In [1]:

```
#Dataset
#import needed libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

#read in csv data
prot_data = pd.read_csv("77_cancer_proteomes_CPTAC_itraq.csv")
clin_data_original = pd.read_csv("clinical_data_breast_cancer.csv",index_col = "C
```

In [2]:

```
#Table of frequencies of target values
print "Number of Samples in Clinical Data:", len(pd.DataFrame(clin_data_original[

freq_target_variable = pd.DataFrame(clin_data_original['AJCC Stage'].value_counts
freq_target_variable.columns = ['Frequency']
freq_target_variable
```

```
Number of Samples in Clinical Data: 105
```

Out[2]:

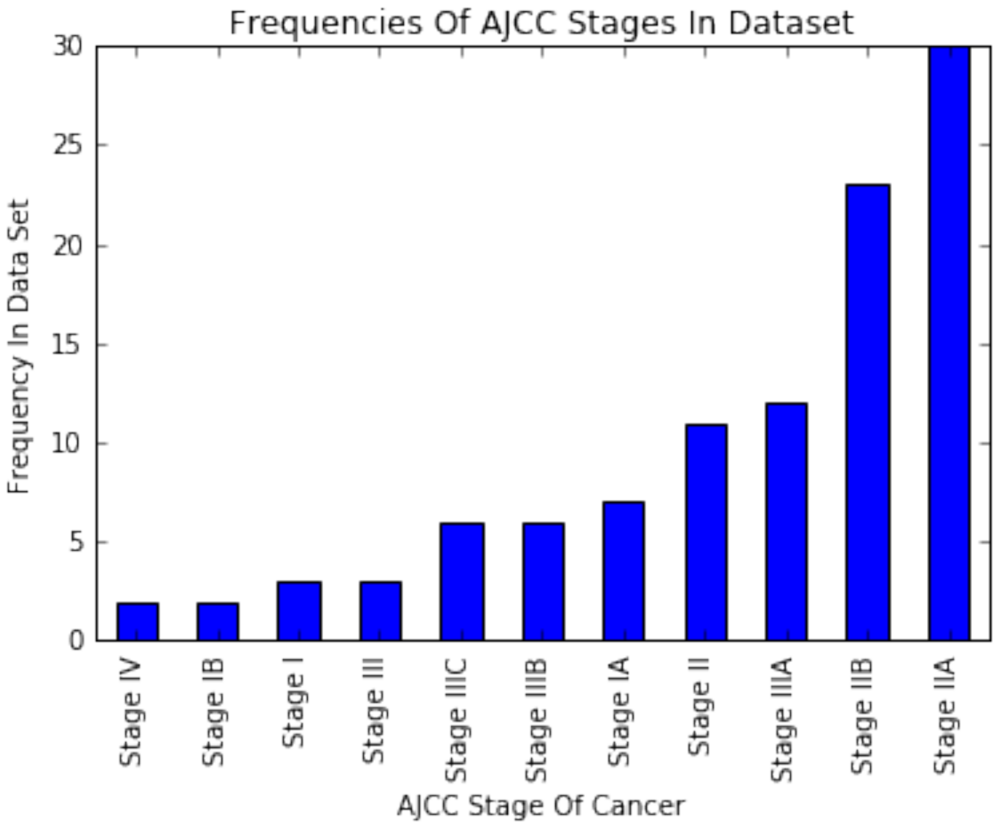
	Frequency
Stage IV	2
Stage IB	2
Stage I	3
Stage III	3
Stage IIIC	6
Stage IIIB	6
Stage IA	7
Stage II	11
Stage IIIA	12
Stage IIB	23
Stage IIA	30

In [3]:

```
#Plot frequencies of target categories
freq_stage_raw = clin_data_original['AJCC Stage'].value_counts(ascending=True)

freq_stage_raw = freq_stage_raw.plot(kind='bar')
freq_stage_raw.set_xlabel("AJCC Stage Of Cancer")
freq_stage_raw.set_ylabel("Frequency In Data Set")
freq_stage_raw.set_title("Frequencies Of AJCC Stages In Dataset")
```

Out[3]:

```
<matplotlib.text.Text at 0x115437f90>
```



In [4]:

```
#Description of protein data, overall statistics on proteins of each patient.
print "Number Of Samples in Protein Data:", len(prot_data.columns)

prot_data.describe().round(2)
```

Number Of Samples in Protein Data: 86

Out[4]:

	AO-A12D.01TCGA	C8-A131.01TCGA	AO-A12B.01TCGA	BH-A18Q.02TCGA	C8-A130.02TCGA	C8 A1
count	11334.00	11335.00	11334.00	12024.00	12025.00	11
mean	0.13	0.13	-0.44	-0.73	-0.04	0.1
std	1.73	1.58	1.63	2.42	1.35	1.6
min	-12.47	-13.16	-9.91	-24.55	-15.00	-12
25%	-0.66	-0.58	-1.33	-1.27	-0.67	-0.
50%	0.08	0.12	-0.32	-0.30	0.02	0.0
75%	0.91	0.85	0.49	0.45	0.72	0.9
max	17.62	12.68	8.29	11.79	6.93	10

8 rows × 83 columns

In [5]:

```
#find decriptions of proteins overall
#read the table row first, for example the mean of the standard deviations would
prot_data.describe().transpose().describe().round(2)
```

Out[5]:

	count	mean	std	min	25%	50%	75%	max
count	83.00	83.00	83.00	83.00	83.00	83.00	83.00	83.00
mean	11238.78	-0.20	1.74	-14.03	-0.95	-0.08	0.71	10.41
std	472.24	0.33	0.26	3.13	0.36	0.19	0.18	2.19
min	9693.00	-1.49	1.31	-24.55	-2.91	-0.95	0.27	6.44
25%	10949.50	-0.35	1.57	-15.40	-1.06	-0.19	0.58	8.76
50%	11280.00	-0.11	1.67	-13.60	-0.87	-0.04	0.71	10.08
75%	11515.50	-0.00	1.87	-12.11	-0.74	0.03	0.83	11.78
max	12025.00	0.49	2.54	-6.33	-0.50	0.31	1.28	17.62

In [6]:

```
#create copy of protein and process it to have a single gene column to use as an
prot_data['gene_symbol'].fillna("NA",inplace = True)
prot_data['gene'] = prot_data['RefSeq_accession_number'] + " - " + prot_data['gen
                    prot_data['gene_symbol']
prot_data = prot_data.set_index('gene')
prot_data = prot_data.drop(['gene_name','gene_symbol','RefSeq_accession_number'],

#drop missing data rows, and transpose data to line up with clin_data
prot_data_reduced = prot_data.dropna(axis = 0)
prot_data_reduced = prot_data_reduced.transpose()

#change naming of prot_data index to line up with clin_data. Move TCGA- to beginn
prot_data_reduced.index = pd.Series([val[10:14] + "-" + val[0:7]
                                     for val in prot_data_reduced.index], index =
prot_data_reduced.index.rename("Complete TCGA ID",inplace = True)

#sort dataframe
prot_data_reduced = prot_data_reduced.sort_index()
```

In [7]:

```
#find decriptions of proteins overall for processed protein data
prot_data_reduced.transpose().describe().transpose().describe().round(2)
```

Out[7]:

	count	mean	std	min	25%	50%	75%	max
count	83	83.00	83.00	83.00	83.00	83.00	83.00	83.00
mean	7994	-0.11	1.46	-11.63	-0.80	-0.05	0.65	8.44
std	0	0.20	0.15	2.25	0.21	0.12	0.13	1.70
min	7994	-0.86	1.08	-16.70	-1.87	-0.55	0.35	5.13
25%	7994	-0.22	1.36	-13.15	-0.86	-0.12	0.57	7.13
50%	7994	-0.11	1.48	-11.65	-0.76	-0.05	0.64	8.35
75%	7994	0.01	1.54	-10.23	-0.67	0.02	0.73	9.56
max	7994	0.39	1.91	-5.71	-0.52	0.23	1.14	13.22

In [8]:

```
#Discover duplicate patient identifiers
prot_data_reduced.index.value_counts().head()
```

Out[8]:

```
TCGA-AO-A12B    2
TCGA-C8-A131    2
TCGA-AO-A12D    2
TCGA-AO-A0JC    1
TCGA-BH-A0DG    1
Name: Complete TCGA ID, dtype: int64
```

In [9]:

```
#renaming duplicate indexes and dropping them
for i in range(1,len(prot_data_reduced)):
    if prot_data_reduced.index[i] == prot_data_reduced.index[i-1]:
        prot_range = prot_data_reduced.index.values
        prot_range[i] = prot_data_reduced.index[i] + "B"
        drop = prot_data_reduced.index[i] + "B"
        prot_data_reduced.set_index(prot_range)
        prot_data_reduced.drop([drop,0])
```

In [10]:

```
#check all duplicates dropped
prot_data_reduced.index.value_counts().head()
```

Out[10]:

```
TCGA-AO-A0JC    1
TCGA-A2-A0EX    1
TCGA-A2-A0EV    1
TCGA-A8-A06N    1
PTAC-263d3f-    1
Name: Complete TCGA ID, dtype: int64
```

In [11]:

```
#Clinical data description
clin_data_original.describe().round(2)
```

Out[11]:

	Age at Initial Pathologic Diagnosis	Days to Date of Last Contact	Days to date of Death	OS event	OS Time	SigClust Unsupervised mRNA	SigClust Intrinsic mRNA	miRNA Cluster
count	105.00	105.00	11.00	105.00	105.00	105.00	105.00	105.00
mean	58.69	788.39	1254.45	0.10	817.65	-4.89	-7.18	4.00
std	13.07	645.28	678.05	0.31	672.03	3.56	5.02	1.59
min	30.00	0.00	160.00	0.00	0.00	-12.00	-13.00	1.00
25%	49.00	240.00	947.50	0.00	240.00	-6.00	-12.00	3.00
50%	58.00	643.00	1364.00	0.00	665.00	-5.00	-6.00	4.00
75%	67.00	1288.00	1627.50	0.00	1305.00	-3.00	-2.00	5.00
max	88.00	2850.00	2483.00	1.00	2850.00	0.00	0.00	7.00

In [12]:

```
#remove clin_data column with NAs
clin_data_original = clin_data_original.dropna(axis = 1)
```

In [13]:

```
clin_data_original.describe().round(2)
```

Out[13]:

	Age at Initial Pathologic Diagnosis	Days to Date of Last Contact	OS event	OS Time	SigClust Unsupervised mRNA	SigClust Intrinsic mRNA	miRNA Clusters	methyl Cluste
count	105.00	105.00	105.00	105.00	105.00	105.00	105.00	105.00
mean	58.69	788.39	0.10	817.65	-4.89	-7.18	4.00	3.34
std	13.07	645.28	0.31	672.03	3.56	5.02	1.59	1.41
min	30.00	0.00	0.00	0.00	-12.00	-13.00	1.00	1.00
25%	49.00	240.00	0.00	240.00	-6.00	-12.00	3.00	2.00
50%	58.00	643.00	0.00	665.00	-5.00	-6.00	4.00	4.00
75%	67.00	1288.00	0.00	1305.00	-3.00	-2.00	5.00	4.00
max	88.00	2850.00	1.00	2850.00	0.00	0.00	7.00	5.00

In [14]:

```
#combine protein data and clinical data to ensure matched indexes and get rid of
#info
combined_table = clin_data_original.join(prot_data_reduced)
```

In [15]:

```
#check for rows in clinical data without protein data
combined_table.describe().round(2)
```

Out[15]:

	Age at Initial Pathologic Diagnosis	Days to Date of Last Contact	OS event	OS Time	SigClust Unsupervised mRNA	SigClust Intrinsic mRNA	miRNA Clusters	methyl Cluste
count	105.00	105.00	105.00	105.00	105.00	105.00	105.00	105.00
mean	58.69	788.39	0.10	817.65	-4.89	-7.18	4.00	3.34
std	13.07	645.28	0.31	672.03	3.56	5.02	1.59	1.41
min	30.00	0.00	0.00	0.00	-12.00	-13.00	1.00	1.00
25%	49.00	240.00	0.00	240.00	-6.00	-12.00	3.00	2.00
50%	58.00	643.00	0.00	665.00	-5.00	-6.00	4.00	4.00
75%	67.00	1288.00	0.00	1305.00	-3.00	-2.00	5.00	4.00
max	88.00	2850.00	1.00	2850.00	0.00	0.00	7.00	5.00

8 rows × 8006 columns

In [16]:

```
#drop these rows
combined_table = combined_table.dropna(axis = 0)
```

In [17]:

```
#Counts of each column now match
combined_table.describe().round(2)
```

Out[17]:

	Age at Initial Pathologic Diagnosis	Days to Date of Last Contact	OS event	OS Time	SigClust Unsupervised mRNA	SigClust Intrinsic mRNA	miRNA Clusters	methyla Cluster
count	77.00	77.00	77.00	77.00	77.00	77.00	77.00	77.00
mean	58.91	846.53	0.09	870.88	-4.66	-7.23	4.03	3.42
std	13.41	692.00	0.29	717.15	3.43	5.01	1.59	1.35
min	30.00	0.00	0.00	0.00	-12.00	-13.00	1.00	1.00
25%	50.00	230.00	0.00	230.00	-5.00	-12.00	3.00	2.00
50%	59.00	769.00	0.00	769.00	-5.00	-6.00	4.00	4.00
75%	67.00	1319.00	0.00	1364.00	-3.00	-2.00	5.00	4.00
max	88.00	2850.00	1.00	2850.00	0.00	0.00	7.00	5.00

8 rows × 8006 columns

In [18]:

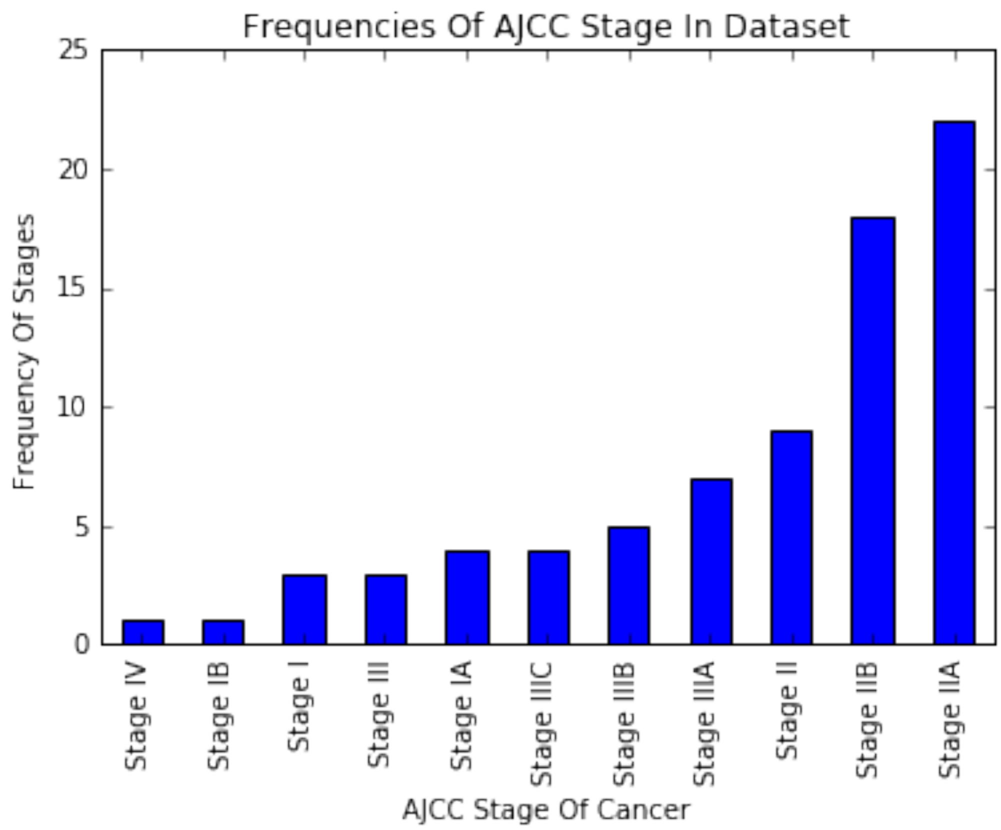
```
#interesting columns for reference
target_column = ['AJCC Stage']
subtarget_columns = ['Metastasis','Tumor','Node']
other_clusterings = ['miRNA Clusters']
```

In [19]:

```
#reduced dataset categories
freq_stage_processed = combined_table['AJCC Stage'].value_counts(ascending=True)

freq_stage_processed = freq_stage_processed.plot(kind='bar')
freq_stage_processed.set_xlabel('AJCC Stage Of Cancer')
freq_stage_processed.set_ylabel('Frequency Of Stages')
freq_stage_processed.set_title('Frequencies Of AJCC Stage In Dataset')
```

Out[19]:

```
<matplotlib.text.Text at 0x10401fa50>
```



In [20]:

```
#reduce subclasses to classes in AJCC Stage
combined_table['AJCC Stage Classes'] = pd.Series([val.replace("B","").replace("A"
                                                  for val in combined_table['AJCC
                                                  index = combined_table.index)
```

In [21]:

```
freq_target_variable['Frequency Without Subdivisions'] = combined_table['AJCC Sta
freq_target_variable.fillna("-",inplace=True)
freq_target_variable.sort_index()
```

Out[21]:

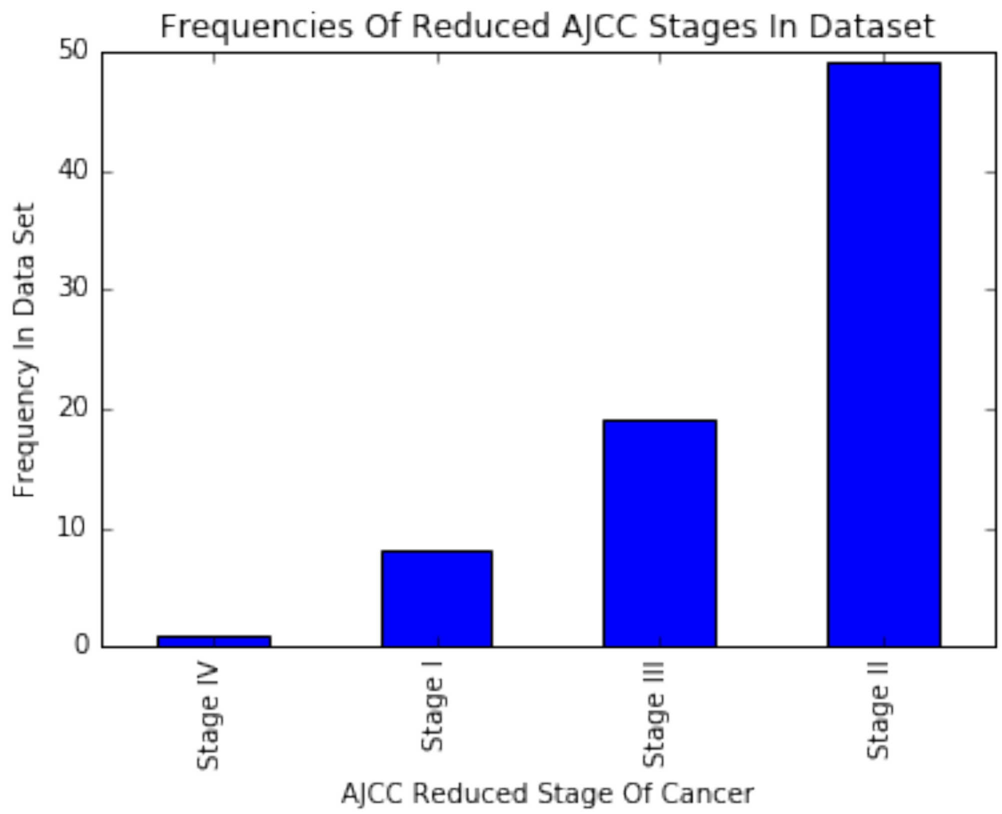
	Frequency	Frequency Without Subdivisions
Stage I	3	8
Stage IA	7	-
Stage IB	2	-
Stage II	11	49
Stage IIA	30	-
Stage IIB	23	-
Stage III	3	19
Stage IIIA	12	-
Stage IIIB	6	-
Stage IIIC	6	-
Stage IV	2	1

In [22]:

```
#AJCC Stage Classes
freq_reduced_stage_processed = combined_table['AJCC Stage Classes'].value_counts(

freq_reduced_stage_processed = freq_reduced_stage_processed.plot(kind='bar')
freq_reduced_stage_processed.set_xlabel("AJCC Reduced Stage Of Cancer")
freq_reduced_stage_processed.set_ylabel("Frequency In Data Set")
freq_reduced_stage_processed.set_title("Frequencies Of Reduced AJCC Stages In Dat
```

Out[22]:

```
<matplotlib.text.Text at 0x11ac15810>
```



In [23]:

```
#under-represented subclasses (those with one entry)
print combined_table['AJCC Stage'][combined_table['AJCC Stage'] == "Stage IV"]
print combined_table['AJCC Stage'][combined_table['AJCC Stage'] == "Stage IB"]
```

```
Complete TCGA ID
TCGA-A2-A0SW    Stage IV
Name: AJCC Stage, dtype: object
Complete TCGA ID
TCGA-C8-A12U    Stage IB
Name: AJCC Stage, dtype: object
```

In [24]:

```
#dropping these as potential outliers
combined_table.drop("TCGA-A2-A0SW", axis = 0, inplace = True)
combined_table.drop("TCGA-C8-A12U", axis = 0, inplace = True)
```

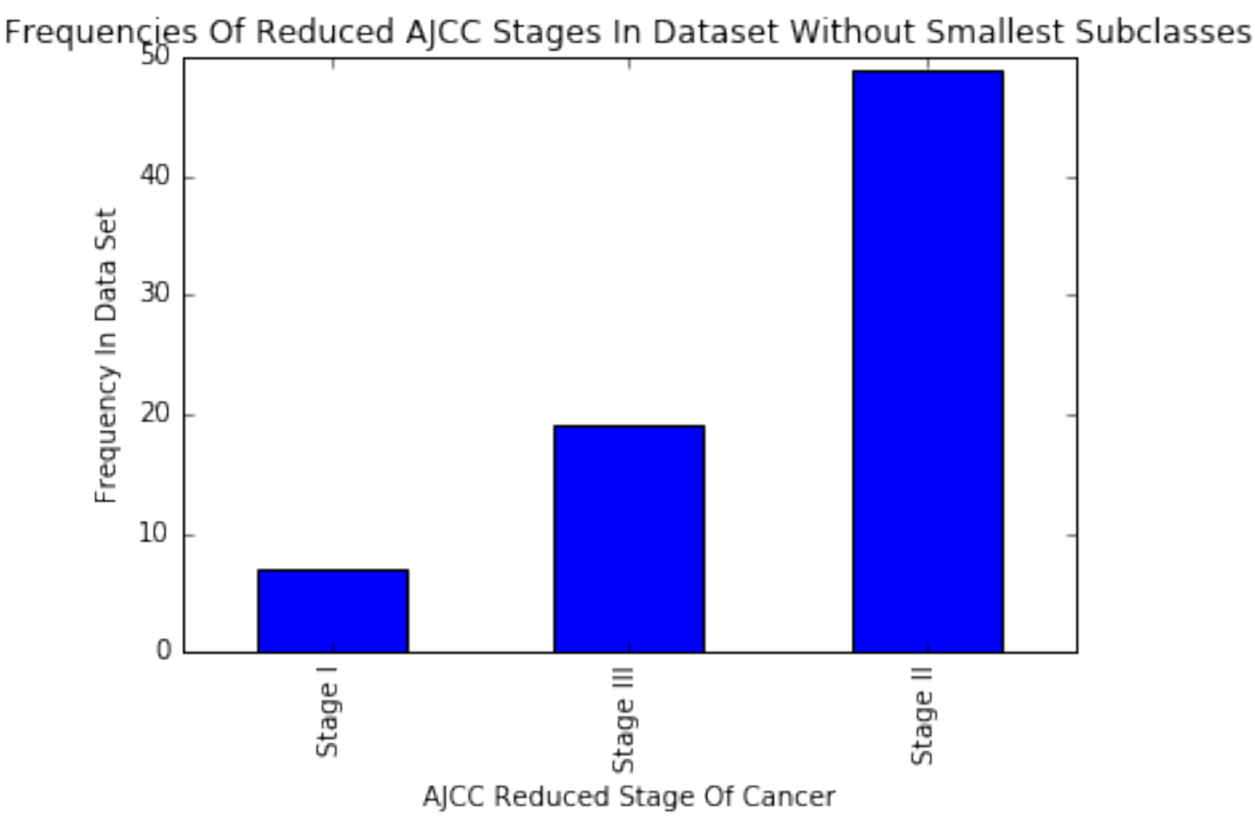
In [25]:

```
print "Frequency Of Target Classes"
print combined_table['AJCC Stage Classes'].value_counts(ascending=True)

freq_reduced_stage_processed_cut = combined_table['AJCC Stage Classes'].value_cou

freq_reduced_stage_processed_cut = freq_reduced_stage_processed_cut.plot(kind='ba
freq_reduced_stage_processed_cut.set_xlabel("AJCC Reduced Stage Of Cancer")
freq_reduced_stage_processed_cut.set_ylabel("Frequency In Data Set")
freq_reduced_stage_processed_cut.set_title("Frequencies Of Reduced AJCC Stages In
```

```
Frequency Of Target Classes
Stage I       7
Stage III    19
Stage II     49
Name: AJCC Stage Classes, dtype: int64
```

Out[25]:

```
<matplotlib.text.Text at 0x11af8ae50>
```



In [26]:

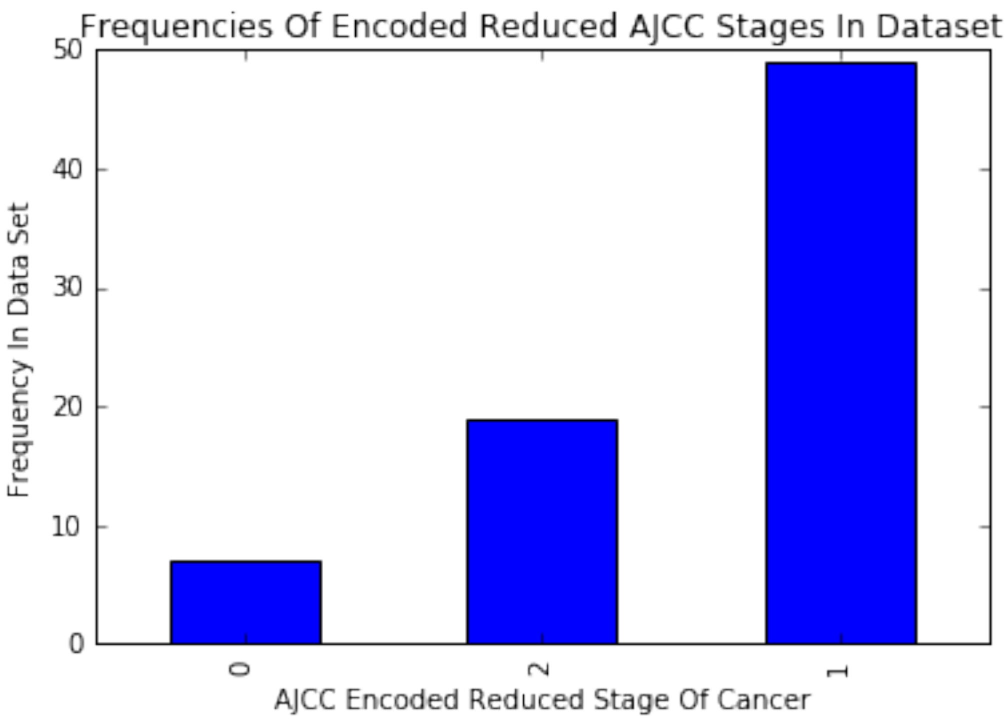
```
#encoding target
from sklearn.preprocessing import LabelEncoder
lbl_enc = LabelEncoder().fit(combined_table['AJCC Stage Classes'])
combined_table['AJCC Stage Classes'] = lbl_enc.transform(combined_table['AJCC Sta
```

In [27]:

```
#Coded targets
freq_reduced_stage_encoded = combined_table['AJCC Stage Classes'].value_counts(as

freq_reduced_stage_encoded = freq_reduced_stage_encoded.plot(kind='bar')
freq_reduced_stage_encoded.set_xlabel("AJCC Encoded Reduced Stage Of Cancer")
freq_reduced_stage_encoded.set_ylabel("Frequency In Data Set")
freq_reduced_stage_encoded.set_title("Frequencies Of Encoded Reduced AJCC Stages
```

Out[27]:

```
<matplotlib.text.Text at 0x11b238ed0>
```



In [28]:

```
#data columns
protein_columns = [val for val in combined_table.columns if "NP_" in val or "XP_"
combined_table_proteins = combined_table[protein_columns]
```

In [29]:

```
#Data Splitting
from sklearn.model_selection import StratifiedShuffleSplit

def split_data(data,target,eval_size):
    kf = StratifiedShuffleSplit(n_splits = 1, test_size = eval_size, random_state
    for train_indice, valid_indice in kf.split(data,target):
        X_train, X_valid = data.iloc[train_indice], data.iloc[valid_indice]
        y_train, y_valid = target.iloc[train_indice],target.iloc[valid_indice]
    return X_train, y_train, X_valid, y_valid
```

In [30]:

```
#Dummy classifier for benchmark
from sklearn.dummy import DummyClassifier

def dummy_clf(val,score):
    X_train_prot, y_train_prot, X_valid_prot, y_valid_prot = split_data(combined_
                                                                         combined_
    dummy_clf = DummyClassifier(strategy = 'most_frequent').fit(X_train_prot,y_tr
    score = score(y_valid_prot,dummy_clf.predict(X_valid_prot),average = 'weighte
    return score
```

In [31]:

```
#import possible scoring metrics
from sklearn.metrics import accuracy_score
from sklearn.metrics import f1_score
from sklearn.metrics import log_loss
from sklearn.metrics import cohen_kappa_score
from sklearn.metrics import hinge_loss
from sklearn.metrics import fbeta_score
from sklearn.metrics import hamming_loss
from sklearn.metrics import precision_score
from sklearn.metrics import recall_score
```

In [32]:

```
#Dummy scores for targets and other categories of interest
exploriative = pd.DataFrame(index = target_column + subtarget_columns + other_clu
exploriative['Unique Values'] = [len(combined_table[val].unique()) for val in exp
exploriative['Mode'] = [combined_table[val].mode().iloc[0] for val in exploriativ
exploriative['Dummy Score'] = [dummy_clf(val,f1_score) for val in exploriative.in
print exploriative
```

```
                    Unique Values       Mode  Dummy Score
AJCC Stage                      9  Stage IIA         0.14
Metastasis                      1         M0         1.00
Tumor                           4         T2         0.53
Node                            4         N0         0.35
miRNA Clusters                  7          4         0.20
AJCC Stage Classes              3          1         0.53

/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/sklearn/met
rics/classification.py:1113: UndefinedMetricWarning: F-score is ill-
defined and being set to 0.0 in labels with no predicted samples.
  'precision', 'predicted', average, warn_for)
```

In [33]:

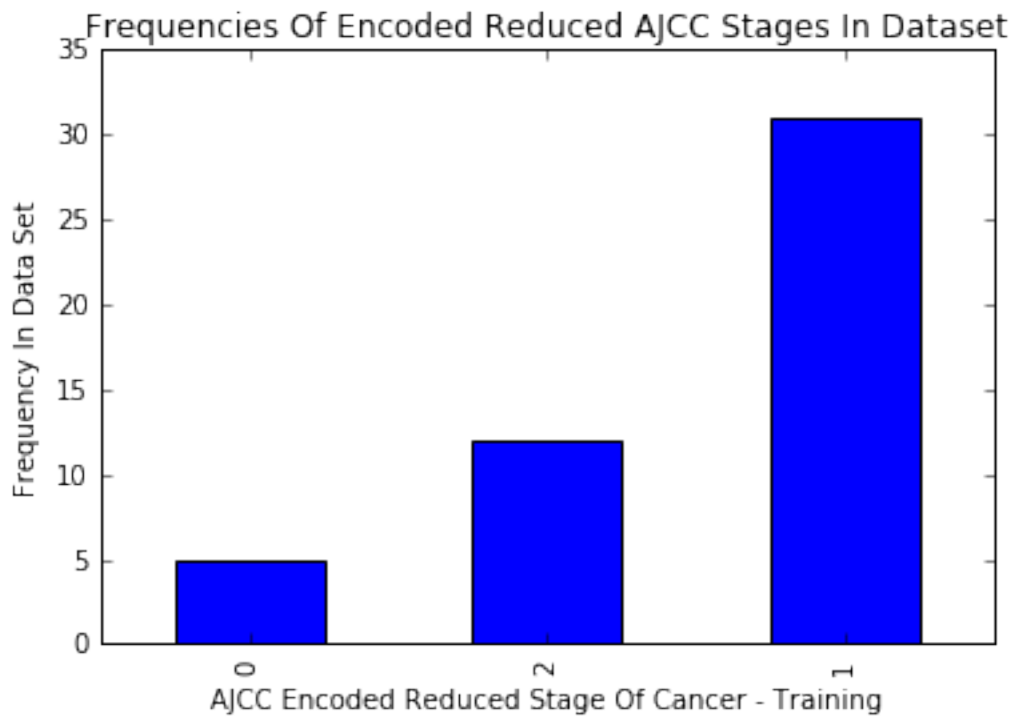
```
#split data into train and test
X_train_prot, y_train_prot, X_valid_prot, y_valid_prot = split_data(combined_tabl
                                                                     combined_tabl
```

In [34]:

```
#Training set sizes
freq_reduced_stage_training_encoded = y_train_prot.value_counts(ascending=True)

freq_reduced_stage_training_encoded = freq_reduced_stage_training_encoded.plot(ki
freq_reduced_stage_training_encoded.set_xlabel("AJCC Encoded Reduced Stage Of Can
freq_reduced_stage_training_encoded.set_ylabel("Frequency In Data Set")
freq_reduced_stage_training_encoded.set_title("Frequencies Of Encoded Reduced AJC
```

Out[34]:

```
<matplotlib.text.Text at 0x11b4ebad0>
```

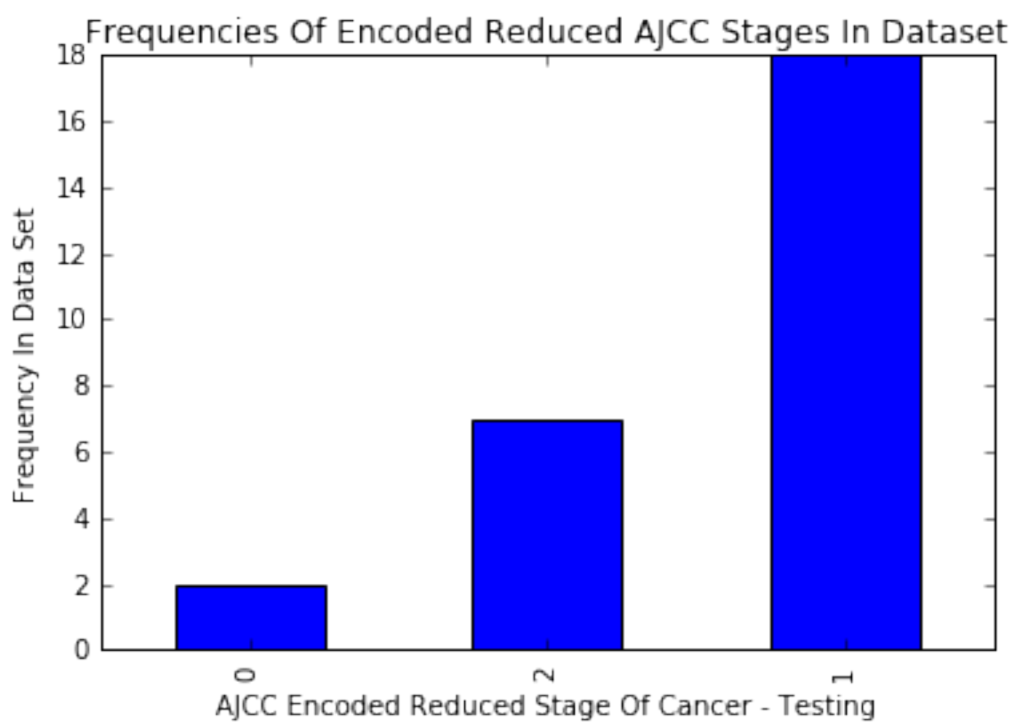


In [35]:

```
#Test set category sizes
freq_reduced_stage_testing_encoded = y_valid_prot.value_counts(ascending=True)

freq_reduced_stage_testing_encoded = freq_reduced_stage_testing_encoded.plot(kind
freq_reduced_stage_testing_encoded.set_xlabel("AJCC Encoded Reduced Stage Of Canc
freq_reduced_stage_testing_encoded.set_ylabel("Frequency In Data Set")
freq_reduced_stage_testing_encoded.set_title("Frequencies Of Encoded Reduced AJCC
```

Out[35]:

```
<matplotlib.text.Text at 0x11c506450>
```



In [36]:

```
#train default algorithms
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.naive_bayes import GaussianNB
from sklearn.svm import SVC
from sklearn.cluster import KMeans
import xgboost as xgb
from xgboost import XGBClassifier

rfc = RandomForestClassifier(random_state = 0)
xgb = XGBClassifier(seed = 0)
lgr = LogisticRegression(random_state = 0)
kmm = KMeans(random_state = 0)
svm = SVC(random_state = 0, probability = True)
gnb = GaussianNB()
```

In [37]:

```
rfc_trained = rfc.fit(X_train_prot,y_train_prot)
xgb_trained = xgb.fit(X_train_prot,y_train_prot)
lgr_trained = lgr.fit(X_train_prot,y_train_prot)
kmm_trained = kmm.fit(X_train_prot,y_train_prot)
gnb_trained = GaussianNB().fit(X_train_prot,y_train_prot)
svm_trained = svm.fit(X_train_prot,y_train_prot)
```

In [38]:

```
#Create Scoring Grid
models = ['Random Forest','Gradient Boosting','Logistic Regression','KMeans','Nai
model_codes = [rfc_trained,xgb_trained,lgr_trained,kmm_trained,gnb_trained,svm_tr
scores = [f1_score,accuracy_score,cohen_kappa_score,log_loss,"score",hinge_loss,f
          precision_score,recall_score]
scoring_names = ['F1 Score','Accuracy','Kappa','Log Loss','Score','Hinge Loss','F
                 'Precision','Recall Score']
scoring_grid = pd.DataFrame(index = models)
```

In [39]:

```
def create_scoring_grid(data,target,scoring_grid,models):
    for i in range(len(scores)):
        score = []
        for j in models:
            if (scores[i] == log_loss or scores[i] == hinge_loss):
                try:
                    score.append(scores[i](target,j.predict_proba(data)).round(2)
                except:
                    score.append("-")
            elif (scores[i] == f1_score or scores[i] == precision_score or scores
                score.append(scores[i](target,j.predict(data),average = 'weighted
            elif (scores[i] == fbeta_score):
                score.append(scores[i](target,j.predict(data),beta = 0.5,average
            elif (scores[i] == "score"):
                try:
                    score.append(j.score(data,target).round(2))
                except:
                    pass
            else:
                score.append(scores[i](target,j.predict(data)).round(2))
        scoring_grid[scoring_names[i]] = score
    return scoring_grid
print create_scoring_grid(X_valid_prot,y_valid_prot,scoring_grid,model_codes)
```

```
/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/sklearn/m
etrics/classification.py:1115: UndefinedMetricWarning: F-score is
ill-defined and being set to 0.0 in labels with no true samples.
  'recall', 'true', average, warn_for)
/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/sklearn/m
etrics/classification.py:1113: UndefinedMetricWarning: Precision i
s ill-defined and being set to 0.0 in labels with no predicted sam
ples.
  'precision', 'predicted', average, warn_for)


                     F1 Score  Accuracy  Kappa Log Loss      Score
Hinge Loss  \
Random Forest            0.53      0.59  -0.03     3.23       0.59
0.91
Gradient Boosting        0.47      0.52  -0.14     1.52       0.52
1.05
Logistic Regression      0.39      0.41  -0.29     2.72       0.41
1.11
KMeans                   0.14      0.15  -0.05        - -399630.90
```

In [40]:

```
from sklearn.model_selection import RandomizedSearchCV
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import make_scorer

def evaluate(data_train,target_train,data_valid,target_valid,score,params,pipes):
    model_codes = []
    models_use = []
    try:
        rfc_tuned = GridSearchCV(pipes['rfc_pipe'],params['rfc_params'],
                                    scoring=score,cv=3).fit(data_train,target_
        model_codes.append(rfc_tuned)
        models_use.append("Random Forest")
    except:
        pass
    try:
        lgr_tuned = GridSearchCV(pipes['lgr_pipe'],params['lgr_params'],
                                    scoring=score,cv=3).fit(data_train,target_
        model_codes.append(lgr_tuned)
        models_use.append("Logistic Regression")
    except:
        pass
    try:
        kmm_tuned = GridSearchCV(pipes['kmm_pipe'],params['kmm_params'],
                              scoring=score,cv=3).fit(data_train,target_train)
        model_codes.append(kmm_tuned)
        models_use.append("KMeans")
    except:
        pass
    try:
        svm_tuned = GridSearchCV(pipes['svm_pipe'],params['svm_params'],
                                    scoring=score,cv=3).fit(data_train,target_
        model_codes.append(svm_tuned)
        models_use.append("Support Vector")
    except:
        pass
    try:
        xgb_tuned = GridSearchCV(pipes['xgb_pipe'],params['xgb_params'],
                              scoring=score,cv=3).fit(data_train,target_train)
        model_codes.append(xgb_tuned)
        models_use.append("XGBoost")
    except:
        pass
    try:
        gnb_tuned = GridSearchCV(pipes['gnb_pipe'],params['gnb_params'],
                              scoring=score,cv=3).fit(data_train,target_train)
        model_codes.append(gnb_tuned)
        models_use.append("Naive Bayes")
    except:
        pass
    scoring_grid_tuned = pd.DataFrame(index = models_use)
    scoring_grid_tuned = create_scoring_grid(data_valid,target_valid,scoring_grid
    return scoring_grid_tuned, model_codes
```

In [41]:

```
from sklearn.decomposition import PCA

pca = PCA(svd_solver = 'full', random_state = 0, n_components = 48)

pca_fitted = pca.fit(X_train_prot,y_train_prot)

X_train_pca = pca_fitted.transform(X_train_prot)
X_train_pca = pd.DataFrame(X_train_pca, index = X_train_prot.index)
X_valid_pca = pca_fitted.transform(X_valid_prot)
X_valid_pca = pd.DataFrame(X_valid_pca, index = X_valid_prot.index)
```

In [42]:

```
kbest_params = {'rfc_params':{},'xgb_params':{},'lgr_params':{},'kmm_params':{},'

for i in kbest_params.values():
    i['kbest__k'] = range(1,49)
```

In [43]:

```
from sklearn.feature_selection import SelectKBest
from sklearn.feature_selection import chi2
from sklearn.feature_selection import f_classif
from sklearn.pipeline import Pipeline

kbest = SelectKBest(f_classif)

kbest_pca_rfc_pipe = Pipeline([('kbest',kbest),('rfc',rfc)])
kbest_pca_xgb_pipe = Pipeline([('kbest',kbest),('xgb',xgb)])
kbest_pca_lgr_pipe = Pipeline([('kbest',kbest),('lgr',lgr)])
kbest_pca_kmm_pipe = Pipeline([('kbest',kbest),('kmm',kmm)])
kbest_pca_svm_pipe = Pipeline([('kbest',kbest),('svm',svm)])
kbest_pca_gnb_pipe = Pipeline([('kbest',kbest),('gnb',gnb)])

kbest_pipes = {'rfc_pipe':kbest_pca_rfc_pipe,'xgb_pipe':kbest_pca_xgb_pipe,'lgr_p
               'kmm_pipe':kbest_pca_kmm_pipe,'svm_pipe':kbest_pca_svm_pipe,'gnb_p
```

In [44]:

```
#find optimum number of PCA features for each algorithm
kbest_pca_scoring_grid, kbest_pca_tuned = evaluate(X_train_pca,y_train_prot,X_val
                                                   kbest_params,kbest_pipes)
```

In [45]:

```
#score and best number of features for each
features_chosen = []
cv_scores = []
tuning_cv_results = pd.DataFrame(index = kbest_pca_scoring_grid.index)
for i in kbest_pca_tuned:
    print i.best_params_
    features_chosen.append(i.best_params_['kbest__k'])
    cv_scores.append(i.best_score_.round(2))
tuning_cv_results['Initial Scores'] = cv_scores
print tuning_cv_results
```

```
{'kbest__k': 29}
{'kbest__k': 4}
{'kbest__k': 11}
{'kbest__k': 1}
{'kbest__k': 4}
{'kbest__k': 46}
                     Initial Scores
Random Forest                  0.60
Logistic Regression            0.58
KMeans                         0.42
Support Vector                 0.54
XGBoost                        0.58
Naive Bayes                    0.51
```

In [46]:

```
#testing set score
kbest_pca_scoring_grid.insert(0, 'K Chosen', features_chosen)
print kbest_pca_scoring_grid
```

```
                    K Chosen  F1 Score  Accuracy  Kappa Log Loss  S
core  \
Random Forest             29      0.53      0.67   0.00      3.2
0.53
Logistic Regression        4      0.55      0.59   0.00     0.87
0.55
KMeans                    11      0.15      0.11  -0.12        -
0.15
Support Vector             1      0.52      0.63  -0.04      0.9
0.52
XGBoost                    4      0.66      0.70   0.28     1.35
0.66
Naive Bayes               46      0.31      0.30  -0.22     1.34
0.31

                    Hinge Loss  Fbeta Score  Hamming Loss  Precision
\
Random Forest             0.88         0.48          0.33       0.44
Logistic Regression       0.89         0.54          0.41       0.56
KMeans                       -         0.20          0.89       0.25
Support Vector            0.96         0.46          0.37       0.44
XGBoost                   0.68         0.65          0.30       0.64
Naive Bayes               1.17         0.33          0.70       0.35

                    Recall Score
Random Forest               0.67
Logistic Regression         0.59
KMeans                      0.11
Support Vector              0.63
XGBoost                     0.70
Naive Bayes                 0.30
```

In [47]:

```
#create feature sets for each algorithm
X_train_kbest_rfc = kbest_pca_tuned[0].best_estimator_.steps[0][1].transform(X_tr
X_train_kbest_lgr = kbest_pca_tuned[1].best_estimator_.steps[0][1].transform(X_tr
X_train_kbest_kmm = kbest_pca_tuned[2].best_estimator_.steps[0][1].transform(X_tr
X_train_kbest_svm = kbest_pca_tuned[3].best_estimator_.steps[0][1].transform(X_tr
X_train_kbest_xgb = kbest_pca_tuned[4].best_estimator_.steps[0][1].transform(X_tr
X_valid_kbest_rfc = kbest_pca_tuned[0].best_estimator_.steps[0][1].transform(X_va
X_valid_kbest_lgr = kbest_pca_tuned[1].best_estimator_.steps[0][1].transform(X_va
X_valid_kbest_kmm = kbest_pca_tuned[2].best_estimator_.steps[0][1].transform(X_va
X_valid_kbest_svm = kbest_pca_tuned[3].best_estimator_.steps[0][1].transform(X_va
X_valid_kbest_xgb = kbest_pca_tuned[4].best_estimator_.steps[0][1].transform(X_va
```

In [48]:

```
#tune XGBClassifier
xgb = XGBClassifier(learning_rate=0.1,seed=0)
xgb_params_cv = {"xgb__n_estimators": range(1,1201)}
params = {'xgb_params':xgb_params_cv}
pipe = {'xgb_pipe':Pipeline([('xgb',xgb)])}
scorer = make_scorer(cohen_kappa_score)

tuned_scoring_grid, tuned = evaluate(X_train_kbest_xgb,y_train_prot,X_valid_kbest
                                             params,pipe)

#test set scoring grid for reference
print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 1'] = ["-","-","-","-",tuned[0].best_score_.round
print tuning_cv_results
```

```
         F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Loss  Fbe
ta Score  \
XGBoost      0.66       0.7   0.28      1.81   0.66        0.67
0.65

         Hamming Loss  Precision  Recall Score
XGBoost           0.3       0.64           0.7
0.635280078215
{'xgb__n_estimators': 670}
                    Initial Scores Tuning Stage 1
Random Forest                 0.60              -
Logistic Regression           0.58              -
KMeans                        0.42              -
Support Vector                0.54              -
XGBoost                       0.58           0.64
Naive Bayes                   0.51              -
```

In [49]:

```
xgb = XGBClassifier(learning_rate=0.1,n_estimators=670,seed=0)
xgb_params_cv = {"xgb__max_depth": range(1,30),"xgb__min_child_weight": range(1,1
params = {'xgb_params':xgb_params_cv}

pipe = {'xgb_pipe':Pipeline([('xgb',xgb)])}

tuned_scoring_grid, tuned = evaluate(X_train_kbest_xgb,y_train_prot,X_valid_kbest
                                     params,pipe)

print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 2'] = ["-","-","-","-",tuned[0].best_score_.round
print tuning_cv_results
```

```
         F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Loss  Fbe
ta Score  \
XGBoost      0.66       0.7   0.28      1.71   0.66        0.71
0.65

         Hamming Loss  Precision  Recall Score
XGBoost           0.3       0.64          0.7
0.670468923186
{'xgb__min_child_weight': 2, 'xgb__max_depth': 3}
                     Initial Scores Tuning Stage 1 Tuning Stage 2
Random Forest                  0.60              -              -
Logistic Regression            0.58              -              -
KMeans                         0.42              -              -
Support Vector                 0.54              -              -
XGBoost                        0.58           0.64           0.67
Naive Bayes                    0.51              -              -
```

In [50]:

```
xgb = XGBClassifier(learning_rate=0.1,n_estimators=670,max_depth=3,min_child_weig
xgb_params_cv = {'xgb__gamma': [i/10.0 for i in range(0,5)]}
params = {'xgb_params':xgb_params_cv}
pipe = {'xgb_pipe':Pipeline([('xgb',xgb)])}

tuned_scoring_grid, tuned = evaluate(X_train_kbest_xgb,y_train_prot,X_valid_kbest
                                     params,pipe)

print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 3'] = ["-","-","-","-",tuned[0].best_score_.round
print tuning_cv_results
```

```
         F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Loss  Fbe
ta Score  \
XGBoost      0.66       0.7   0.28      1.71   0.66        0.71
0.65

         Hamming Loss  Precision  Recall Score
XGBoost           0.3       0.64           0.7
0.670468923186
{'xgb__gamma': 0.0}
                     Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                 0.60              -              -
Logistic Regression           0.58              -              -
KMeans                        0.42              -              -
Support Vector                0.54              -              -
XGBoost                       0.58           0.64           0.67
Naive Bayes                   0.51              -              -

                    Tuning Stage 3
Random Forest                    -
Logistic Regression              -
KMeans                           -
Support Vector                   -
XGBoost                       0.67
Naive Bayes                      -
```

In [51]:

```
xgb = XGBClassifier(learning_rate=0.1,n_estimators=670,max_depth=3,min_child_weig
xgb_params_cv = {"xgb__subsample": [i for i in range(1,11)],
                 "xgb__colsample_bytree": [i for i in range(1,11)]}
params = {'xgb_params':xgb_params_cv}

pipe = {'xgb_pipe':Pipeline([('xgb',xgb)])}

tuned_scoring_grid, tuned = evaluate(X_train_kbest_xgb,y_train_prot,X_valid_kbest
                                     params,pipe)

print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 4'] = ["-","-","-","-",tuned[0].best_score_.round
print tuning_cv_results
```

```
         F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Loss  Fbe
ta Score  \
XGBoost      0.66       0.7   0.28      1.71   0.66        0.71
0.65

         Hamming Loss  Precision  Recall Score
XGBoost           0.3       0.64           0.7
0.670468923186
{'xgb__colsample_bytree': 1, 'xgb__subsample': 1}
                    Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                 0.60              -              -
Logistic Regression           0.58              -              -
KMeans                        0.42              -              -
Support Vector                0.54              -              -
XGBoost                       0.58           0.64           0.67
Naive Bayes                   0.51              -              -

                   Tuning Stage 3 Tuning Stage 4
Random Forest                   -              -
Logistic Regression             -              -
KMeans                          -              -
Support Vector                  -              -
XGBoost                      0.67           0.67
Naive Bayes                     -              -
```

In [52]:

```
xgb = XGBClassifier(learning_rate=0.05,max_depth=3,min_child_weight=2,gamma=0.0,s
xgb_params_cv = {'xgb__n_estimators':range(1,1200)}
params = {'xgb_params':xgb_params_cv}
pipe = {'xgb_pipe':Pipeline([('xgb',xgb)])}

xgb_tuned_scoring_grid, xgb_tuned = evaluate(X_train_kbest_xgb,y_train_prot,X_val
                                             'f1_weighted',params,pipe)

print xgb_tuned_scoring_grid

for i in xgb_tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 5'] = ["-","-","-","-",xgb_tuned[0].best_score_.r
print tuning_cv_results
```

```
         F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Loss  Fbe
ta Score  \
XGBoost      0.66       0.7   0.28      1.65   0.66        0.71
0.65

         Hamming Loss  Precision  Recall Score
XGBoost           0.3       0.64          0.7
0.693466758684
{'xgb__n_estimators': 850}
                    Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                 0.60              -              -
Logistic Regression           0.58              -              -
KMeans                        0.42              -              -
Support Vector                0.54              -              -
XGBoost                       0.58           0.64           0.67
Naive Bayes                   0.51              -              -

                   Tuning Stage 3 Tuning Stage 4 Tuning Stage 5
Random Forest                   -              -              -
Logistic Regression             -              -              -
KMeans                          -              -              -
Support Vector                  -              -              -
XGBoost                      0.67           0.67           0.69
Naive Bayes                     -              -              -
```

In [53]:

```
for i in xgb_tuned:
    xgb_tuned_params = i.best_estimator_.steps[0][1]
print xgb_tuned_params
```

```
XGBClassifier(base_score=0.5, colsample_bytree=1, gamma=0.0,
       learning_rate=0.05, max_delta_step=0, max_depth=3,
       min_child_weight=2, n_estimators=850, nthread=-1,
       objective='multi:softprob', seed=0, silent=True, subsample=1)
```

In [54]:

```
#Final Classifier test set scores
xgb_final_classifier = xgb_tuned[0]
final_models_use = ['XGBoost']
final_models = [xgb_final_classifier]
final_classifier_scores = pd.DataFrame(index = final_models_use)
final_test_scores = create_scoring_grid(X_valid_kbest_xgb,y_valid_prot,final_clas
print final_test_scores
```

```
         F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Loss  Fbe
ta Score  \
XGBoost      0.66       0.7   0.28      1.65   0.66        0.71
0.65

         Hamming Loss  Precision  Recall Score
XGBoost           0.3       0.64           0.7
```

In [55]:

```
#tune model 2, random forest
rfc = RandomForestClassifier(random_state=0)
rfc_params_cv = {'rfc__n_estimators':range(100,200)}
params = {'rfc_params':rfc_params_cv}
pipe = {'rfc_pipe':Pipeline([('rfc',rfc)])}

tuned_scoring_grid, tuned = evaluate(X_train_kbest_rfc,y_train_prot,X_valid_kbest
                                                              y_valid_prot,'f1_weight

print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 1']['Random Forest'] = tuned[0].best_score_.round
print tuning_cv_results
```

```
               F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Los
s  \
Random Forest      0.53      0.67      0      0.92   0.53        0.8
3

               Fbeta Score  Hamming Loss  Precision  Recall Score
Random Forest         0.48          0.33       0.44          0.67
0.506982600733
{'rfc__n_estimators': 103}
                     Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                 0.60           0.51              -
Logistic Regression           0.58              -              -
KMeans                        0.42              -              -
Support Vector                0.54              -              -
XGBoost                       0.58           0.64           0.67
Naive Bayes                   0.51              -              -

                    Tuning Stage 3 Tuning Stage 4 Tuning Stage 5
Random Forest                    -              -              -
Logistic Regression              -              -              -
KMeans                           -              -              -
Support Vector                   -              -              -
XGBoost                       0.67           0.67           0.69
Naive Bayes                      -              -              -

/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/ipykernel/_
_main__.py:16: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: http://pandas.pydata.org/panda
s-docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-
view-versus-copy)
```

In [56]:

```
rfc = RandomForestClassifier(random_state=0,n_estimators=103)
rfc_params_cv = {'rfc__max_features':["sqrt",None,'auto',0.2],
                 'rfc__min_samples_leaf':range(1,11)}
params = {'rfc_params':rfc_params_cv}
pipe = {'rfc_pipe':Pipeline([('rfc',rfc)])}

tuned_scoring_grid, tuned = evaluate(X_train_kbest_rfc,y_train_prot,X_valid_kbest
                                                            y_valid_prot,'f1_weight

print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 2']['Random Forest'] = tuned[0].best_score_.round
print tuning_cv_results
```

```
               F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Los
s  \
Random Forest      0.58      0.67   0.08      1.12   0.58        0.7
6

               Fbeta Score  Hamming Loss  Precision  Recall Score
Random Forest         0.57          0.33       0.58          0.67
0.536728395062
{'rfc__max_features': None, 'rfc__min_samples_leaf': 1}
                     Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                 0.60           0.51           0.54
Logistic Regression           0.58              -              -
KMeans                        0.42              -              -
Support Vector                0.54              -              -
XGBoost                       0.58           0.64           0.67
Naive Bayes                   0.51              -              -

                    Tuning Stage 3 Tuning Stage 4 Tuning Stage 5
Random Forest                    -              -              -
Logistic Regression              -              -              -
KMeans                           -              -              -
Support Vector                   -              -              -
XGBoost                       0.67           0.67           0.69
Naive Bayes                      -              -              -

/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/ipykernel/_
_main__.py:16: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: http://pandas.pydata.org/panda
s-docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-
view-versus-copy)
```

In [57]:

```
rfc = RandomForestClassifier(random_state=0,n_estimators=103,max_features=None,mi
rfc_params_cv = {'rfc__min_samples_split':range(1,11),
                 'rfc__max_depth':range(1,11)}
params = {'rfc_params':rfc_params_cv}
pipe = {'rfc_pipe':Pipeline([('rfc',rfc)])}

rfc_tuned_scoring_grid, rfc_tuned= evaluate(X_train_kbest_rfc,y_train_prot,X_vali
                                              'f1_weighted',params,pipe)

print rfc_tuned_scoring_grid

for i in rfc_tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 3']['Random Forest'] = tuned[0].best_score_.round
print tuning_cv_results
```

```
               F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Los
s  \
Random Forest      0.58      0.67   0.08      1.03   0.58        0.7
7

               Fbeta Score  Hamming Loss  Precision  Recall Score
Random Forest         0.57          0.33       0.58          0.67
0.57075617284
{'rfc__min_samples_split': 7, 'rfc__max_depth': 3}
                     Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                 0.60           0.51           0.54
Logistic Regression           0.58              -              -
KMeans                        0.42              -              -
Support Vector                0.54              -              -
XGBoost                       0.58           0.64           0.67
Naive Bayes                   0.51              -              -

                    Tuning Stage 3 Tuning Stage 4 Tuning Stage 5
Random Forest                 0.54              -              -
Logistic Regression              -              -              -
KMeans                           -              -              -
Support Vector                   -              -              -
XGBoost                       0.67           0.67           0.69
Naive Bayes                      -              -              -

/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/ipykernel/_
_main__.py:16: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: http://pandas.pydata.org/panda
s-docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-
view-versus-copy)
```

In [58]:

```
for i in rfc_tuned:
    rfc_best_params = i.best_estimator_.steps[0][1]
print rfc_best_params
```

```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion=
'gini',
            max_depth=3, max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=7, min_weight_fraction_leaf=0.0,
            n_estimators=103, n_jobs=1, oob_score=False, random_stat
e=0,
            verbose=0, warm_start=False)
```

In [59]:

```
#Final Classifier
rfc_final_classifier = rfc_tuned[0]
final_models_use = ['Random Forest Classifier']
final_models = [rfc_final_classifier]
final_classifier_scores = pd.DataFrame(index = final_models_use)
scoring_temp = create_scoring_grid(X_valid_kbest_rfc,y_valid_prot,final_classifie
final_test_scores = pd.concat([final_test_scores,scoring_temp])
print final_test_scores
```

```
                          F1 Score  Accuracy  Kappa  Log Loss  Score
\
XGBoost                       0.66      0.70   0.28      1.65   0.66
Random Forest Classifier      0.58      0.67   0.08      1.03   0.58

                          Hinge Loss  Fbeta Score  Hamming Loss  Pre
cision  \
XGBoost                         0.71         0.65          0.30
0.64
Random Forest Classifier        0.77         0.57          0.33
0.58

                          Recall Score
XGBoost                           0.70
Random Forest Classifier          0.67
```

In [60]:

```
#train model 3, logistic regression
lgr = LogisticRegression(random_state=0,class_weight='balanced')
lgr_params_cv = {'lgr__penalty':['l1','l2'],
                 "lgr__C":[0.7,0.8,0.9,1.0,1.1,1.2,1.3]}
params = {'lgr_params':lgr_params_cv}
pipe = {'lgr_pipe':Pipeline([('lgr',lgr)])}

lgr_tuned_scoring_grid, lgr_tuned = evaluate(X_train_kbest_lgr,y_train_prot,X_val
                                             'f1_weighted',params,pipe)

print lgr_tuned_scoring_grid

for i in lgr_tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 1']['Logistic Regression'] = tuned[0].best_score_
print tuning_cv_results
```

```
                     F1 Score  Accuracy  Kappa  Log Loss  Score  Hin
ge Loss  \
Logistic Regression      0.56      0.56    0.1      0.96   0.56
0.98

                     Fbeta Score  Hamming Loss  Precision  Recall Sc
ore
Logistic Regression         0.56          0.44       0.57          0
.56
0.705218855219
{'lgr__C': 1.0, 'lgr__penalty': 'l2'}
                     Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                  0.60           0.51           0.54
Logistic Regression            0.58           0.54              -
KMeans                         0.42              -              -
Support Vector                 0.54              -              -
XGBoost                        0.58           0.64           0.67
Naive Bayes                    0.51              -              -

                    Tuning Stage 3 Tuning Stage 4 Tuning Stage 5
Random Forest                 0.54              -              -
Logistic Regression              -              -              -
KMeans                           -              -              -
Support Vector                   -              -              -
XGBoost                       0.67           0.67           0.69
Naive Bayes                      -              -              -

/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/ipykernel/_
_main__.py:17: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: http://pandas.pydata.org/panda
s-docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-
view-versus-copy)
```

In [61]:

```
for i in lgr_tuned:
    lgr = i.best_estimator_.steps[0][1]
print lgr
```

```
LogisticRegression(C=1.0, class_weight='balanced', dual=False,
          fit_intercept=True, intercept_scaling=1, max_iter=100,
          multi_class='ovr', n_jobs=1, penalty='l2', random_state=0,
          solver='liblinear', tol=0.0001, verbose=0, warm_start=Fals
e)
```

In [62]:

```
#Final Classifier
lgr_final_classifier = lgr_tuned[0]
final_models_use = ['Logistic Regression']
final_models = [lgr_final_classifier]
final_classifier_scores = pd.DataFrame(index = final_models_use)
scoring_temp = create_scoring_grid(X_valid_kbest_lgr,y_valid_prot,final_classifie
final_test_scores = pd.concat([final_test_scores,scoring_temp])
print final_test_scores
```

```
                          F1 Score  Accuracy  Kappa  Log Loss  Score
\
XGBoost                       0.66      0.70   0.28      1.65   0.66
Random Forest Classifier      0.58      0.67   0.08      1.03   0.58
Logistic Regression           0.56      0.56   0.10      0.96   0.56

                          Hinge Loss  Fbeta Score  Hamming Loss  Pre
cision  \
XGBoost                         0.71         0.65          0.30
0.64
Random Forest Classifier        0.77         0.57          0.33
0.58
Logistic Regression             0.98         0.56          0.44
0.57

                          Recall Score
XGBoost                           0.70
Random Forest Classifier          0.67
Logistic Regression               0.56
```

In [63]:

```
#Final model, SVM
svm = SVC(random_state=0,probability = True,class_weight='balanced')
svm_params_cv = {"svm__kernel":['poly','rbf','linear','sigmoid']}
params = {'svm_params':svm_params_cv}
pipe = {'svm_pipe':Pipeline([('svm',svm)])}

tuned_scoring_grid, tuned = evaluate(X_train_kbest_svm,y_train_prot,X_valid_kbest
                                     params,pipe)

print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 1']['Support Vector'] = tuned[0].best_score_.roun
print tuning_cv_results
```

```
                F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Lo
ss  \
Support Vector      0.52      0.63  -0.04      0.82   0.52        0.
88

                Fbeta Score  Hamming Loss  Precision  Recall Score
Support Vector         0.46          0.37       0.44          0.63
0.613647342995
{'svm__kernel': 'poly'}
                     Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                  0.60           0.51           0.54
Logistic Regression            0.58           0.54              -
KMeans                         0.42              -              -
Support Vector                 0.54           0.61              -
XGBoost                        0.58           0.64           0.67
Naive Bayes                    0.51              -              -

                    Tuning Stage 3 Tuning Stage 4 Tuning Stage 5
Random Forest                 0.54              -              -
Logistic Regression              -              -              -
KMeans                           -              -              -
Support Vector                   -              -              -
XGBoost                       0.67           0.67           0.69
Naive Bayes                      -              -              -

/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/ipykernel/_
_main__.py:16: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: http://pandas.pydata.org/panda
s-docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-
view-versus-copy)
```

In [64]:

```
svm = SVC(random_state=0,kernel='poly',class_weight='balanced',probability=True)
svm_params_cv = {"svm__C":[0.001,0.01,0.1]}
params = {'svm_params':svm_params_cv}
pipe = {'svm_pipe':Pipeline([('svm',svm)])}

tuned_scoring_grid, tuned = evaluate(X_train_kbest_svm,y_train_prot,X_valid_kbest
                                         params,pipe)

print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 2']['Support Vector'] = tuned[0].best_score_.roun
print tuning_cv_results
```

```
                F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Lo
ss  \
Support Vector      0.52      0.63  -0.06      0.82   0.52        0.
88

                Fbeta Score  Hamming Loss  Precision  Recall Score
Support Vector         0.46          0.37       0.44          0.63
0.68309178744
{'svm__C': 0.001}
                     Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                  0.60           0.51           0.54
Logistic Regression            0.58           0.54              -
KMeans                         0.42              -              -
Support Vector                 0.54           0.61           0.68
XGBoost                        0.58           0.64           0.67
Naive Bayes                    0.51              -              -

                    Tuning Stage 3 Tuning Stage 4 Tuning Stage 5
Random Forest                 0.54              -              -
Logistic Regression              -              -              -
KMeans                           -              -              -
Support Vector                   -              -              -
XGBoost                       0.67           0.67           0.69
Naive Bayes                      -              -              -

/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/ipykernel/_
_main__.py:15: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: http://pandas.pydata.org/panda
s-docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-
view-versus-copy)
```

In [65]:

```
svm = SVC(random_state=0,kernel='poly',C=0.001,class_weight='balanced',probabilit
svm_params_cv = {"svm__gamma":[0.05,0.1,0.3,0.5,0.7,0.9,1.0,'auto']}
params = {'svm_params':svm_params_cv}
pipe = {'svm_pipe':Pipeline([('svm',svm)])}

svm_tuned_scoring_grid, svm_tuned = evaluate(X_train_kbest_svm,y_train_prot,X_val
                                             'f1_weighted',params,pipe)

print tuned_scoring_grid

for i in tuned:
    print i.best_score_
    print i.best_params_

tuning_cv_results['Tuning Stage 3']['Support Vector'] = tuned[0].best_score_.roun
print tuning_cv_results
```

```
                F1 Score  Accuracy  Kappa  Log Loss  Score  Hinge Lo
ss  \
Support Vector      0.52      0.63  -0.06      0.82   0.52        0.
88

                Fbeta Score  Hamming Loss  Precision  Recall Score
Support Vector         0.46          0.37       0.44          0.63
0.68309178744
{'svm__C': 0.001}
                     Initial Scores Tuning Stage 1 Tuning Stage 2  \
Random Forest                  0.60           0.51           0.54
Logistic Regression            0.58           0.54              -
KMeans                         0.42              -              -
Support Vector                 0.54           0.61           0.68
XGBoost                        0.58           0.64           0.67
Naive Bayes                    0.51              -              -

                    Tuning Stage 3 Tuning Stage 4 Tuning Stage 5
Random Forest                 0.54              -              -
Logistic Regression              -              -              -
KMeans                           -              -              -
Support Vector                0.68              -              -
XGBoost                       0.67           0.67           0.69
Naive Bayes                      -              -              -

/Users/WonderWaffle/anaconda/lib/python2.7/site-packages/ipykernel/_
_main__.py:15: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: http://pandas.pydata.org/panda
s-docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-
view-versus-copy)
```

In [66]:

```
for i in svm_tuned:
    svm = i.best_estimator_.steps[0][1]
print svm
```

```
SVC(C=0.001, cache_size=200, class_weight='balanced', coef0=0.0,
  decision_function_shape=None, degree=3, gamma=0.1, kernel='poly',
  max_iter=-1, probability=True, random_state=0, shrinking=True, tol
=0.001,
  verbose=False)
```

In [67]:

```
#Final Classifier
svm_final_classifier = svm_tuned[0]
final_models_use = ['Support Vector']
final_models = [svm_final_classifier]
final_classifier_scores = pd.DataFrame(index = final_models_use)
scoring_temp = create_scoring_grid(X_valid_kbest_svm,y_valid_prot,final_classifie
final_test_scores = pd.concat([final_test_scores,scoring_temp])
print final_test_scores
```

```
                          F1 Score  Accuracy  Kappa  Log Loss  Score
\
XGBoost                       0.66      0.70   0.28      1.65   0.66
Random Forest Classifier      0.58      0.67   0.08      1.03   0.58
Logistic Regression           0.56      0.56   0.10      0.96   0.56
Support Vector                0.52      0.63  -0.06      0.82   0.52

                          Hinge Loss  Fbeta Score  Hamming Loss  Pre
cision  \
XGBoost                         0.71         0.65          0.30
0.64
Random Forest Classifier        0.77         0.57          0.33
0.58
Logistic Regression             0.98         0.56          0.44
0.57
Support Vector                  0.87         0.46          0.37
0.44

                          Recall Score
XGBoost                           0.70
Random Forest Classifier          0.67
Logistic Regression               0.56
Support Vector                    0.63
```

In [68]:

```
final_models = [gnb_trained]
final_classifier_scores = pd.DataFrame(index = ['Naive Bayes'])
scoring_temp = create_scoring_grid(X_valid_prot,y_valid_prot,final_classifier_sco
final_test_scores = pd.concat([final_test_scores,scoring_temp])
dummy_clf = DummyClassifier(strategy = 'most_frequent').fit(X_train_prot,y_train_
final_models = [dummy_clf]
final_classifier_scores = pd.DataFrame(index = ['Dummy Classifier        '])
```

```
scoring_temp = create_scoring_grid(x_valid_prot,y_valid_prot,final_classifier_sco
print scoring_temp
final_test_scores = pd.concat([final_test_scores,scoring_temp])
print final_test_scores
```

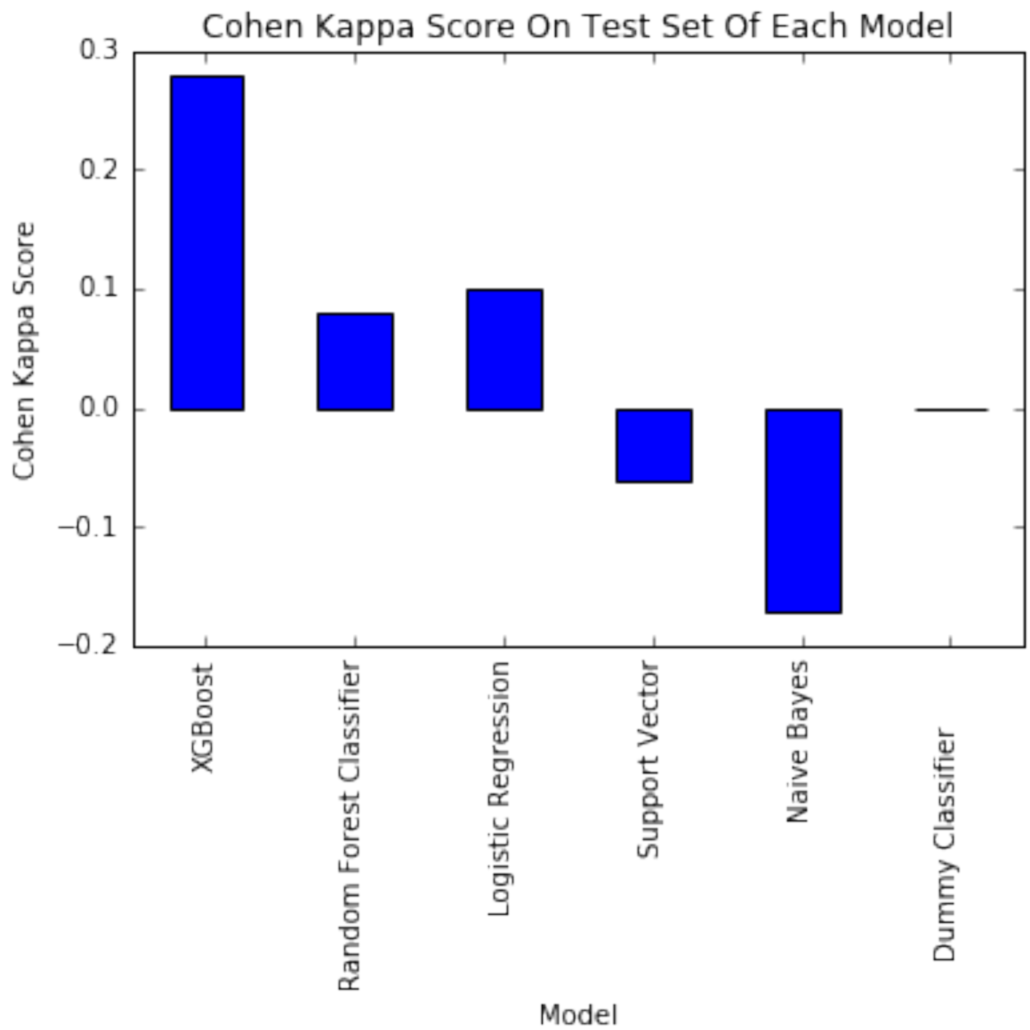
```
                          F1 Score  Accuracy  Kappa  Log Loss  Score
\
Dummy Classifier              0.53      0.67      0     11.51   0.67

                          Hinge Loss  Fbeta Score  Hamming Loss  Pre
cision  \
Dummy Classifier                0.67         0.48          0.33
0.44

                          Recall Score
Dummy Classifier                  0.67
                          F1 Score  Accuracy  Kappa  Log Loss  Score
\
XGBoost                       0.66      0.70   0.28      1.65   0.66
Random Forest Classifier      0.58      0.67   0.08      1.03   0.58
Logistic Regression           0.56      0.56   0.10      0.96   0.56
Support Vector                0.52      0.63  -0.06      0.82   0.52
Naive Bayes                   0.48      0.56  -0.17     15.35   0.56
Dummy Classifier              0.53      0.67   0.00     11.51   0.67

                          Hinge Loss  Fbeta Score  Hamming Loss  Pre
cision  \
XGBoost                         0.71         0.65          0.30
0.64
Random Forest Classifier        0.77         0.57          0.33
0.58
Logistic Regression             0.98         0.56          0.44
0.57
Support Vector                  0.87         0.46          0.37
0.44
Naive Bayes                     0.89         0.44          0.44
0.42
Dummy Classifier                0.67         0.48          0.33
0.44

                          Recall Score
XGBoost                           0.70
Random Forest Classifier          0.67
Logistic Regression               0.56
Support Vector                     0.63
Naive Bayes                       0.56
Dummy Classifier                  0.67
```

In [69]:

```
#Accuracy Score
final_test_model_accuracy = final_test_scores['Kappa']

final_test_model_accuracy = final_test_model_accuracy.plot(kind='bar',color=['b',
final_test_model_accuracy.set_xlabel("Model")
final_test_model_accuracy.set_ylabel("Cohen Kappa Score")
final_test_model_accuracy.set_title("Cohen Kappa Score On Test Set Of Each Model"
```

Out[69]:

```
<matplotlib.text.Text at 0x11c6657d0>
```

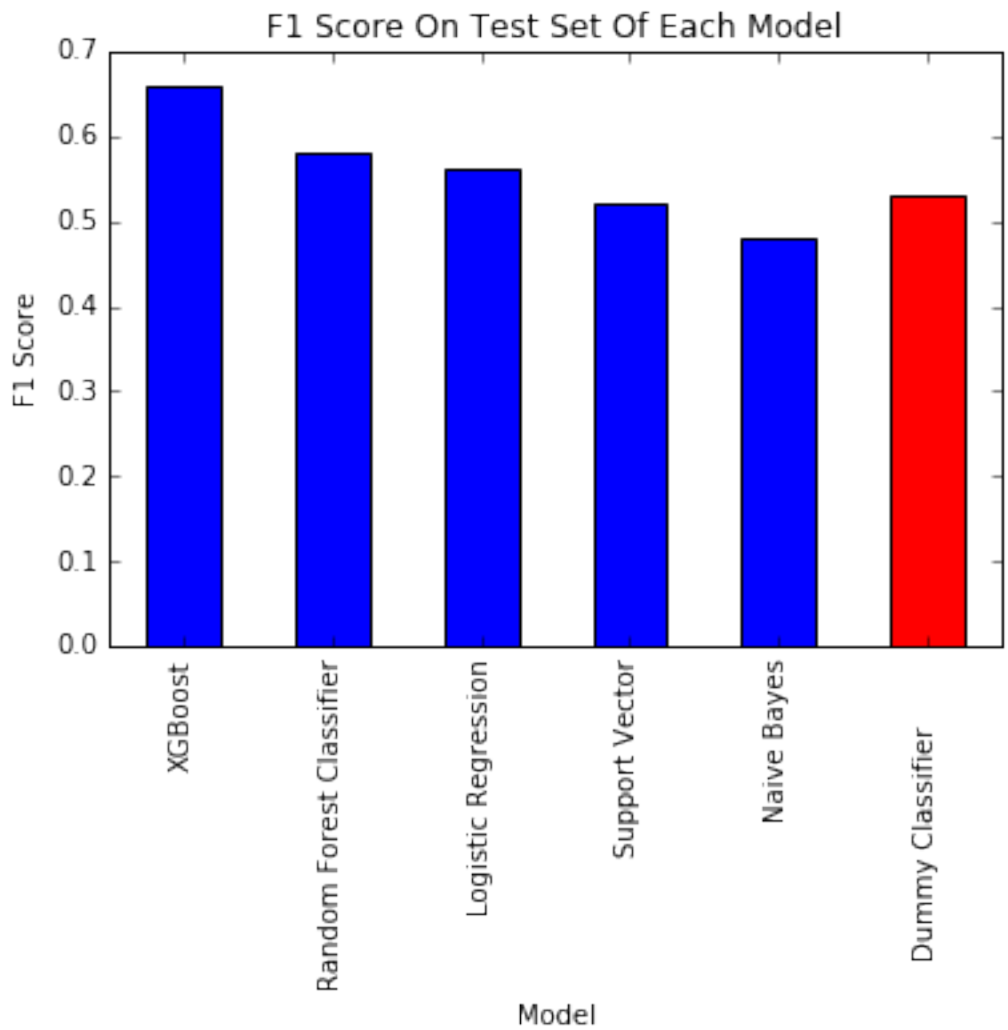


In [70]:

```
#F1 Score
final_test_model_f1score = final_test_scores['F1 Score']

final_test_model_f1score = final_test_model_f1score.plot(kind='bar',color=['b','b
final_test_model_f1score.set_xlabel("Model")
final_test_model_f1score.set_ylabel("F1 Score")
final_test_model_f1score.set_title("F1 Score On Test Set Of Each Model")
```

Out[70]:

```
<matplotlib.text.Text at 0x115d7ae90>
```

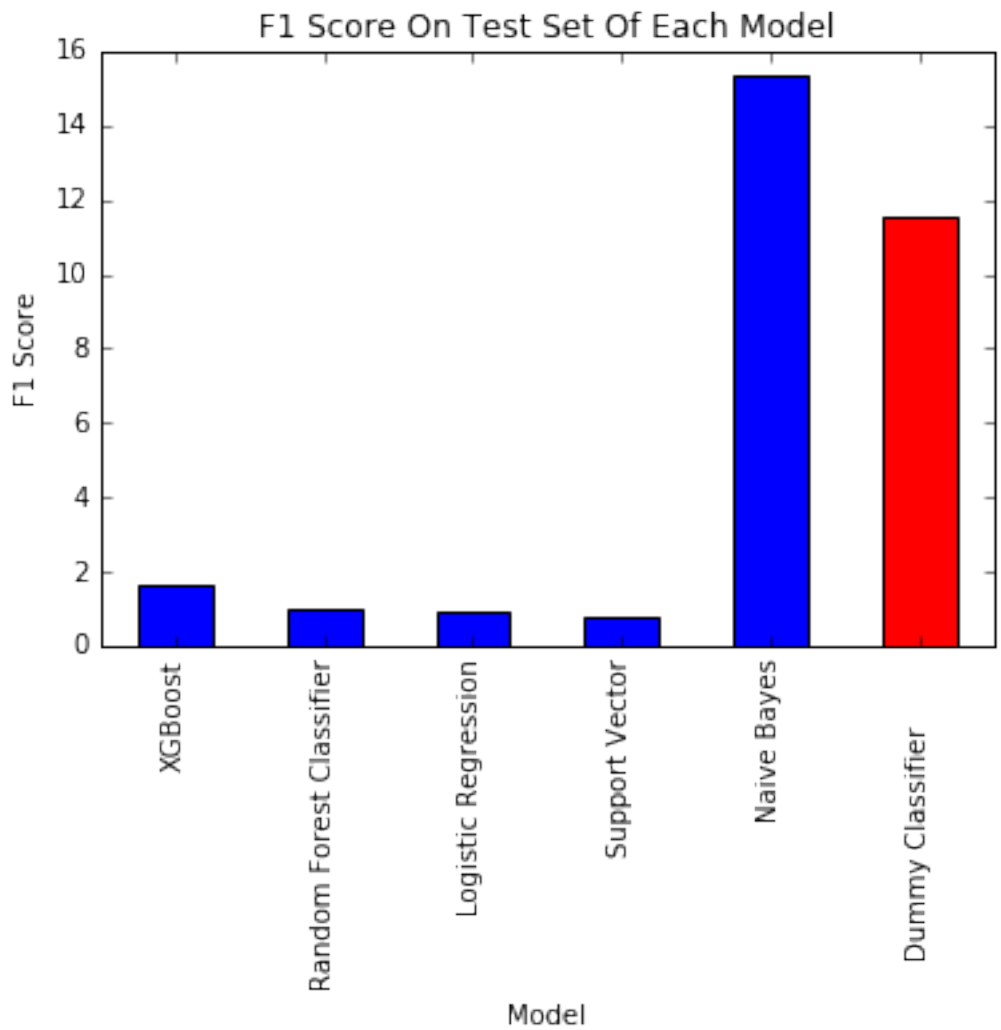


In [71]:

```
#Log Loss
final_test_model_log_loss = final_test_scores['Log Loss']

final_test_model_log_loss = final_test_model_log_loss.plot(kind='bar',color=['b',
final_test_model_log_loss.set_xlabel("Model")
final_test_model_log_loss.set_ylabel("F1 Score")
final_test_model_log_loss.set_title("F1 Score On Test Set Of Each Model")
```

Out[71]:

<matplotlib.text.Text at 0x11a694bd0>



In [72]:

```
from sklearn.metrics import confusion_matrix
confusion_matrix_final_model = pd.DataFrame(confusion_matrix(y_valid_prot,
                                                              xgb_final_classifier
                                            index=['Stage 1','Stage 2','Stage 3']
confusion_matrix_final_model.columns = ['Stage 1','Stage 2','Stage 3']
confusion_matrix_final_model.index.rename("Actual", inplace = True)
confusion_matrix_final_model.columns.rename("Predicted", inplace = True)
print confusion_matrix_final_model
```

```
Predicted  Stage 1  Stage 2  Stage 3
Actual
Stage 1          0        2        0
Stage 2          0       16        2
Stage 3          0        4        3
```

In [73]:

```
#Focus is far too much on the most populous Stage
```