5831037159381623
index: 15 prediction: 1.0 with prob 0.5227957964542795
index: 16 prediction: 1.0 with prob 0.5170290314529387
index: 17 prediction: 1.0 with prob 0.6631686777533011
index: 18 prediction: 1.0 with prob 0.5381583163932905
index: 19 prediction: 1.0 with prob 0.5423283126272441
index: 20 prediction: 1.0 with prob 0.5015076964994869
index: 21 prediction: 1.0 with prob 0.677058702029918
index: 22 prediction: 1.0 with prob 0.4953540085148355
index: 23 prediction: 1.0 with prob 0.6831672520804852
index: 24 prediction: 1.0 with prob 0.663898520048484
index: 25 prediction: 1.0 with prob 0.4471642789913593
index: 26 decide 1 with prob 0.3644196549583994
index: 27 prediction: 2.0 with prob 0.4019770586135675
index: 28 prediction: 1.0 with prob 0.574564880930581
index: 29 prediction: 1.0 with prob 0.5915431676983596
index: 30 prediction: 1.0 with prob 0.5986497845071115
index: 31 prediction: 1.0 with prob 0.48449396754232116
index: 32 prediction: 3.0 with prob 0.5031941186216644
index: 33 decide 1 with prob 0.44427889036478463
index: 34 prediction: 2.0 with prob 0.4500886713961323
index: 35 decide 3 with prob 0.375691813430255
index: 36 prediction: 1.0 with prob 0.5542376641413406
index: 37 prediction: 1.0 with prob 0.48682808821534285
index: 38 prediction: 1.0 with prob 0.5155860026676886
index: 39 decide 1 with prob 0.33349920355181484
index: 40 prediction: 1.0 with prob 0.5587368336603991
index: 41 prediction: 3.0 with prob 0.6400750601505459
index: 42 prediction: 3.0 with prob 0.5412858171800126
index: 43 prediction: 3.0 with prob 0.6692116156836488
index: 44 decide 3 with prob 0.5717850653122429
index: 45 prediction: 1.0 with prob 0.568899286841352
index: 46 prediction: 1.0 with prob 0.5468488780266109
index: 47 prediction: 1.0 with prob 0.5372773272064114
index: 48 prediction: 1.0 with prob 0.68065563637553
index: 49 prediction: 1.0 with prob 0.50187768993327
index: 50 prediction: 1.0 with prob 0.5849653161872965
index: 51 prediction: 1.0 with prob 0.6834680823733464
index: 52 prediction: 1.0 with prob 0.5194157852326506
index: 53 prediction: 1.0 with prob 0.5023022689522103
index: 54 prediction: 1.0 with prob 0.6319436263811183
index: 55 prediction: 1.0 with prob 0.7767379674757713
index: 56 prediction: 2.0 with prob 0.53042454861307
index: 57 prediction: 1.0 with prob 0.4584216246954228
index: 58 prediction: 1.0 with prob 0.5448885219245242
index: 59 prediction: 1.0 with prob 0.5812563741162318
index: 60 prediction: 1.0 with prob 0.5484771000445746
index: 61 prediction: 1.0 with prob 0.584606659304932

index: 62 prediction: 1.0 with prob 0.6391096004160792
index: 63 prediction: 1.0 with prob 0.6128670154892529
index: 64 prediction: 2.0 with prob 0.4941721401158989
index: 65 prediction: 2.0 with prob 0.5293814037244385
index: 66 prediction: 1.0 with prob 0.6504378155122599
index: 67 prediction: 3.0 with prob 0.5826780604479644
index: 68 prediction: 1.0 with prob 0.5849157742422236
index: 69 prediction: 1.0 with prob 0.7477846071114214
index: 70 prediction: 1.0 with prob 0.7344580473572003
index: 71 prediction: 1.0 with prob 0.4939572057366976
index: 72 prediction: 1.0 with prob 0.5611544246858352
index: 73 prediction: 1.0 with prob 0.5984626495039331
index: 74 prediction: 1.0 with prob 0.4482242160229572
index: 75 prediction: 3.0 with prob 0.5734732304278893
index: 76 prediction: 1.0 with prob 0.548317906009681
index: 77 prediction: 3.0 with prob 0.5618760105551107
index: 78 prediction: 1.0 with prob 0.6054893953446602
index: 79 prediction: 1.0 with prob 0.6217359145458681
index: 80 prediction: 4.0 with prob 0.6176532137957701
index: 81 decide 3 with prob 0.40139533033783414
index: 82 prediction: 2.0 with prob 0.3406912857984127
index: 83 prediction: 1.0 with prob 0.6196319060982077
index: 84 decide 3 with prob 0.4488088279334886
index: 85 prediction: 3.0 with prob 0.5268115353509695
index: 86 prediction: 1.0 with prob 0.6042887743286204
index: 87 prediction: 1.0 with prob 0.6190115721653517
index: 88 prediction: 1.0 with prob 0.5671757279580381
index: 89 prediction: 1.0 with prob 0.5368446348716404
index: 90 prediction: 1.0 with prob 0.6464236934624902
index: 91 prediction: 1.0 with prob 0.5001501231755798
index: 92 prediction: 1.0 with prob 0.5806136511652377
index: 93 prediction: 4.0 with prob 0.7397587738182091
index: 94 prediction: 1.0 with prob 0.5275331326043972
index: 95 prediction: 1.0 with prob 0.5911471269610444
index: 96 decide 1 with prob 0.5436354610147949
index: 97 prediction: 1.0 with prob 0.6645523350271165
index: 98 prediction: 4.0 with prob 0.3806835162846578
index: 99 prediction: 1.0 with prob 0.6615388897363154
index: 100 prediction: 1.0 with prob 0.6771449864921094
index: 101 prediction: 1.0 with prob 0.6882359783720613
index: 102 prediction: 1.0 with prob 0.48918119955887984
index: 103 prediction: 1.0 with prob 0.6949631728934702
index: 104 prediction: 3.0 with prob 0.5139334658530784
index: 105 prediction: 1.0 with prob 0.6496061219481237
index: 106 prediction: 1.0 with prob 0.5355294979950274
index: 107 prediction: 1.0 with prob 0.6316890810916571
index: 108 decide 3 with prob 0.4767774867453492
index: 109 prediction: 3.0 with prob 0.5603107206457932
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index: 9174 prediction: 4.0 with prob 0.9497876564986292
index: 9175 prediction: 4.0 with prob 0.7159658711955882
index: 9176 prediction: 1.0 with prob 0.4264543701825032
index: 9177 prediction: 2.0 with prob 0.6760260099722761
index: 9178 prediction: 4.0 with prob 0.6622275435068725
index: 9179 prediction: 1.0 with prob 0.44692621018113277
index: 9180 prediction: 4.0 with prob 0.8729895827140716
index: 9181 prediction: 4.0 with prob 0.8115803252697742

```

index: 9182 prediction: 4.0 with prob 0.8662679689009176
index: 9183 prediction: 4.0 with prob 0.8505127665113253
index: 9184 prediction: 4.0 with prob 0.9469792007118941
index: 9185 prediction: 4.0 with prob 0.6918601316881121
index: 9186 prediction: 4.0 with prob 0.47473914708660636
index: 9187 prediction: 4.0 with prob 0.9308812392417228
index: 9188 prediction: 4.0 with prob 0.9860135925921601
index: 9189 prediction: 4.0 with prob 0.9848208466271905
index: 9190 prediction: 4.0 with prob 0.6124237485376706
index: 9191 prediction: 4.0 with prob 0.9550493889987298
index: 9192 prediction: 4.0 with prob 0.9341680841022414
index: 9193 prediction: 4.0 with prob 0.9095511313154886
index: 9194 prediction: 4.0 with prob 0.7188852601029172
index: 9195 prediction: 4.0 with prob 0.799233752443988
index: 9196 prediction: 4.0 with prob 0.8997027585363737
index: 9197 prediction: 4.0 with prob 0.8897609556696232
index: 9198 prediction: 4.0 with prob 0.8223918245909572
index: 9199 prediction: 4.0 with prob 0.9016219992518577
index: 9200 prediction: 4.0 with prob 0.9970517543095393
index: 9201 prediction: 4.0 with prob 0.9999978026372733
index: 9202 prediction: 4.0 with prob 0.6700001823458309
index: 9203 prediction: 4.0 with prob 0.7329411168829112
index: 9204 prediction: 4.0 with prob 0.8189136791444145
index: 9205 prediction: 4.0 with prob 0.6919893460437131
index: 9206 prediction: 4.0 with prob 0.7551372101398145
index: 9207 prediction: 4.0 with prob 0.8628843197630727
index: 9208 prediction: 4.0 with prob 0.8889881394271834
index: 9209 prediction: 4.0 with prob 0.9956912841463976
index: 9210 prediction: 4.0 with prob 0.9816148872615446
index: 9211 prediction: 4.0 with prob 0.9832655291235379
index: 9212 prediction: 4.0 with prob 0.9921319890154435
index: 9213 prediction: 4.0 with prob 0.9592963248040703
index: 9214 prediction: 4.0 with prob 0.9729458340717195
index: 9215 prediction: 4.0 with prob 0.9434333652711713
index: 9216 prediction: 4.0 with prob 0.9101159205303582
index: 9217 prediction: 4.0 with prob 0.4315292904772117
index: 9218 prediction: 4.0 with prob 0.9606521294009962
index: 9219 prediction: 4.0 with prob 0.7657865313389989
index: 9220 prediction: 4.0 with prob 0.787991154425773
index: 9221 prediction: 4.0 with prob 0.7131150910426033

```

```

In [34]: totalCorrect=0
         for i in range(len(analysed)):
             if myPredsTrain[i][0]==enc.categories[i]:
                 totalCorrect+=1
         print('correct assignments:', totalCorrect)
         print('score:', totalCorrect/len(analysed)*100)
         finalCorr=np.corrcoef(myPredsTrain[:,0], enc.categories)
         print('correlation coefficient:', finalCorr[1,0])
         avgConf=np.average(myPredsTrain[:,1])
         print('average confidence:', avgConf)

```

```

correct assignments: 7118
score: 77.18499240945566
correlation coefficient: 0.6726454186881841
average confidence: 0.629607099334387

```

```
In [35]: def KF_svc(X,y,cost=1.0,gamma='scale',k=10):
    kf = KFold(n_splits=k, shuffle=True)
    model_scores=np.zeros(k)
    corr=np.zeros(k)
    #iterator
    it=iter(np.arange(k))

    model=svm.SVC(C=cost, kernel='rbf', gamma=gamma, probability=True)
    for train_index, test_index in kf.split(X, y):
        #split the dataset into two parts: (k-1)/k*n and (1/k)*n
        i=next(it)
        print('iteration', i)

        #split data
        X_train, X_test=X[train_index], X[test_index]
        y_train, y_test=y[train_index], y[test_index]
        #fit model
        model.fit(X_train, y_train)
        model_scores[i]=model.score(X_test,y_test)
        pred=model.predict(X_test)
        corr[i]=np.corrcoef(pred, y_test)[1,0]

    return model, model_scores, corr
```

```
In [36]: model7, score7, corr7=KF_svc(composition, enc.categories);
```

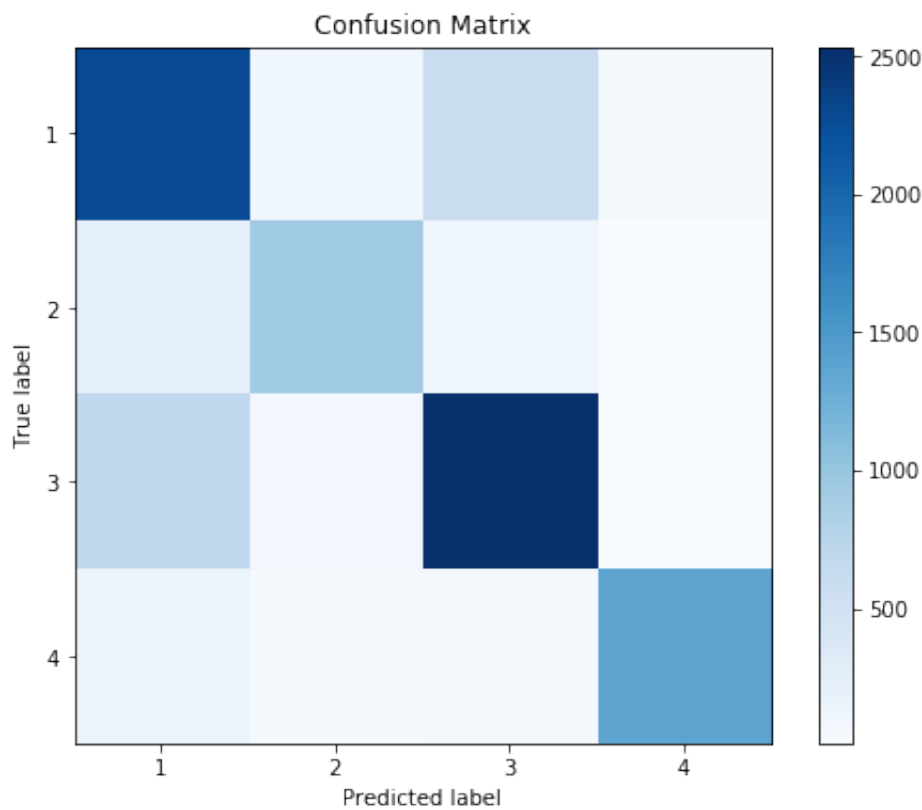
```
iteration 0
iteration 1
iteration 2
iteration 3
iteration 4
iteration 5
iteration 6
iteration 7
iteration 8
iteration 9
```

```
In [37]: for i in range(10):
          print(i, 'score:', np.round(score7[i],3), 'correlation:', np.ro
und(corr7[i],3))
          print('average score:', np.mean(score7))
          print('average coefficient:', np.mean(corr7))
```

```
0 score: 0.621 correlation: 0.432
1 score: 0.649 correlation: 0.503
2 score: 0.644 correlation: 0.473
3 score: 0.567 correlation: 0.391
4 score: 0.625 correlation: 0.499
5 score: 0.597 correlation: 0.431
6 score: 0.616 correlation: 0.434
7 score: 0.6 correlation: 0.419
8 score: 0.618 correlation: 0.446
9 score: 0.585 correlation: 0.413
average score: 0.6121182459348112
average coefficient: 0.44406434609830087
```

```
In [41]: labels=range(1,5)
          rates=confusion_matrix(y_true=enc.categories, y_pred= myPredsTrain[
          :,0], labels=labels)
          #plot heatmap
          cmap = 'hot'
          cmap='Blues'

          plt.figure(figsize=(8, 6))
          tick_marks = np.arange(len(labels))
          plt.xticks(tick_marks, labels)
          plt.yticks(tick_marks, labels)
          plt.imshow(rates, cmap, interpolation='nearest')
          plt.title('Confusion Matrix')
          plt.colorbar()
          plt.ylabel('True label')
          plt.xlabel('Predicted label')
          plt.show()
```



```
In [42]: predictions=myPredsTrain[:,0]
x=np.arange(len(dataCyto))
y1=predictions[0:len(dataCyto)]
y2=enc.categories[0:len(dataCyto)]
x1=x
x2=x
plt.plot(x1, y1, 'ro',label = "predictions")
plt.plot(x2, y2, label = "labels")
plt.xlabel('protein')
plt.ylabel('categories')
plt.title('compare predictions with labels\nCategory 1-Cytosolic')
plt.legend()
plt.figure(figsize=(30,10))
plt.show()

x=np.arange(len(dataCyto),len(dataCyto)+len(dataMito))
y1=predictions[len(dataCyto):len(dataCyto)+len(dataMito)]
y2=enc.categories[len(dataCyto):len(dataCyto)+len(dataMito)]
x1=x
x2=x
plt.plot(x1, y1, 'ro',label = "predictions")
plt.plot(x2, y2, label = "labels")
plt.xlabel('protein')
plt.ylabel('categories')
plt.title('compare predictions with labels\nCategory- Mitochondrial')
plt.legend()
plt.figure(figsize=(30,10))
plt.show()

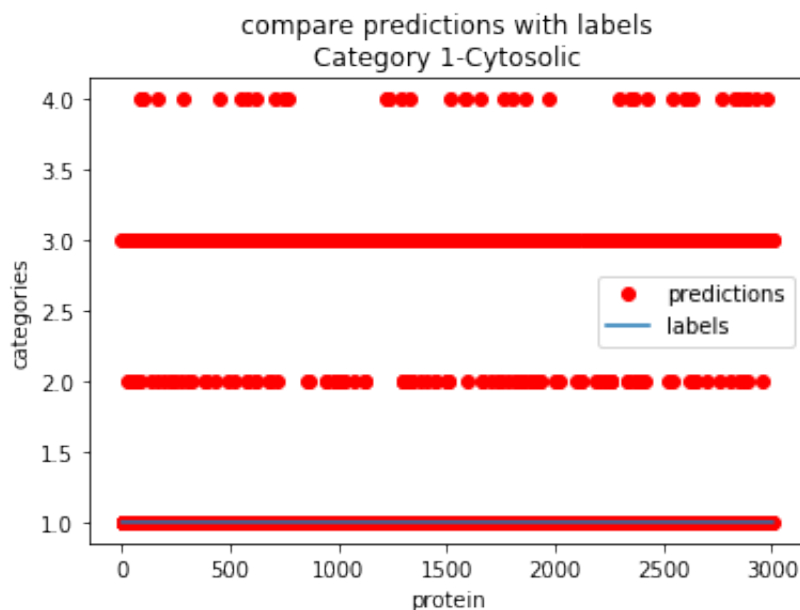
x=np.arange(len(dataCyto)+len(dataMito),len(dataCyto)+len(dataMito)+len(dataNucleus))
y1=predictions[len(dataCyto)+len(dataMito):len(dataCyto)+len(dataMi
```

```

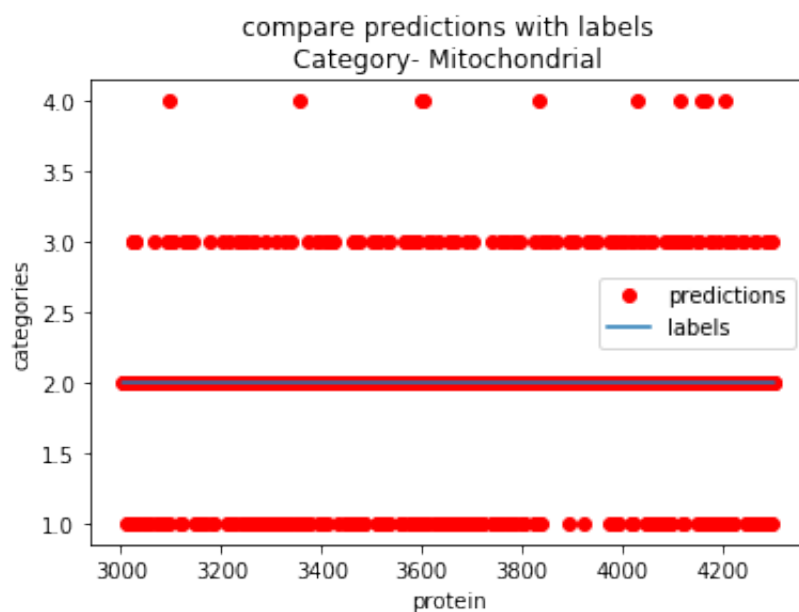
to)+len(dataNucleus)]
y2=enc.categories[len(dataCyto)+len(dataMito):len(dataCyto)+len(dat
aMito)+len(dataNucleus)]
x1=x
x2=x
plt.plot(x1, y1, 'ro',label = "predictions")
plt.plot(x2, y2, label = "labels")
plt.xlabel('protein')
plt.ylabel('categories')
plt.title('compare predictions with labels\nCategory 3-Nuclear')
plt.legend()
plt.figure(figsize=(30,10))
plt.show()

x=np.arange(len(dataCyto)+len(dataMito)+len(dataNucleus), 9222)
y1=predictions[len(dataCyto)+len(dataMito)+len(dataNucleus):]
y2=enc.categories[len(dataCyto)+len(dataMito)+len(dataNucleus):]
x1=x
x2=x
plt.plot(x1, y1, 'ro',label = "predictions")
plt.plot(x2, y2, label = "labels")
plt.xlabel('protein')
plt.ylabel('categories')
plt.title('compare predictions with labels\nCategory 4-Secreted')
plt.legend()
plt.figure(figsize=(30,10))
plt.show()

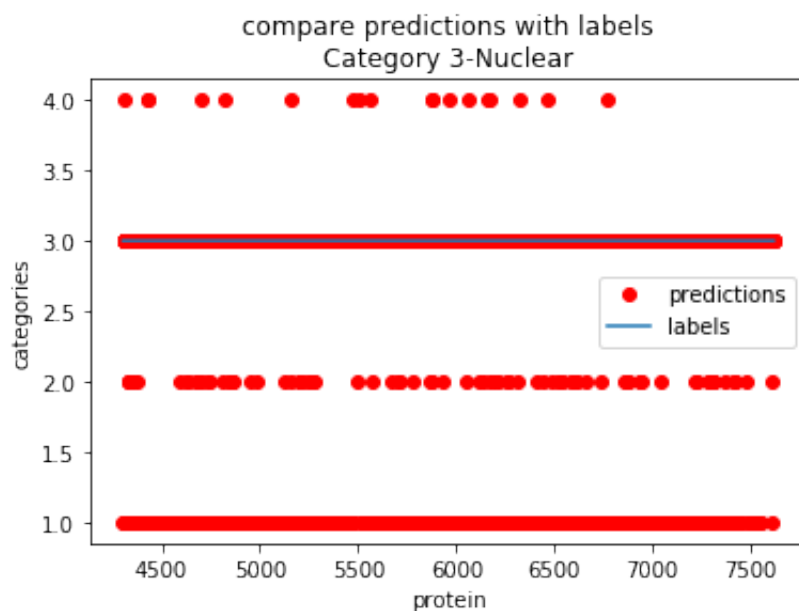
```



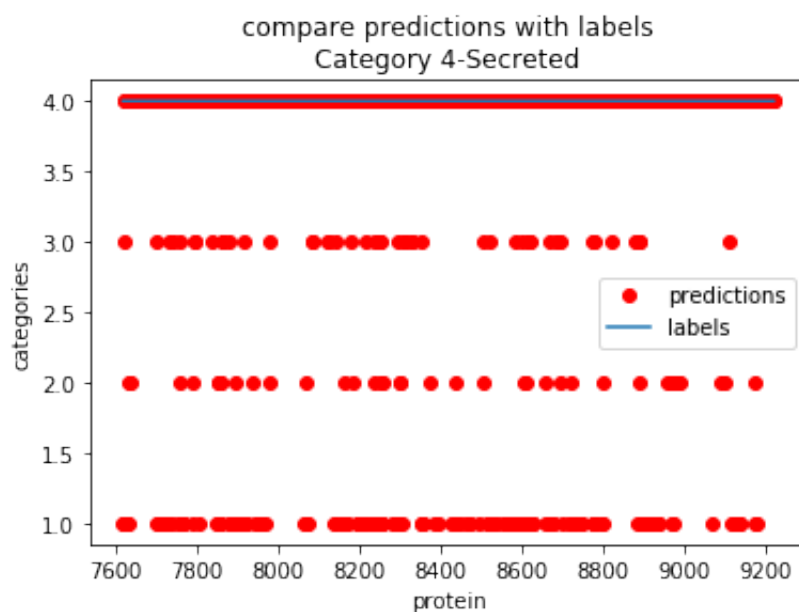
<Figure size 2160x720 with 0 Axes>



<Figure size 2160x720 with 0 Axes>



<Figure size 2160x720 with 0 Axes>



Testing

Make some predictions

```
In [43]: print('model 1:')
print('prediction:', model.predict([composition[0]]))
print('probClass1, probClass2, probClass3, probClass 4')
print(model.predict_proba([composition[0]]))
print('\nmodel 6:')
print('prediction:', model6.predict([composition[0]]))
print('probClass1, probClass2, probClass3, probClass 4')
print(model6.predict_proba([composition[0]]))
```

```
model 1:
prediction: [1.]
probClass1, probClass2, probClass3, probClass 4
[[0.46911443 0.0383588 0.46527591 0.02725086]]
```

```
model 6:
prediction: [3.]
probClass1, probClass2, probClass3, probClass 4
[[0.42489438 0.04610659 0.48956874 0.03943029]]
```

Analyse test data

```
In [44]: dataBlind=[]
for record in SeqIO.parse("blind.fasta.txt", "fasta"):
    dataBlind.append(record)
print('blind:', len(dataBlind))
```

```
blind: 20
```

```
In [45]: blind=[]
for i in range(len(dataBlind)):
    analysed_seq=ProteinAnalysis(str(dataBlind[i].seq))
    blind.append(analysed_seq)
```

```
In [46]: compBlind=np.zeros((len(dataBlind), 20))
for i in range(len(dataBlind)):
    dict=blind[i].get_amino_acids_percent()
    for pos,aa in enumerate(dict.values()):
        compBlind[i,pos]=aa
```

Calculate predictions for NuSVC model

```
In [47]: preds=np.zeros(len(dataBlind))
         for i in range(len(dataBlind)):
             preds[i]=model.predict([compBlind[i]])

         probs=np.zeros((len(dataBlind), 4))
         for i in range(len(dataBlind)):
             probs[i]=model.predict_proba([compBlind[i]])

         predProbs=np.array(np.argmax(probs, axis=1)+1)
```

```
In [48]: predProbs
```

```
Out[48]: array([1, 4, 4, 1, 4, 3, 1, 1, 1, 1, 2, 3, 4, 1, 3, 3, 4, 1, 1, 3])
```

```
In [49]: print("Predictions for SVC model")
         for i in range(len(dataBlind)):
             if preds[i]==predProbs[i]:
                 print('index:', i, 'prediction:', preds[i])
             else:
                 print('index:', i, 'predicts:', preds[i], 'from probability:',
                       predProbs[i], probs[i, int(predProbs[i]-1)])
```

Predictions for SVC model

```
index: 0 prediction: 1.0
index: 1 prediction: 4.0
index: 2 prediction: 4.0
index: 3 prediction: 1.0
index: 4 prediction: 4.0
index: 5 prediction: 3.0
index: 6 predicts: 2.0 from probability: 1 0.37694485726362037
index: 7 prediction: 1.0
index: 8 prediction: 1.0
index: 9 prediction: 1.0
index: 10 prediction: 2.0
index: 11 prediction: 3.0
index: 12 prediction: 4.0
index: 13 prediction: 1.0
index: 14 prediction: 3.0
index: 15 prediction: 3.0
index: 16 prediction: 4.0
index: 17 prediction: 1.0
index: 18 prediction: 1.0
index: 19 prediction: 3.0
```

```
In [50]: for i in range(len(dataBlind)):
        if preds[i]==1:
            print(dataBlind[i].name, 'Cytosolic, Confidence', np.round(
np.max(probs[i])*100), '%')
        elif preds[i]==2:
            print(dataBlind[i].name, 'Mitochondrial, Confidence', np.ro
und(np.max(probs[i])*100), '%')
        elif preds[i]==3:
            print(dataBlind[i].name, 'Nuclear, Confidence', np.round(np
.max(probs[i])*100), '%')
        elif preds[i]==4:
            print(dataBlind[i].name, 'Secreted, Confidence', np.round(n
p.max(probs[i])*100), '%')
```

```
SEQ677 Cytosolic, Confidence 46.0 %
SEQ231 Secreted, Confidence 75.0 %
SEQ871 Secreted, Confidence 55.0 %
SEQ388 Cytosolic, Confidence 46.0 %
SEQ122 Secreted, Confidence 64.0 %
SEQ758 Nuclear, Confidence 55.0 %
SEQ333 Mitochondrial, Confidence 38.0 %
SEQ937 Cytosolic, Confidence 69.0 %
SEQ351 Cytosolic, Confidence 45.0 %
SEQ202 Cytosolic, Confidence 40.0 %
SEQ608 Mitochondrial, Confidence 52.0 %
SEQ402 Nuclear, Confidence 46.0 %
SEQ433 Secreted, Confidence 99.0 %
SEQ821 Cytosolic, Confidence 46.0 %
SEQ322 Nuclear, Confidence 67.0 %
SEQ982 Nuclear, Confidence 71.0 %
SEQ951 Secreted, Confidence 35.0 %
SEQ173 Cytosolic, Confidence 53.0 %
SEQ862 Cytosolic, Confidence 42.0 %
SEQ224 Nuclear, Confidence 68.0 %
```

Calculcate predictions for combined model

```
In [51]: preds6=np.zeros(len(dataBlind))
        for i in range(len(dataBlind)):
            preds6[i]=model6.predict([compBlind[i]])

        probs6=np.zeros((len(dataBlind), 4))
        for i in range(len(dataBlind)):
            probs6[i]=model6.predict_proba([compBlind[i]])

        predProbs6=np.array(np.argmax(probs6, axis=1)+1)
```

```
In [52]: print("Predictions for combined model")
         for i in range(len(dataBlind)):
             if preds6[i]==predProbs6[i]:
                 print('index:', i, 'prediction:', preds6[i])
             else:
                 print('index:',i, 'predicts:', preds6[i], 'from probability
: ', predProbs6[i], probs6[i,int(predProbs6[i]-1)])
```

Predictions for combined model

```
index: 0 predicts: 4.0 from probability: 1 0.38485204262738076
index: 1 prediction: 4.0
index: 2 prediction: 4.0
index: 3 prediction: 1.0
index: 4 prediction: 4.0
index: 5 prediction: 3.0
index: 6 prediction: 2.0
index: 7 prediction: 1.0
index: 8 prediction: 1.0
index: 9 predicts: 2.0 from probability: 1 0.3559566482274185
index: 10 prediction: 2.0
index: 11 prediction: 3.0
index: 12 prediction: 4.0
index: 13 prediction: 1.0
index: 14 prediction: 3.0
index: 15 prediction: 3.0
index: 16 predicts: 4.0 from probability: 3 0.36998374800371653
index: 17 prediction: 1.0
index: 18 prediction: 1.0
index: 19 prediction: 3.0
```

```
In [53]: for i in range(len(dataBlind)):
        if preds6[i]==1:
            print(dataBlind[i].name, 'Cytosolic, Confidence', np.round(
np.max(probs6[i])*100), '%')
        elif preds6[i]==2:
            print(dataBlind[i].name, 'Mitochondrial, Confidence', np.ro
und(np.max(probs6[i])*100), '%')
        elif preds6[i]==3:
            print(dataBlind[i].name, 'Nuclear, Confidence', np.round(np
.max(probs6[i])*100), '%')
        elif preds6[i]==4:
            print(dataBlind[i].name, 'Secreted, Confidence', np.round(n
p.max(probs6[i])*100), '%')
```

```
SEQ677 Secreted, Confidence 38.0 %
SEQ231 Secreted, Confidence 61.0 %
SEQ871 Secreted, Confidence 51.0 %
SEQ388 Cytosolic, Confidence 44.0 %
SEQ122 Secreted, Confidence 43.0 %
SEQ758 Nuclear, Confidence 57.0 %
SEQ333 Mitochondrial, Confidence 39.0 %
SEQ937 Cytosolic, Confidence 69.0 %
SEQ351 Cytosolic, Confidence 41.0 %
SEQ202 Mitochondrial, Confidence 36.0 %
SEQ608 Mitochondrial, Confidence 46.0 %
SEQ402 Nuclear, Confidence 45.0 %
SEQ433 Secreted, Confidence 82.0 %
SEQ821 Cytosolic, Confidence 52.0 %
SEQ322 Nuclear, Confidence 66.0 %
SEQ982 Nuclear, Confidence 80.0 %
SEQ951 Secreted, Confidence 37.0 %
SEQ173 Cytosolic, Confidence 45.0 %
SEQ862 Cytosolic, Confidence 42.0 %
SEQ224 Nuclear, Confidence 60.0 %
```

Compare the two predictions

```

In [54]: ## if the two models agree then great, otherwise pick the prediction with max probability
print("Compare two predictions:")
myPreds=np.zeros((len(dataBlind), 2))

for i in range(len(dataBlind)):
    if preds[i]==preds6[i]:
        ans=preds[i]
        ansprob=max(probs[i, int(preds[i]-1)], probs6[i, int(preds6[i]-1)])
        print('index:', i, 'prediction:', ans, 'with prob', ansprob)
    else:
        a=np.max(probs[i])
        b=np.max(probs6[i])
        if a>b:
            ans=np.argmax(probs[i])+1
            ansprob=np.max(probs[i])
        else:
            ans=np.argmax(probs6[i])+1
            ansprob=np.max(probs6[i])
        print('index:',i, 'decide', ans, 'with prob', ansprob)
    myPreds[i]=ans,ansprob

```

Compare two predictions:

```

index: 0 decide 1 with prob 0.46479573742752245
index: 1 prediction: 4.0 with prob 0.7511174737621287
index: 2 prediction: 4.0 with prob 0.552585390415783
index: 3 prediction: 1.0 with prob 0.4588595917157157
index: 4 prediction: 4.0 with prob 0.6370291183739843
index: 5 prediction: 3.0 with prob 0.5717144404198428
index: 6 prediction: 2.0 with prob 0.3869057337474161
index: 7 prediction: 1.0 with prob 0.6925715030285949
index: 8 prediction: 1.0 with prob 0.4511865829276436
index: 9 decide 1 with prob 0.4039928268318301
index: 10 prediction: 2.0 with prob 0.5213453903216065
index: 11 prediction: 3.0 with prob 0.46283552265431516
index: 12 prediction: 4.0 with prob 0.9938994156180484
index: 13 prediction: 1.0 with prob 0.5183125436060017
index: 14 prediction: 3.0 with prob 0.6651989692070015
index: 15 prediction: 3.0 with prob 0.7955694177857213
index: 16 prediction: 4.0 with prob 0.34924163966033067
index: 17 prediction: 1.0 with prob 0.5262799893747406
index: 18 prediction: 1.0 with prob 0.4180816073615914
index: 19 prediction: 3.0 with prob 0.6772829762455578

```

```
In [55]: print(myPreds)
```

```
[[1.      0.46479574]
 [4.      0.75111747]
 [4.      0.55258539]
 [1.      0.45885959]
 [4.      0.63702912]
 [3.      0.57171444]
 [2.      0.38690573]
 [1.      0.6925715 ]
 [1.      0.45118658]
 [1.      0.40399283]
 [2.      0.52134539]
 [3.      0.46283552]
 [4.      0.99389942]
 [1.      0.51831254]
 [3.      0.66519897]
 [3.      0.79556942]
 [4.      0.34924164]
 [1.      0.52627999]
 [1.      0.41808161]
 [3.      0.67728298]]
```

Final Predictions


```
In [56]: for i in range(len(dataBlind)):
        if myPreds[i,0]==1:
            print(dataBlind[i].name, 'Cytosolic, Confidence', np.round(
myPreds[i,1]*100, 1), '%')
        elif myPreds[i,0]==2:
            print(dataBlind[i].name, 'Mitochondrial, Confidence', np.ro
und(myPreds[i,1]*100,1), '%')
        elif myPreds[i,0]==3:
            print(dataBlind[i].name, 'Nuclear, Confidence', np.round(my
Preds[i,1]*100,1), '%')
        elif myPreds[i,0]==4:
            print(dataBlind[i].name, 'Secreted, Confidence', np.round(m
yPreds[i,1]*100,1), '%')
```

```
SEQ677 Cytosolic, Confidence 46.5 %
SEQ231 Secreted, Confidence 75.1 %
SEQ871 Secreted, Confidence 55.3 %
SEQ388 Cytosolic, Confidence 45.9 %
SEQ122 Secreted, Confidence 63.7 %
SEQ758 Nuclear, Confidence 57.2 %
SEQ333 Mitochondrial, Confidence 38.7 %
SEQ937 Cytosolic, Confidence 69.3 %
SEQ351 Cytosolic, Confidence 45.1 %
SEQ202 Cytosolic, Confidence 40.4 %
SEQ608 Mitochondrial, Confidence 52.1 %
SEQ402 Nuclear, Confidence 46.3 %
SEQ433 Secreted, Confidence 99.4 %
SEQ821 Cytosolic, Confidence 51.8 %
SEQ322 Nuclear, Confidence 66.5 %
SEQ982 Nuclear, Confidence 79.6 %
SEQ951 Secreted, Confidence 34.9 %
SEQ173 Cytosolic, Confidence 52.6 %
SEQ862 Cytosolic, Confidence 41.8 %
SEQ224 Nuclear, Confidence 67.7 %
```

Further testing

(only run if you want to test on further data)

Analyse the data

```
In [ ]: furtherData=[]

#####change the filename to match the file you want to test
##For further information see README.md
for record in SeqIO.parse("filename.txt", "fasta"):
    furtherData.append(record)
print('furtherData:', len(furtherData))

furtherSequences=[]
for i in range(len(furtherData)):
    analysed_seq=ProteinAnalysis(str(furtherData[i].seq))
    furtherSequences.append(analysed_seq)

compFurther=np.zeros((len(furtherData), 20))
for i in range(len(furtherData)):
    dict=furtherSequences[i].get_amino_acids_percent()
    for pos,aa in enumerate(dict.values()):
        compFurther[i,pos]=aa
```

Make predictions on further data

```

In [ ]: #model 1
predsF=np.zeros(len(furtherData))
for i in range(len(furtherData)):
    predsF[i]=model.predict([compFurther[i]])

probsF=np.zeros((len(furtherData), 4))
for i in range(len(furtherData)):
    probsF[i]=model.predict_proba([compFurther[i]])

predProbsF=np.array(np.argmax(probsF, axis=1)+1)

#model 6
preds6F=np.zeros(len(furtherData))
for i in range(len(furtherData)):
    preds6F[i]=model6.predict([compFurther[i]])

probs6F=np.zeros((len(furtherData), 4))
for i in range(len(furtherData)):
    probs6F[i]=model6.predict_proba([compFurther[i]])

predProbs6F=np.array(np.argmax(probs6F, axis=1)+1)

print("Predictions:")
myPredsF=np.zeros((len(furtherData), 2))

for i in range(len(furtherData)):
    if predsF[i]==preds6F[i]:
        ans=predsF[i]
        ansprob=max(probsF[i, int(predsF[i]-1)], probs6F[i, int(preds6F[i]-1)])
    else:
        a=np.max(probsF[i])
        b=np.max(probs6F[i])
        if a>b:
            ans=np.argmax(probsF[i])+1
            ansprob=np.max(probsF[i])
        else:
            ans=np.argmax(probs6F[i])+1
            ansprob=np.max(probs6F[i])
    myPredsF[i]=ans,ansprob

for i in range(len(furtherData)):
    if myPredsF[i,0]==1:
        print(furtherData[i].name, 'Cytosolic, Confidence', np.round(myPredsF[i,1]*100), '%')
    elif myPredsF[i,0]==2:
        print(furtherData[i].name, 'Mitochondrial, Confidence', np.round(myPredsF[i,1]*100), '%')
    elif myPredsF[i,0]==3:
        print(furtherData[i].name, 'Nuclear, Confidence', np.round(myPredsF[i,1]*100), '%')
    elif myPredsF[i,0]==4:
        print(furtherData[i].name, 'Secreted, Confidence', np.round(myPredsF[i,1]*100), '%')

```

