ML_2Type

establish a 2 type classifier for E/NE data. 'effc': 0=E; 1=NE

In [1]:
```
import pandas as pd
import matplotlib.pyplot as plt
from sklearn import decomposition as skldec #for PCA
import numpy as np
import seaborn as sns
import os
import time

from sklearn.linear_model import SGDClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC

save_dir = 'input your file dir' #r'E:\Github'
```

Function

In [2]:
```
from sklearn.model_selection import GridSearchCV

def GridSearch_result(ML, X, y, param_grid, cv=3, score="accuracy"):
    start = time.time()
    grid_search = GridSearchCV(ML, param_grid, cv=cv, scoring=score, refit=True)
    grid_search.fit(X, y)
    end = time.time()
    print("Run Time:%s s" % (end-start))
    return [grid_search.best_params_, grid_search.best_estimator_]
```

In [3]:
```
from sklearn.metrics import confusion_matrix
from sklearn.metrics import accuracy_score
from sklearn.metrics import roc_curve
from sklearn.model_selection import cross_val_predict
```

```
from sklearn.metrics import roc_auc_score  #AUC

def ML_result(ML, X, y, label, roc=0, feedback=0, save_dir=None,
              cmap=sns.color_palette('tab10'), cv=3, ):
    "Input: ML classifier. "
    "fit, and Output confusion_matrix, accuracy_score / roc_curve"

    ML.fit(X, y)
    y_pred = cross_val_predict(ML, X, y, cv=cv)

    conf_mat = confusion_matrix(y, y_pred)
    accu = accuracy_score(y, y_pred)
    if roc != 0:
        if roc == "rf":
            y_probas_forest = cross_val_predict(ML, X, y, cv=cv, method="predict_proba")
            y_scores = y_probas_forest[:, 1] # score = proba of positive class
        if roc == "sgd":
            y_scores = cross_val_predict(ML, X, y, cv=cv, method="decision_function")
        fpr, tpr, thresholds = roc_curve(y, y_scores)
        auc = roc_auc_score(y, y_scores)
        plot_roc_curve([fpr], [tpr], label=[label], auc=[auc], cmap=cmap, save_dir=save_dir)
        plt.show()
        if feedback == 1:
            return {"conf_mat":conf_mat, "accu":accu, "auc":auc, "fpr":fpr, "tpr":tpr}
        else:
            return {"conf_mat":conf_mat, "accu":accu, "auc":auc}
    return {"conf_mat":conf_mat, "accu":accu }
```

In [4]:

```
def plot_roc_curve(fpr, tpr, label, auc, cmap=None, save_dir=None):
    fig, ax1 = plt.subplots(dpi=110)
    for i in range(len(fpr)):
        Label="%s : %0.3f" % (label[i], auc[i])  #align
        if cmap==None:
            ax1.plot(fpr[i], tpr[i], label=Label, linewidth=2.5,)
        else:
            ax1.plot(fpr[i], tpr[i], color=cmap[i], label=Label, linewidth=2.5,)

    ax1.plot([0, 1], [0, 1], linestyle='--', color='0.4')
    plt.rcParams['font.sans-serif'] = ['Arial']
    ax1.tick_params(axis='both', labelsize=13, labelcolor="k")
```

```
    plt.xlabel('False Positive Rate', fontsize=14, fontweight="bold")
    plt.ylabel('True Positive Rate', fontsize=14, fontweight="bold")
    plt.legend(loc="lower right", prop={"size": 12,"weight":"bold",'family':'Arial'}, frameon=False)
    if save_dir != None:
        fig.savefig(os.path.join(save_dir, str(time.time())+'.png'), bbox_inches='tight', dpi=150)
```

In [5]:

```
def conf_mat_heatmap(conf_mat, rect_set, title, ticklabel=['E','NE'],
                     cmap=None, density=True, save_dir=None,):
    'draw conf_matrix heatmap'
    fig = plt.figure(dpi=130, figsize=(2.5, 2.5))
    ax1 = fig.add_subplot(111)

    if cmap == None:  #return matplotlib colormap
        cmap = sns.cubehelix_palette(rot=0.2, gamma=0.5, dark=0.3, light=1, as_cmap=True)
    if density == False:
        h = sns.heatmap(data=conf_mat, xticklabels=ticklabel, yticklabels=ticklabel, annot=True,
                        linewidths=1, linecolor="0.7", cbar=False, #turn off color bar
                        #annot_kws={'size':11,'weight':600,'family':"Arial",'color':"k"},
                        square=True, cmap=cmap, ax=ax1)
    elif density == True:
        density_mat = conf_mat/np.sum(conf_mat, axis=1).reshape(conf_mat.shape[0], -1)
        h = sns.heatmap(data=density_mat, xticklabels=ticklabel, yticklabels=ticklabel, annot=True,
                        fmt=".1%", linewidths=1, linecolor="0.7", cbar=False,
                        #annot_kws={'size':11,'weight':600,'family':"Arial",'color':"k"},
                        square=True, vmin=0, vmax=1, cmap=cmap, ax=ax1)
    ax1.tick_params(width=2, length=4, colors="k")
    rect = plt.Rectangle(xy=rect_set["xy1"], width=rect_set["width1"], height=rect_set["height1"],
                         fill=False, edgecolor="k", linewidth=rect_set["linewidth1"])
    ax1.add_patch(rect)

    rect_cb = [1, 0.13, 0.11, 0.74] # color bar
    cbar_ax = fig.add_axes(rect_cb)
    cb = h.figure.colorbar(h.collections[0], cax=cbar_ax) #show colorbar
    cb.ax.tick_params(direction='in', labelsize=10, length=4, width=1, colors="k",
                      left=True, right=True)
    rect2 = plt.Rectangle(xy=rect_set["xy2"], width=rect_set["width2"], height=rect_set["height2"],
                         fill=False, edgecolor="k", linewidth=rect_set["linewidth2"] )
    cbar_ax.add_patch(rect2)

    font1 = {'family':'Arial', 'color':'k', 'weight':'bold', 'size': 12}
```

```
    accu = conf_mat.trace()/conf_mat.sum()
    ax1.set_xlabel('Accuracy Score:{:.1%}'.format(accu), font1);#
    ax1.set_ylabel("Actual", font1);#
    ax1.set_title(str(title)+'\n Predicted', font1);  #
    if save_dir != None:
        plt.savefig(os.path.join(save_dir, title+'.png'), bbox_inches='tight', dpi=150)

rect_set={"xy1":(0.015,0.017), "width1":1.96, "height1":1.96,"linewidth1":2.2,
                    "xy2":(0.03,0.004), "width2":0.97, "height2":0.99,"linewidth2":1.1}
rect_set2={"xy1":(0.023,0.017), "width1":2.94, "height1":2.96,"linewidth1":2.2,
                    "xy2":(0.03,0.004), "width2":0.97, "height2":0.99,"linewidth2":1.1}
```

import data

In [7]:
```
file_path = os.path.join(save_dir,'ML_dataset.xlsx')
df = pd.read_excel(file_path, sheet_name='adj_effc_2t', index_col=0)
df.dropna(inplace=True)
df.head()
```

Out[7]:

id	cancer	sample_id	LAa	LAErr	SZa	SZErr	CLa	CLErr	effc	kill
81	CCom	A3	1.51085	0.13405	1.34627	0.02986	1.83637	0.22148	1	0.30000
16	GC	5	1.03143	0.22530	1.20558	0.06233	0.82232	0.09236	1	0.07000
60	KC	A6	0.11333	0.01206	1.15431	0.10533	0.02664	0.00668	0	0.97336
37	PaC	6	0.81366	0.01794	1.14430	0.09914	0.97903	0.07454	1	0.00000
90	GC	A2	1.71732	0.40495	1.12907	0.01176	1.44957	0.08896	1	0.04000

In [8]:
```
#split data
df3 = df.loc[:, ["LAa","LAErr","SZa","SZErr","CLa","CLErr"]]
df3.head()
```

Out[8]:

id	LAa	LAErr	SZa	SZErr	CLa	CLErr
81	1.51085	0.13405	1.34627	0.02986	1.83637	0.22148
16	1.03143	0.22530	1.20558	0.06233	0.82232	0.09236
60	0.11333	0.01206	1.15431	0.10533	0.02664	0.00668
37	0.81366	0.01794	1.14430	0.09914	0.97903	0.07454
90	1.71732	0.40495	1.12907	0.01176	1.44957	0.08896

Visualization

In [228…

```
index3 = ["CLa","LAa","SZa","CLErr","LAErr","SZErr","effc"]
df_c = df.loc[:, index3]
corr_matrix = df_c.corr()
corr_matrix["effc"].sort_values(ascending=False)
```

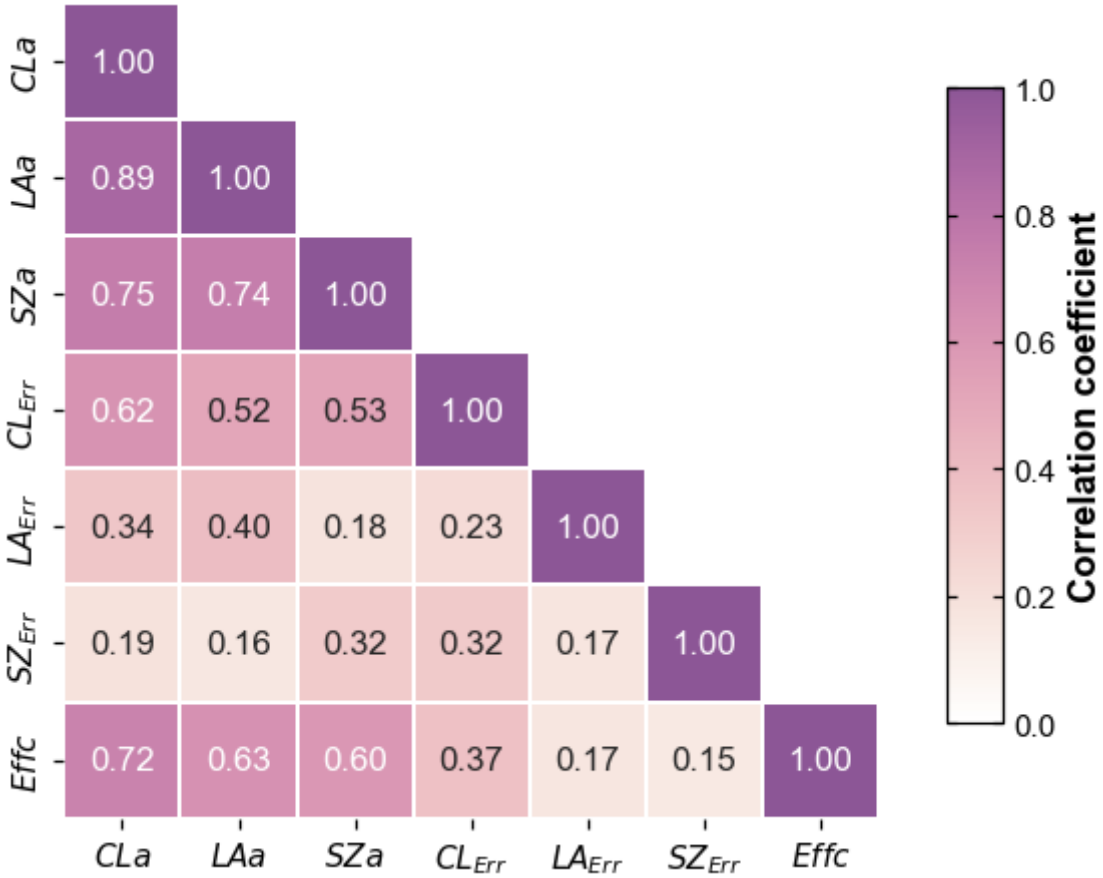
Out[228]:

```
effc     1.000000
CLa      0.716707
LAa      0.631748
SZa      0.598631
CLErr    0.371904
LAErr    0.167493
SZErr    0.148016
Name: effc, dtype: float64
```

In [395…

```
fig = plt.figure(dpi=110, )
ax1 = fig.add_subplot(111)
cmap = sns.cubehelix_palette(rot=0.4, hue=0.9, gamma=0.7, dark=0.3, light=1, as_cmap=True)
mask = np.triu(np.ones_like(corr_matrix, dtype=bool), 1)
g=sns.heatmap(data=corr_matrix, vmax=1, vmin=0, linewidth=1, linecolor="w", cmap=cmap,
              annot = True, fmt="0.2f", square=True, mask=mask, cbar=False,
              ax=ax1, annot_kws={'size':11, 'family':"Arial"},)
```

```
rect = [0.85, 0.2, 0.04, 0.6]   #x, y, x_width, y_height
cbar_ax = fig.add_axes(rect)
cb = g.figure.colorbar(g.collections[0], cax=cbar_ax)  #share colorbar
cb.ax.tick_params(direction='in', color="k", length=3, left=True, right=True)
cb.set_label('Correlation coefficient', font={'family':'Arial', 'size':12, 'weight': 'bold'})
labels = ['$CLa$','$LAa$','$SZa$','$CL_{Err}$','$LA_{Err}$','$SZ_{Err}$',"$Effc$"]
ax1.set_yticklabels(labels);
ax1.set_xticklabels(labels);
#fig.savefig(os.path.join(save_dir, str(time.time())+'.png'), dpi=150, bbox_inches='tight')
```



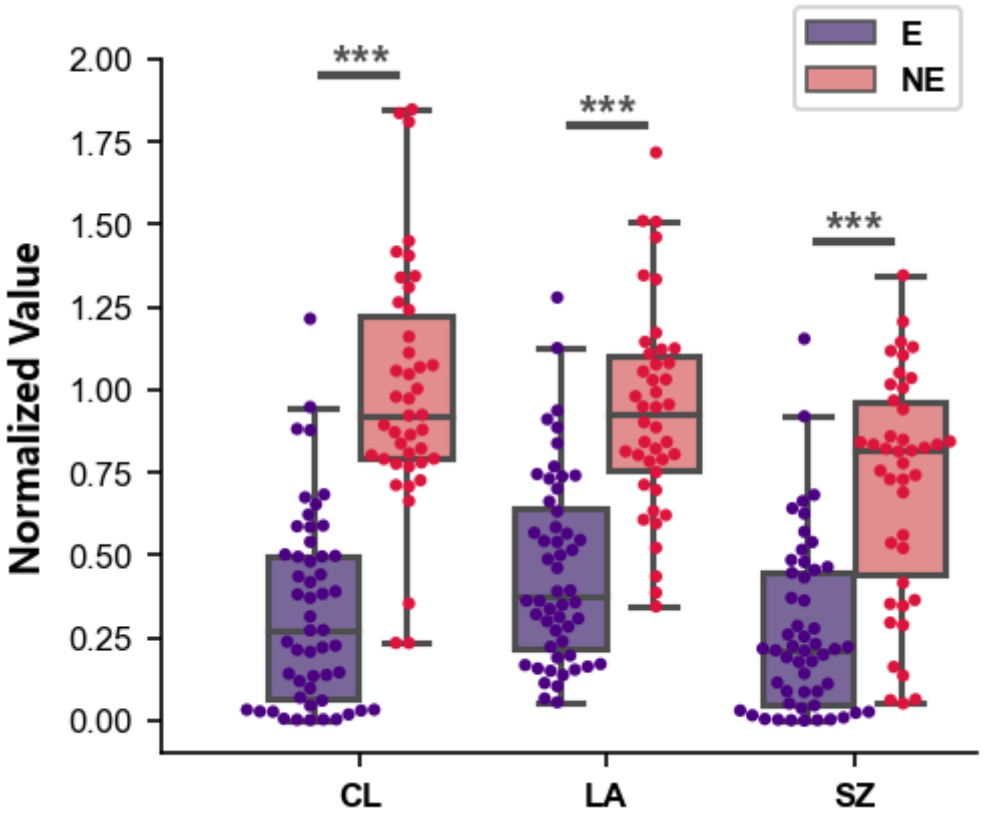
In [41]:
```
def plot_sig(xstart, xend, ystart, yend, sig, ax, vert=True):
    '''
    to draw significance markers*
```

```
    sig: list. Control the shape of these annotation
    vert: bool. whether draw vertical line.
    '''
    for i in range(len(xstart)):
        if vert[i] == True:
            x = np.ones((2)) * xstart[i]
            y = np.arange(ystart[i], yend[i]+0.1, yend[i]-ystart[i])
            ax.plot(x, y, label="$y$", linewidth=1, color="0.3")
            x = np.ones((2))*xend[i]
            y = np.arange(ystart[i], yend[i]+0.1, yend[i]-ystart[i])
            ax.plot(x, y, label="$y$", linewidth=1, color="0.3")

        x = np.arange(xstart[i], xend[i]+0.1, xend[i]-xstart[i])#draw horizontal line.
        y = yend[i] + 0*x
        ax.plot(x, y, label="$y$", linewidth=2, color="0.3")

        x0 = (xstart[i] + xend[i])/2
        y0=yend[i]
        ax.annotate(r'%s'% sig[i], xy=(x0, y0),   # %s string
                    fontsize=10, fontweight="bold", fontfamily="Microsoft YaHei",
                   color="0.3", va="baseline", ha="center")
    plt.show()
```

In [45]:

```
#boxplot
df4 = pd.read_excel(os.path.join(save_dir,'boxplot.xlsx'),
                    sheet_name="kill_adj", index_col=0)
fig = plt.figure(figsize=(3.5,3), dpi=150)
ax1 = fig.add_subplot(111)

c1 = ["#765EA3", "lightcoral"]
c2 = ["indigo", "crimson"]
a = sns.boxplot(x="Attri", y="val", hue="effc", data=df4, ax=ax1,
                linewidth=1.5, width=0.75, showfliers=False, dodge=True, palette=c1);
b = sns.swarmplot(x="Attri", y="val", hue="effc", data=df4,  palette=c2,
                  size=3, dodge=True, ax=ax1);

handles = ax1.get_legend_handles_labels()
ax1.legend(handles = handles[0][0:2], bbox_to_anchor=(1, 1.1),
           labels=["E","NE"], prop={"size":8, 'weight':"bold"})
plt.ylabel("Normalized Value", fontsize=9, fontweight="600", fontfamily="Microsoft YaHei")
```

```
plt.xlabel(None)
ax1.set_xticklabels(["CL","LA","SZ"], fontweight="600", fontfamily="Arial")
plt.tick_params(axis='both', direction='out', labelsize=8)
plt.ylim(-0.1,2)
plt.xlim(-0.8,2.5)
ax1.spines['right'].set_visible(False)
ax1.spines['top'].set_visible(False)

plot_sig([-0.15,0.85,1.85], [0.15,1.15,2.15], [1.8,1.7,1.4], [1.95,1.8,1.45],
         ['***','***','***'], ax1, [0,0,0])
#fig.savefig(os.path.join(save_dir, str(time.time())+'.png'), dpi=200, bbox_inches='tight')
```



In [4]:
```
#PCA
pca = skldec.PCA()
```

```
pca.fit(df3)
result = pca.transform(df3)

data = pd.DataFrame(result)
data['label'] = np.array(df.effc)
data
```

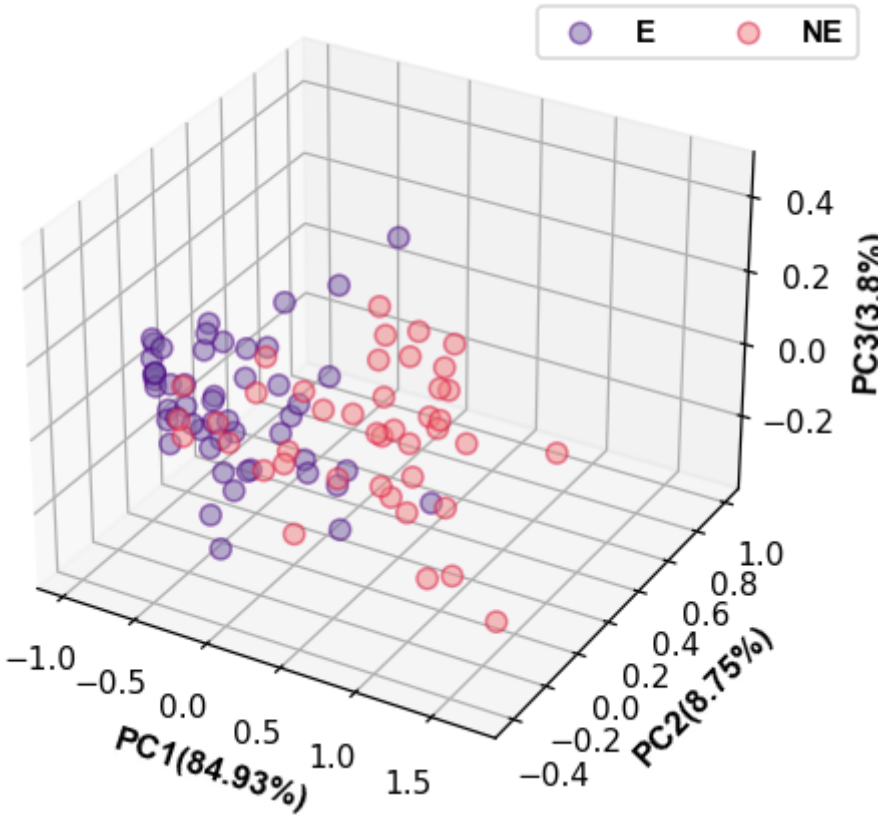
Out[4]:

	0	1	2	3	4	5	label
0	1.716002	0.035878	0.096184	-0.075637	0.030290	0.066523	1
1	0.693676	0.447050	-0.164975	0.000187	0.155484	0.054385	1
2	-0.382791	0.994978	0.081704	-0.052080	0.068707	-0.002045	0
3	0.644134	0.411908	0.115701	-0.068697	-0.004609	-0.032591	1
4	1.459682	-0.078248	-0.342719	0.014896	0.255272	0.043671	1
...	...	...	...	...	...	...	...
89	-0.932429	-0.016139	0.000975	-0.049787	-0.014419	0.018728	0
90	-0.917494	-0.027223	0.025770	-0.043373	0.002811	0.022065	0
91	-0.941914	-0.014663	0.013553	-0.044438	0.003312	0.022242	0
92	-0.968697	-0.001484	0.049589	-0.049317	0.004837	0.020648	0
93	-0.900291	-0.038045	-0.005015	-0.052099	-0.017647	0.020763	0

94 rows × 7 columns

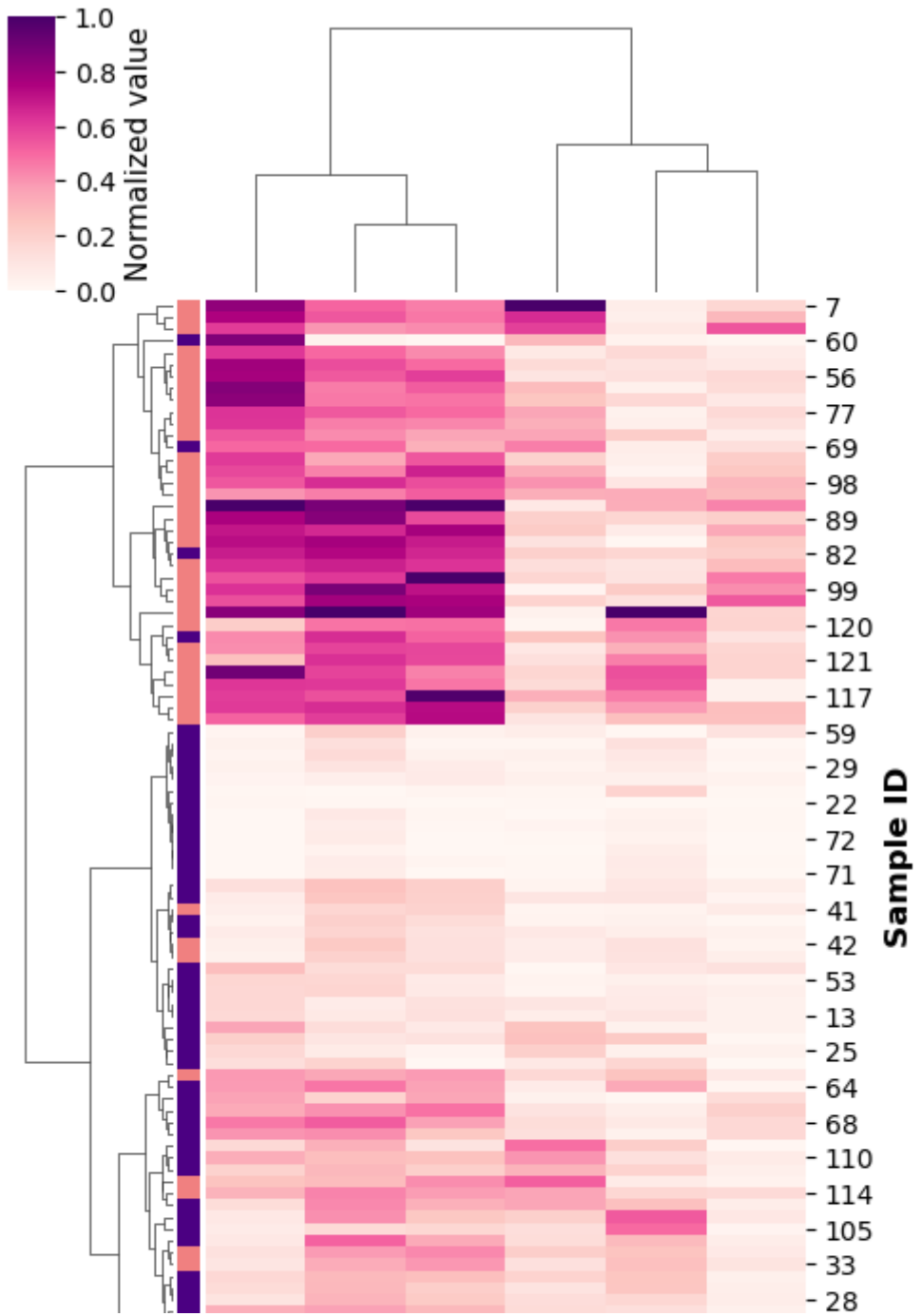
In [52]:
```
fig_a = plt.figure(dpi=110)
ax = fig_a.add_subplot(111, projection='3d') #3D scatter
d1 = data.loc[data['label']==0]
d2 = data.loc[data['label']==1]

ax.scatter(d1.iloc[:, 0], d1.iloc[:, 1], d1.iloc[:, 2], c="#765EA3", alpha=0.5,
           edgecolor="indigo", s=45, label='E')
ax.scatter(d2.iloc[:, 0], d2.iloc[:, 1], d2.iloc[:, 2], c="lightcoral", alpha=0.5,
           edgecolor="crimson", s=45, label='NE')
```

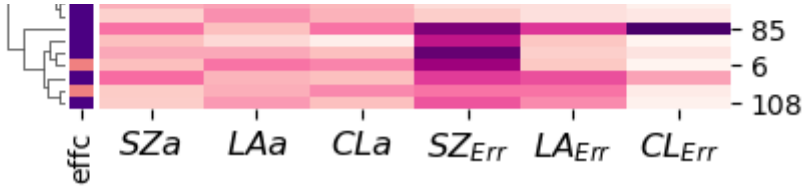
```
x_label = 'PC1(%s%%)' % round(pca.explained_variance_ratio_[0]*100.0, 2);
y_label = 'PC2(%s%%)' % round(pca.explained_variance_ratio_[1]*100.0, 2);
z_label = 'PC3(%s%%)' % round(pca.explained_variance_ratio_[2]*100.0, 2);
font1 = {'family':'Arial', 'size':11, "color":"k", 'weight':'bold',}
ax.legend(bbox_to_anchor=(1.1, 0.98), ncol=2, prop={"size":10, "weight":"bold", 'family':'Arial'})
ax.tick_params(labelsize=10, color="k")
ax.set_xlabel(x_label, font1)
ax.set_ylabel(y_label, font1)
ax.set_zlabel(z_label, font1)
plt.show()
fig_a.savefig(os.path.join(save_dir, str(time.time())+'.png'), dpi=150, )
```



In [153…

```
#clustermap
my_palette = dict(zip(df.effc.unique(), ["lightcoral", "indigo"]))#lightcoral:NE; indigo:E
row_colors = df.effc.map(my_palette)
h=sns.clustermap(df3, method ='ward', metric='euclidean', standard_scale=1, vmax=1, vmin=0,
                 cmap='RdPu', row_colors=row_colors,
                 figsize=(5, 8), dendrogram_ratio=0.2, cbar_kws={'anchor':(1,1),}
                )
h.cax.tick_params(labelsize=10, color="k", right=True)
h.cax.set_ylabel('Normalized value', fontsize=11)
h.ax_heatmap.tick_params(axis='y', labelsize=10)
h.ax_heatmap.set_ylabel('Sample ID', fontsize=12, fontweight='bold')
xlabel = ['$SZa$','$LAa$','$CLa$','$SZ_{Err}$','$LA_{Err}$','$CL_{Err}$']
h.ax_heatmap.set_xticklabels(xlabel, fontsize=12,);
#h.savefig(os.path.join(save_dir, str(time.time())+'.png'), dpi=150, )
```


Normalized value
1.0
0.8
0.6
0.4
0.2
0.0
Sample ID
7
60
56
77
69
98
89
82
99
120
121
117
59
29
22
72
71
41
42
53
13
25
64
68
110
114
105
33
28



two type classifier

data process & Visualization

use average to fill nan. 1-CLa as kill if kill == nan

In [9]:
```
from sklearn.model_selection import StratifiedShuffleSplit

def split_train_test(dataframe, dataframe_y, test_size=0.2, random_state=42):
    split = StratifiedShuffleSplit(test_size=test_size, random_state=random_state)
    for train_index, test_index in split.split(dataframe, dataframe_y):
        train_set = dataframe.iloc[train_index]
        test_set = dataframe.iloc[test_index]
    return train_set, test_set
```

In [10]:
```
start_train_set, start_test_set = split_train_test(df, df["effc"])
start_train_set.head()
```

Out[10]:

id	cancer	sample_id	LAa	LAErr	SZa	SZErr	CLa	CLErr	effc	kill
80	CCom	A2	0.73102	0.02199	0.45568	0.03990	0.88166	0.10193	0	0.49000
76	BC	A6	0.88654	0.06394	0.83419	0.02892	0.78035	0.03184	1	0.21965
75	BC	A5	0.74513	0.01565	0.53963	0.04687	0.43542	0.08215	0	0.56458
31	STS	A4	0.80518	0.13636	0.53674	0.11692	0.97353	0.14199	1	0.10000
9	GCa	A1	0.13751	0.01783	0.02638	0.01450	0.13777	0.01425	0	0.33000

In [11]:
```
train_set_2 = start_train_set.loc[:, ["LAa","CLa","SZa","effc"]]
test_set_2 = start_test_set.loc[:, ["LAa","CLa","SZa","effc"]]

index3 = ["LAa","LAErr","SZa","SZErr","CLa","CLErr","effc"]
train_set_3 = start_train_set.loc[:, index3]
test_set_3 = start_test_set.loc[:, index3]
train_set_3.head(8)
```

Out[11]:

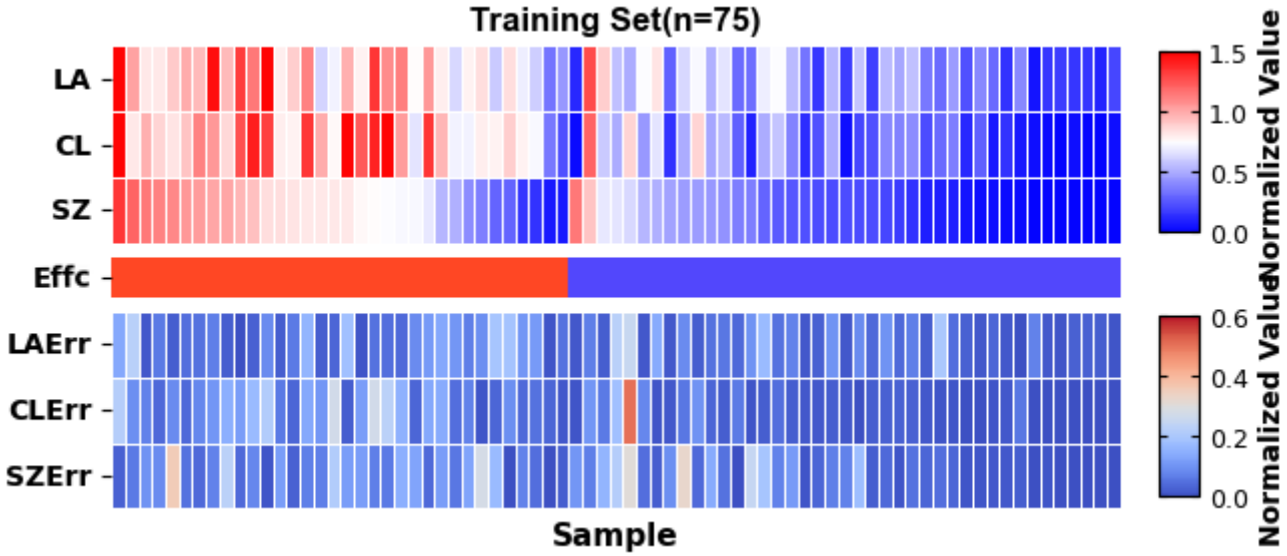
id	LAa	LAErr	SZa	SZErr	CLa	CLErr	effc
80	0.73102	0.02199	0.45568	0.03990	0.88166	0.10193	0
76	0.88654	0.06394	0.83419	0.02892	0.78035	0.03184	1
75	0.74513	0.01565	0.53963	0.04687	0.43542	0.08215	0
31	0.80518	0.13636	0.53674	0.11692	0.97353	0.14199	1
9	0.13751	0.01783	0.02638	0.01450	0.13777	0.01425	0
33	0.60747	0.10823	0.13574	0.04558	0.72641	0.05372	1
10	0.48793	0.03798	0.17683	0.00914	0.38125	0.02639	0
4	0.58451	0.08473	0.21197	0.17402	0.20764	0.00256	0

In [12]:
```
def num_cat(dataframe, column="effc"):
    data_num = dataframe.drop(column, axis=1)
    list_cat = dataframe[column].tolist()
    data_cat = np.array(list_cat)
    return data_num, data_cat
```

In [13]:
```
X_train_3, y_train_3 = num_cat(train_set_3, column="effc")
X_test_3, y_test_3 = num_cat(test_set_3, column="effc")
```

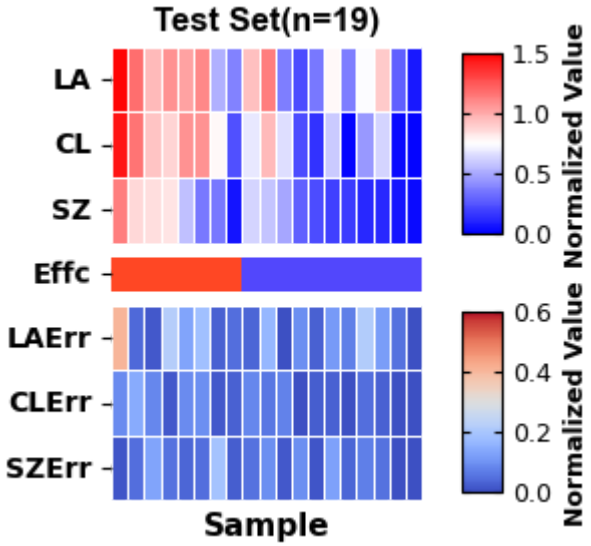
In [147…
```
fig = plt.figure(dpi=100, figsize=(6.5,3))
grid = fig.add_gridspec(3, 1, hspace=0.1, height_ratios=[4,0.8,4])
ax1 = plt.subplot(grid[0,:])
ax2 = plt.subplot(grid[2,:])
ax0 = plt.subplot(grid[1,:])
############## heatmap123
data = train_set_3.sort_values(by = ['effc',"SZa"], ascending=False)
h=sns.heatmap(data=data[["LAa","CLa","SZa"]].T,
            ax=ax1,
            vmin=0, vmax=1.5,
            linewidth=0.7,
            linecolor="w",
            cmap=sns.color_palette('bwr',n_colors=100),
            cbar=False,
            cbar_kws={ 'label':'Normalized Value', 'extend':'both',},
           )
g=sns.heatmap(data=data[["LAErr","CLErr","SZErr"]].T,
            ax=ax2,
            linewidth=0.7,
            vmin=0, vmax=0.6,
            linecolor="w",
            cmap=sns.color_palette('coolwarm',n_colors=100),
            cbar=False
           )
sns.heatmap(data=np.array(data["effc"]).reshape(1,-1), #reshape to form 2D array
            ax=ax0,
            linewidth=0,
            linecolor="w",
            cmap=sns.color_palette('rainbow',n_colors=10),
            cbar=False
```

```
           )
ax0.set_xlabel(None)
ax0.set_xticks([]);
ax0.set_yticklabels(["Effc"], rotation=1, fontweight="bold")
############ cbar
rect = [0.93, 0.57, 0.03, 0.3]   #x, y, width, height
cbar_ax = fig.add_axes(rect)
cb = h.figure.colorbar(h.collections[0], cax=cbar_ax)  #share colorbar
cb.ax.tick_params(direction='in', labelsize=9, color="k", length=3, left=True, right=True)
cb.ax.set_ylabel( 'Normalized Value',fontweight="bold", fontsize=10)
####################
rect2 = [0.93, 0.13, 0.03, 0.3]
cbar_ax2 = fig.add_axes(rect2)
cb2 = g.figure.colorbar(g.collections[0], cax=cbar_ax2)
cb2.ax.tick_params(direction='in', labelsize=9, color="k", length=3,
                   left=True, right=True)
cb2.ax.set_ylabel( 'Normalized Value', fontweight="bold", fontsize=10)
################### set axis
font1 = {'family': 'Arial',  #Microsoft JhengHei
         'color': 'k',
         'weight': 'bold', }
ax1.set_title("Training Set(n=%s)" % train_set_3.shape[0], font1);
ax1.set_yticklabels(["LA","CL","SZ"], fontweight="bold", rotation=0)
ax2.set_yticklabels(["LAErr","CLErr","SZErr"], fontweight="bold")
ax1.set_xlabel(None)
ax2.set_xlabel("Sample", fontweight="bold", fontsize=11)
ax1.set_xticks([]);
ax2.set_xticks([]);

fig.savefig(os.path.join(save_dir, str(time.time())+'.svg'), bbox_inches='tight', dpi=150)
```



In [22]:
```
fig = plt.figure(dpi=100, figsize=(2,3))
grid = fig.add_gridspec(3, 1, hspace=0.1, height_ratios=[4,0.7,4])
ax1 = plt.subplot(grid[0,:])
ax2 = plt.subplot(grid[2,:])
ax0 = plt.subplot(grid[1,:])
############### heatmap123
data = test_set_3.sort_values(by = ['effc',"SZa"], ascending=False)
h=sns.heatmap(data=data[["LAa","CLa","SZa"]].T,
              ax=ax1,
              vmin=0,vmax=1.5,
              linewidth=0.7,
              linecolor="w",
              cmap=sns.color_palette('bwr', n_colors=100),
              cbar=False,
              cbar_kws={ 'label':'Normalized Value', 'extend':'both',},
             )
g=sns.heatmap(data=data[["LAErr","CLErr","SZErr"]].T,
              ax=ax2,
              linewidth=0.7,
              vmin=0,vmax=0.6,
              linecolor="w",
              cmap=sns.color_palette('coolwarm', n_colors=100),
```

```
            cbar=False)
sns.heatmap(data=np.array(data["effc"]).reshape(1,-1),
            ax=ax0,
            linewidth=0,
            linecolor="w",
            cmap=sns.color_palette('rainbow', n_colors=10),
            cbar=False)
ax0.set_xlabel(None)
ax0.set_xticks([]);
ax0.set_yticklabels(["Effc"], rotation=1, fontweight="bold")
############ cbar
rect = [1, 0.57, 0.1, 0.3]
cbar_ax = fig.add_axes(rect)
cb = h.figure.colorbar(h.collections[0], cax=cbar_ax)
cb.ax.tick_params(direction='in', labelsize=9, color="k",length=3,
                  left=True, right=True)
cb.ax.set_ylabel( 'Normalized Value', fontweight="bold", fontsize=9)
###################
rect2 = [1, 0.14, 0.1, 0.3]
cbar_ax2 = fig.add_axes(rect2)
cb2 = g.figure.colorbar(g.collections[0], cax=cbar_ax2)
cb2.ax.tick_params(direction='in', labelsize=9, color="k", length=3,
                  left=True, right=True)
cb2.ax.set_ylabel( 'Normalized Value', fontweight="bold", fontsize=9)
################### set axis
font1 = {'family':'Arial', 'color':'k', 'weight':'bold',}
ax1.set_title("Test Set (n=%s)" % test_set_3.shape[0], font1);
ax1.set_yticklabels(["LA","CL","SZ"], fontweight="bold", rotation=0)
ax2.set_yticklabels(["LAErr","CLErr","SZErr"], fontweight="bold")
ax1.set_xlabel(None)
ax2.set_xlabel("Sample", fontweight="bold", fontsize=11)
ax1.set_xticks([]);
ax2.set_xticks([]);
fig.savefig(os.path.join(save_dir, str(time.time())+'.svg'), bbox_inches='tight', dpi=150)
```



Model Training

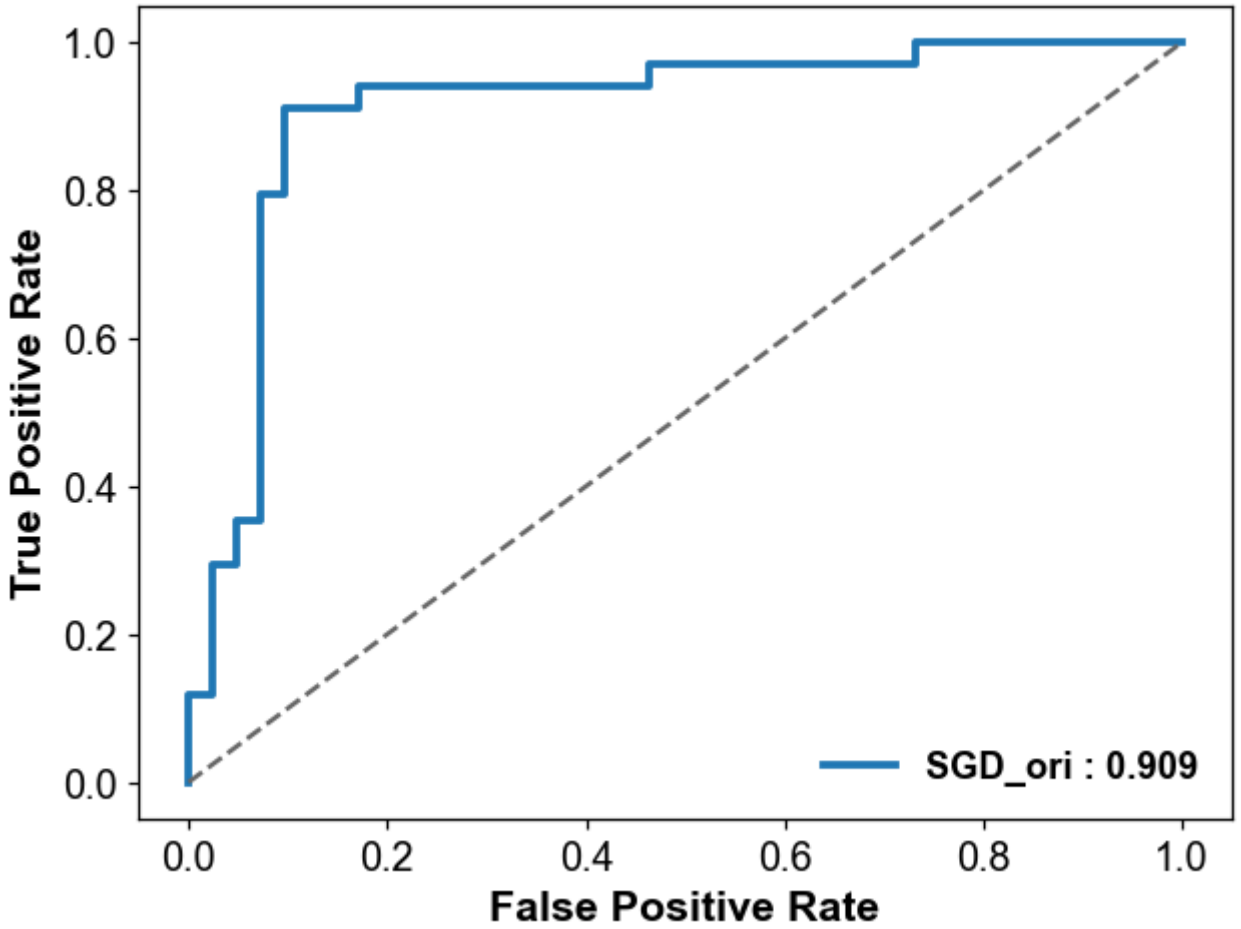
3 algorithms: SGD, RF, SVM. mulitmode (=3) data

without parameter tuning

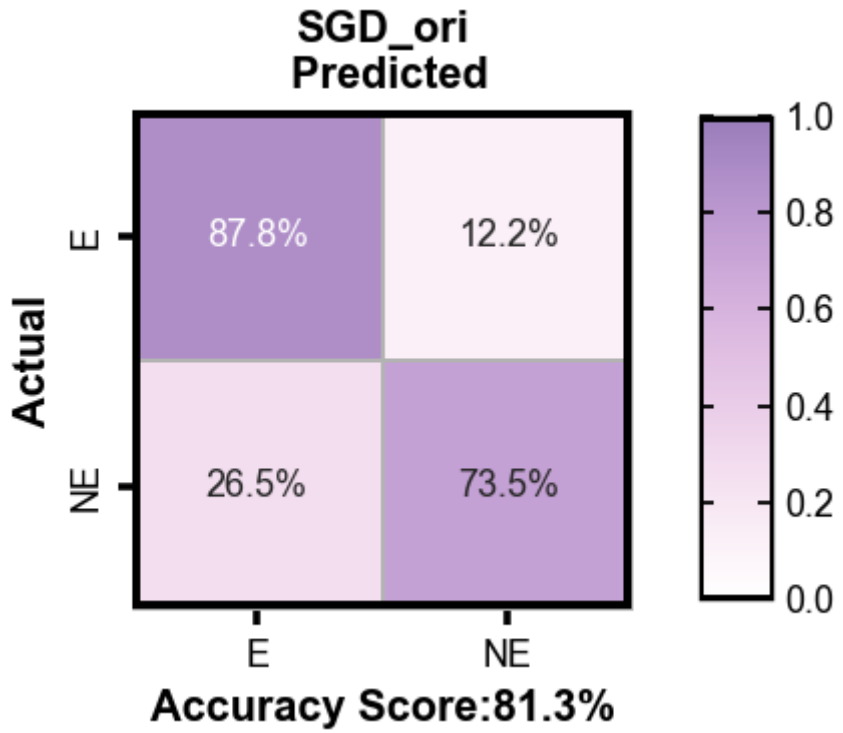
SGD

In [403…

```
sgd_clf3 = SGDClassifier(random_state=42)
r_s = ML_result(sgd_clf3, X_train_3, y_train_3, "SGD_ori", roc="sgd", feedback=1, save_dir=save_dir,)
```



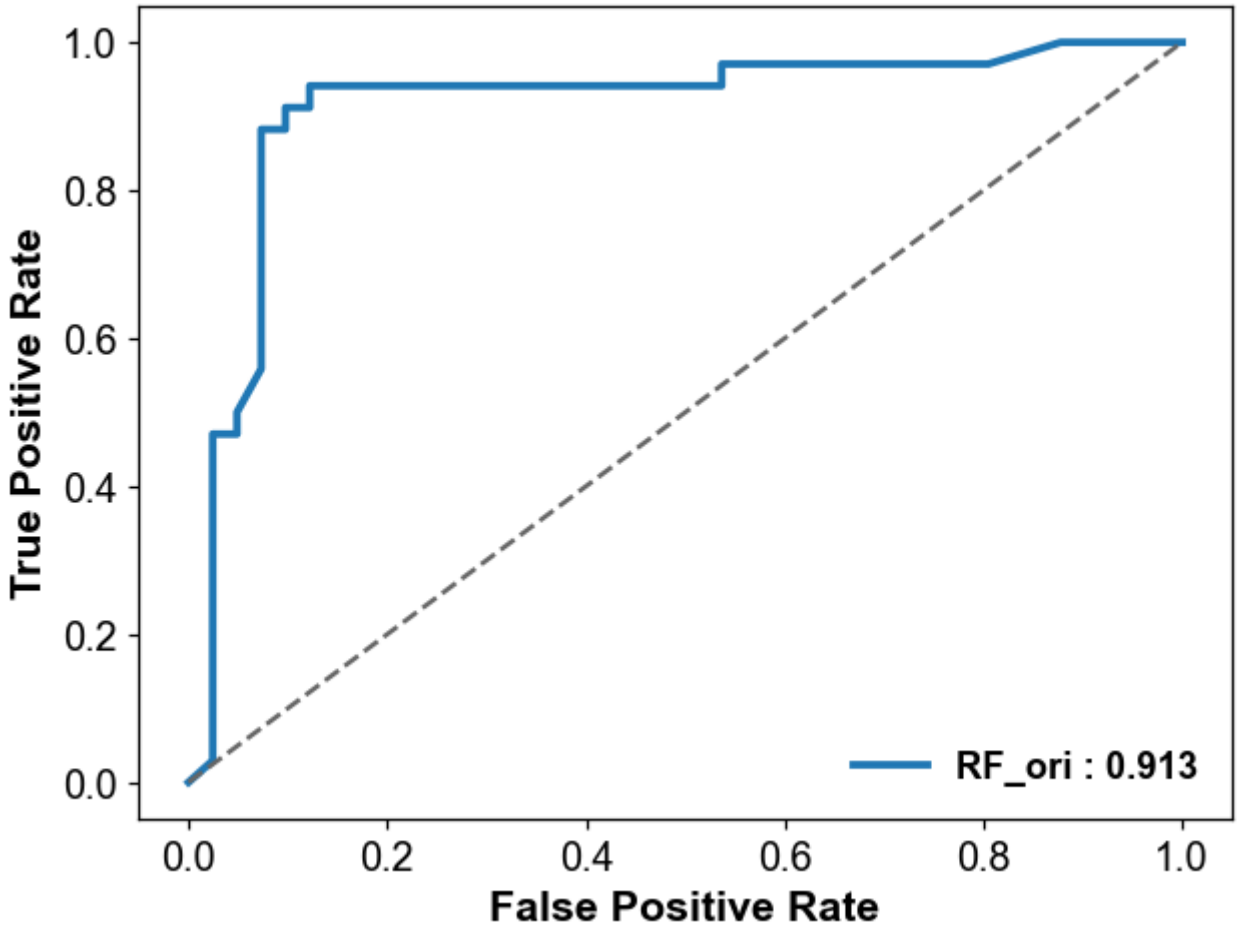
In [398…
```
conf_mat_heatmap(r_s["conf_mat"], rect_set=rect_set, title="SGD_ori", save_dir=save_dir)
```



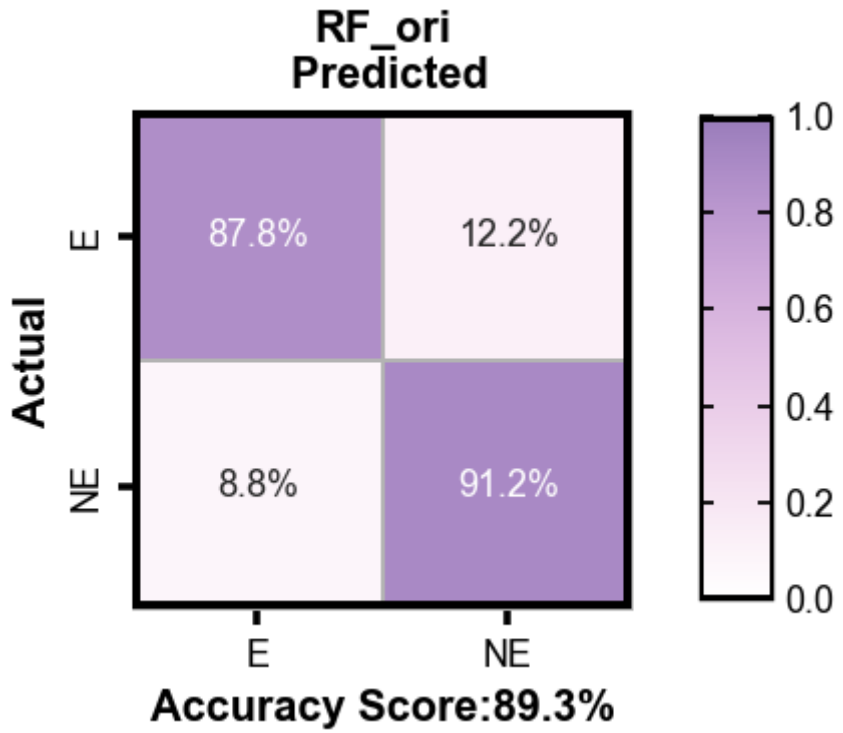
RF

In [399…

```
forest_clf3 = RandomForestClassifier(random_state=42)
r_f = ML_result(forest_clf3, X_train_3, y_train_3, "RF_ori", roc="rf", feedback=1, save_dir=save_dir)
```



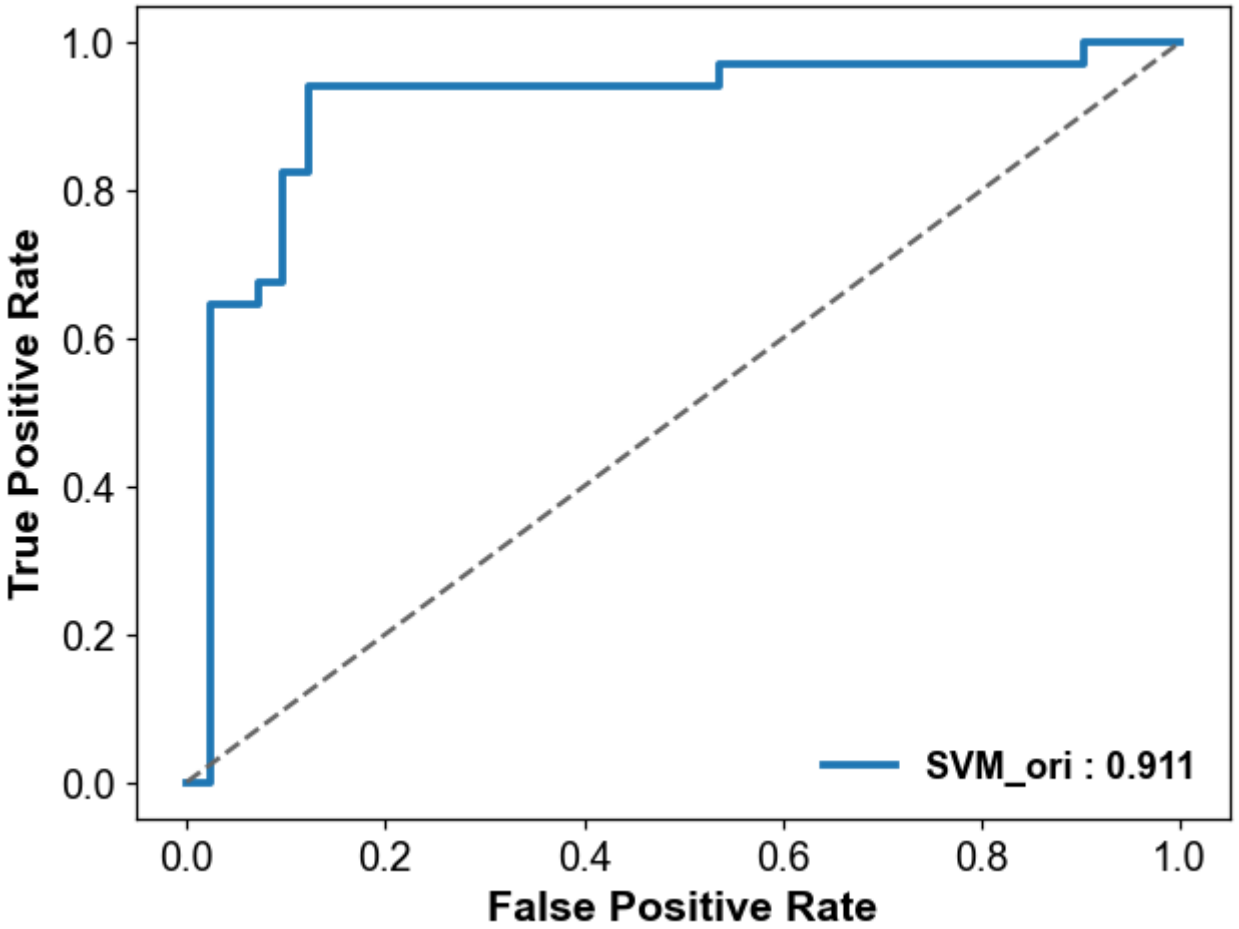
In [317…
```
conf_mat_heatmap(r_f["conf_mat"], rect_set=rect_set, title="RF_ori", save_dir=save_dir)
```



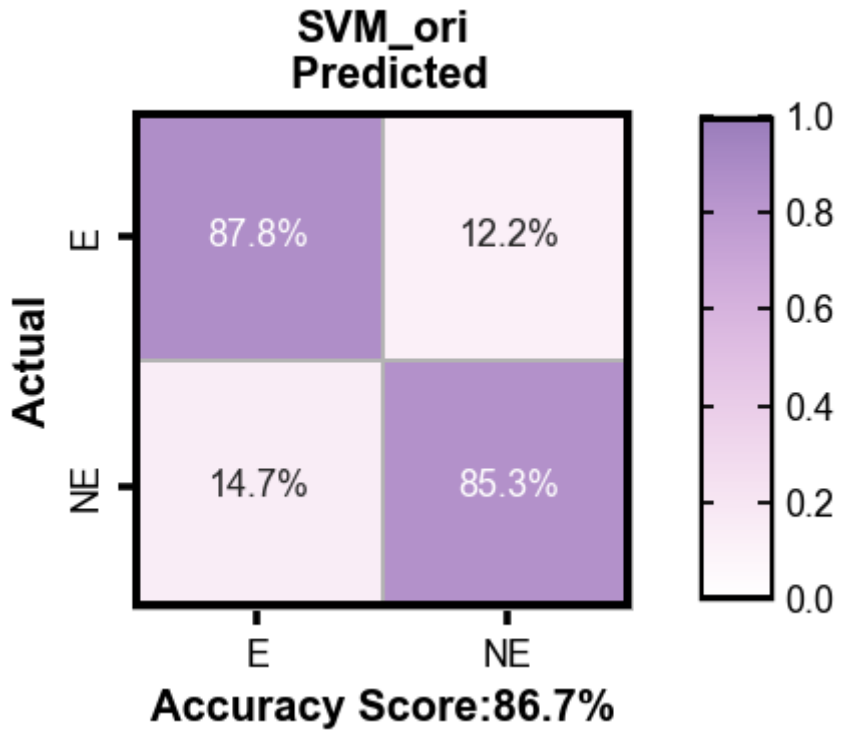
SVM

In [400…

```
svc3 = SVC(probability=True, random_state=42)
r_v = ML_result(svc3, X_train_3, y_train_3, "SVM_ori", roc="rf", feedback=1, save_dir=save_dir)
```



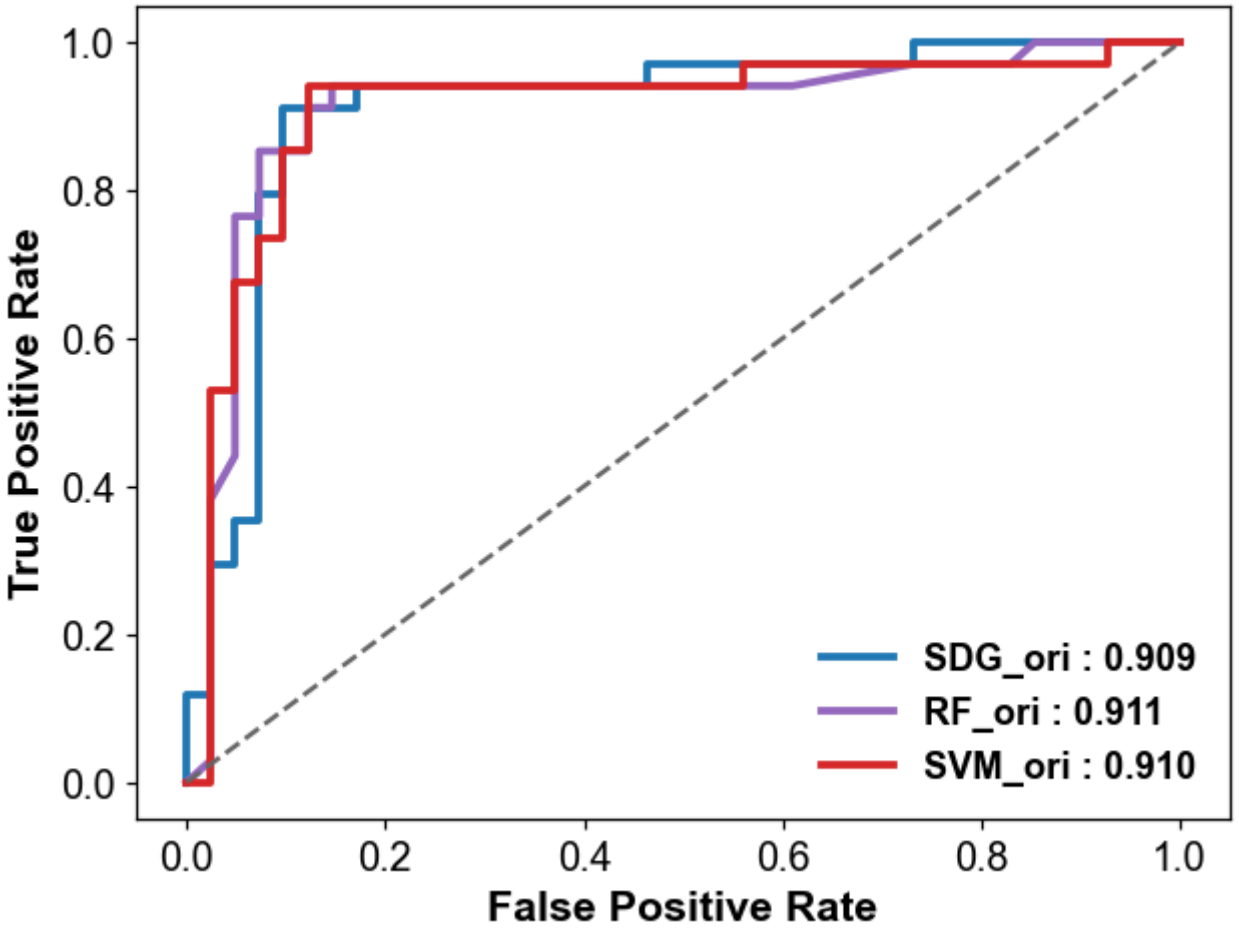
In [320…
```
conf_mat_heatmap(r_v["conf_mat"], rect_set=rect_set, title="SVM_ori", save_dir=save_dir)
```



re-paint

In [337…

```
plot_roc_curve([r_s["fpr"], r_f["fpr"], r_v["fpr"]],
               [r_s["tpr"], r_f["tpr"], r_v["tpr"]],
               ["SDG_ori", "RF_ori", "SVM_ori"],
               [r_s["auc"], r_f["auc"], r_v["auc"]], save_dir=save_dir,
               cmap=[plt.get_cmap('tab10')(0),plt.get_cmap('tab10')(4),plt.get_cmap('tab10')(3)], )
```



GridSearch

triple modal data

SGD

best_SGDClassifier(alpha=0.055564444444444444, eta0=0.26126315789473686,
learning_rate='invscaling', loss='log', n_jobs=-1, penalty='l1',
power_t=0.07357142857142857, random_state=42)

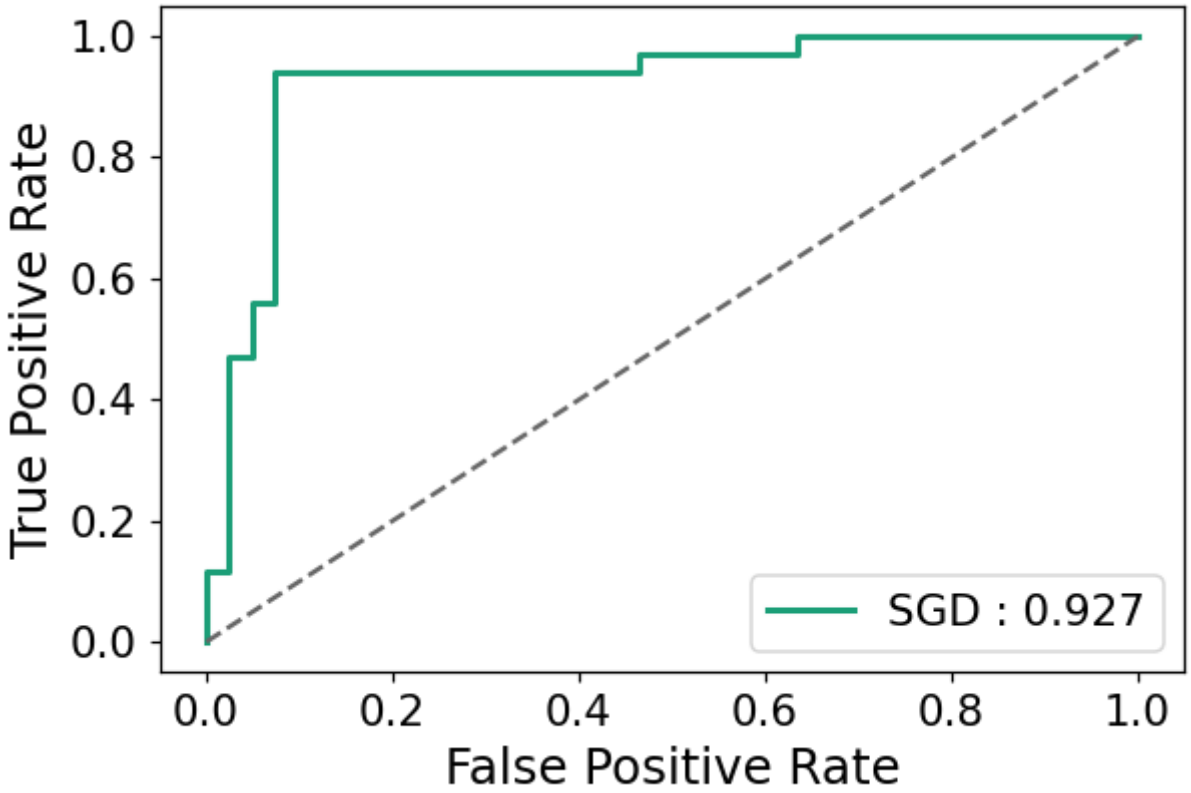
In [976…
```
#trainable parameters
sgd_clf = SGDClassifier(random_state=42, n_jobs=-1)
sgd_clf.get_params()
```

Out[976]:
```
{'alpha': 0.0001,
 'average': False,
 'class_weight': None,
 'early_stopping': False,
 'epsilon': 0.1,
 'eta0': 0.0,
 'fit_intercept': True,
 'l1_ratio': 0.15,
 'learning_rate': 'optimal',
 'loss': 'hinge',
 'max_iter': 1000,
 'n_iter_no_change': 5,
 'n_jobs': -1,
 'penalty': 'l2',
 'power_t': 0.5,
 'random_state': 42,
 'shuffle': True,
 'tol': 0.001,
 'validation_fraction': 0.1,
 'verbose': 0,
 'warm_start': False}
```

In [27]:
```
param=[{"learning_rate": ['constant','optimal','invscaling'],
        'penalty': ['l2','l1','elasticnet'],
        "eta0":np.linspace(0.01,0.5,num=10),
        "loss":["hinge","modified_huber","log"],
        "alpha":np.linspace(0.0001,0.09,num=10),
        "power_t":np.linspace(0.001,0.1,num=10),
        "class_weight":[None,"balanced"],
        "l1_ratio":np.linspace(0.1,0.9,num=10)
       }]

sgdbest = GridSearch_result(sgd_clf, X_train_3, y_train_3, param)
print(sgdbest)
```

```
Re_best_sgd = ML_result(sgdbest[1], X_train_3, y_train_3, "SGD", roc="sgd", feedback=1, save_dir=save_dir)
```

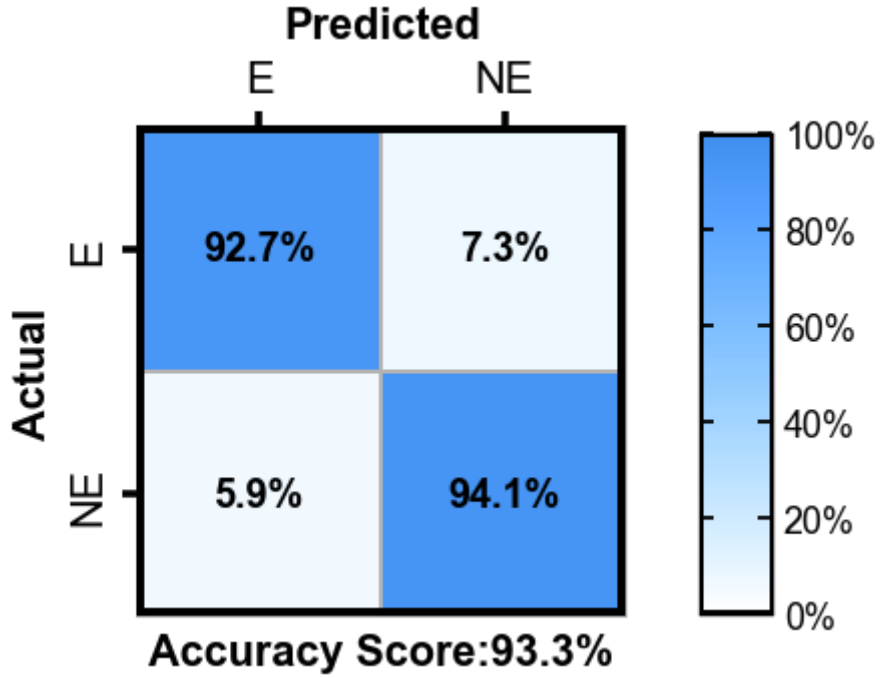
```
Run Time:1806.9934689998627 s
[{'alpha': 0.055564444444444444, 'class_weight': None, 'eta0': 0.26126315789473686, 'learning_rate': 'invscaling', 'loss': 'lo
g', 'penalty': 'l1', 'power_t': 0.07357142857142857}, SGDClassifier(alpha=0.055564444444444444, eta0=0.26126315789473686,
              learning_rate='invscaling', loss='log', n_jobs=-1, penalty='l1',
              power_t=0.07357142857142857, random_state=42)]
```



Out[27]:
```
{'conf_mat': array([[38,  3],
        [ 2, 32]], dtype=int64),
 'accu': 0.9333333333333333,
 'auc': 0.9268292682926829}
```

In [62]:
```
conf_mat_heatmap(Re_best_sgd['conf_mat'], rect_set=rect_set, title="SGD", save_dir=save_dir)
```

```
D:\Anaconda\lib\site-packages\ipykernel_launcher.py:44: UserWarning: FixedFormatter should only be used together with FixedLocator
```



RF

best_RandomForestClassifier(max_depth=2, max_features=3, min_samples_leaf=6, n_estimators=3, n_jobs=-1, random_state=42)

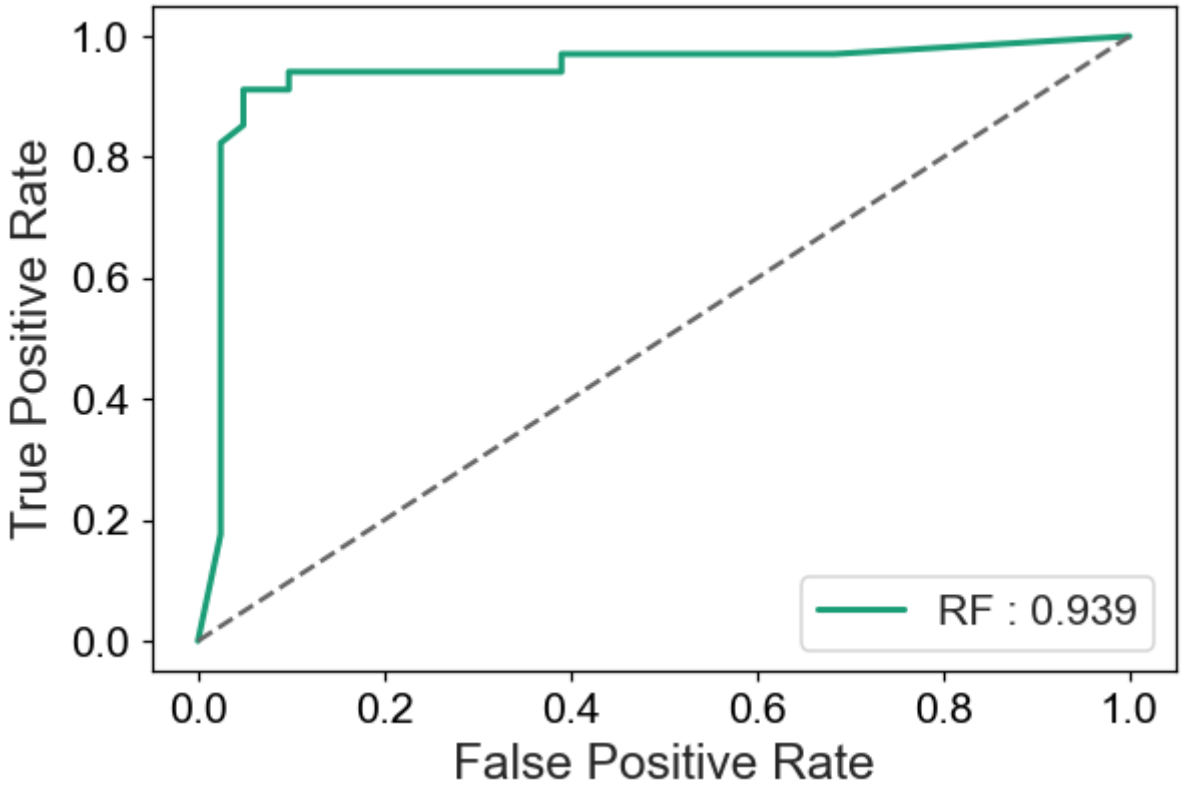
In [980…

```
#trainable parameters
forest_clf = RandomForestClassifier(n_jobs=-1, random_state=42)
forest_clf.get_params()
```

Out[980]:
```
{'bootstrap': True,
 'ccp_alpha': 0.0,
 'class_weight': None,
 'criterion': 'gini',
 'max_depth': None,
 'max_features': 'auto',
 'max_leaf_nodes': None,
 'max_samples': None,
 'min_impurity_decrease': 0.0,
 'min_samples_leaf': 1,
 'min_samples_split': 2,
 'min_weight_fraction_leaf': 0.0,
 'n_estimators': 5,
 'n_jobs': None,
 'oob_score': False,
 'random_state': None,
 'verbose': 0,
 'warm_start': False}
```

In [66]:
```
param2 = [{'n_estimators': range(2,18),
           "max_depth":[None, 2, 3, 5],
           "max_features":["auto", 6, 5, 4, 3],
           "min_samples_split":[2, 3, 4, 6],
           "min_samples_leaf":[6, 8, 10, 5]
          }]
rfbest = GridSearch_result(forest_clf, X_train_3, y_train_3, param2, score="roc_auc")
print(rfbest)
ML_result(rfbest[1], X_train_3, y_train_3, "RF", roc="rf", feedback=1, save_dir=save_dir)
```

```
Run Time:2376.3678488731384 s
[{'max_depth': 2, 'max_features': 3, 'min_samples_leaf': 6, 'min_samples_split': 2, 'n_estimators': 3}, RandomForestClassifier
(max_depth=2, max_features=3, min_samples_leaf=6,
                       n_estimators=3, n_jobs=-1, random_state=42)]
```



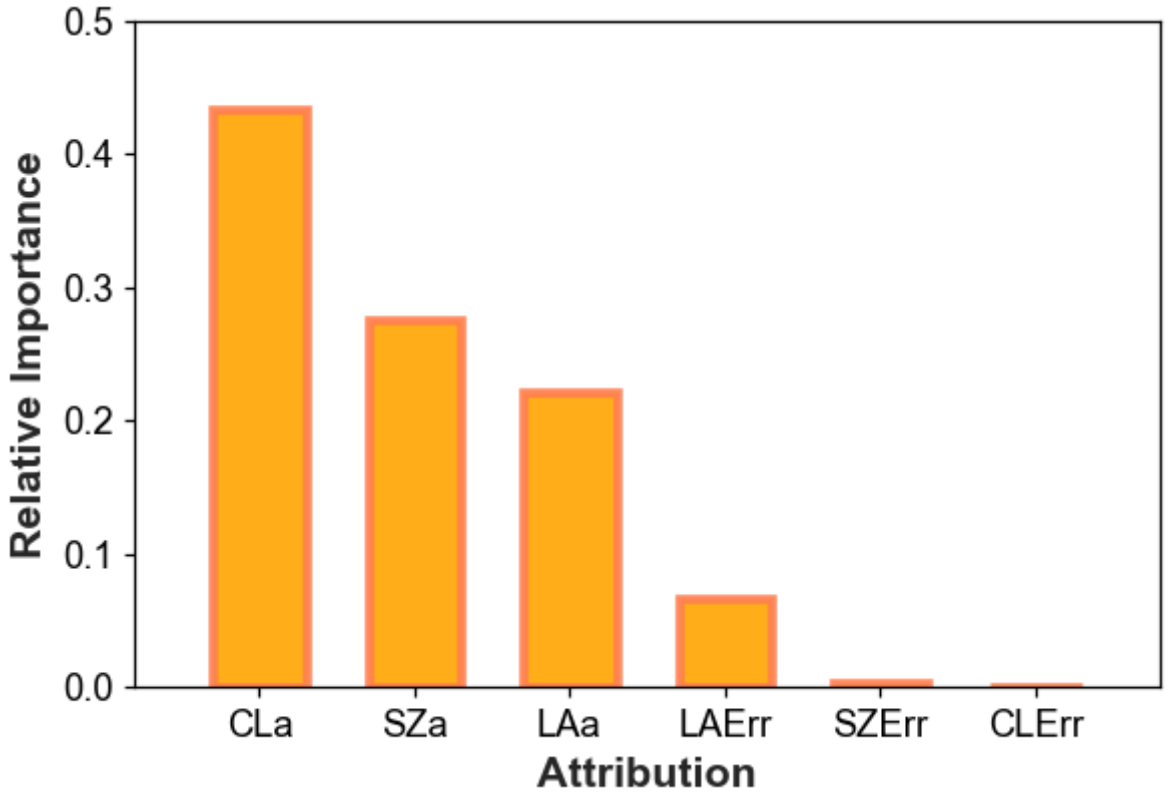
Out[66]:
```
{'conf_mat': array([[38,  3],
       [ 3, 31]], dtype=int64),
 'accu': 0.92,
 'auc': 0.9390243902439024}
```

In [219…
```
#feature importance. sum=100
rf_impo = rfbest[1].feature_importances_
impo_df = pd.DataFrame(sorted(zip(rf_impo, X_train_3.columns), reverse=True))
print(impo_df)

plt.rcParams['axes.labelsize'] = 14
plt.rcParams['xtick.labelsize'] = 12
plt.rcParams['ytick.labelsize'] = 12
sns.set_style("ticks", {"axes.edgecolor": "k", 'xtick.color': 'k',
                        'ytick.color': 'k',})
fig, ax1 = plt.subplots(dpi=110,)
```

```
ax1.set_ylabel('Relative Importance', fontweight="bold")
ax1.set_xlabel('Attribution', fontweight="bold")
ax1.set_xlim(-0.8, 5.8)
ax1.set_ylim(0, 0.5)
ax1.bar(x=impo_df[1], height=impo_df[0], width=0.6,
        color='orange',alpha=0.9, edgecolor='coral', linewidth=3, )
```

```
          0      1
0  0.433293    CLa
1  0.275099    SZa
2  0.222177    LAa
3  0.066863  LAErr
4  0.002568  SZErr
5  0.000000  CLErr
```

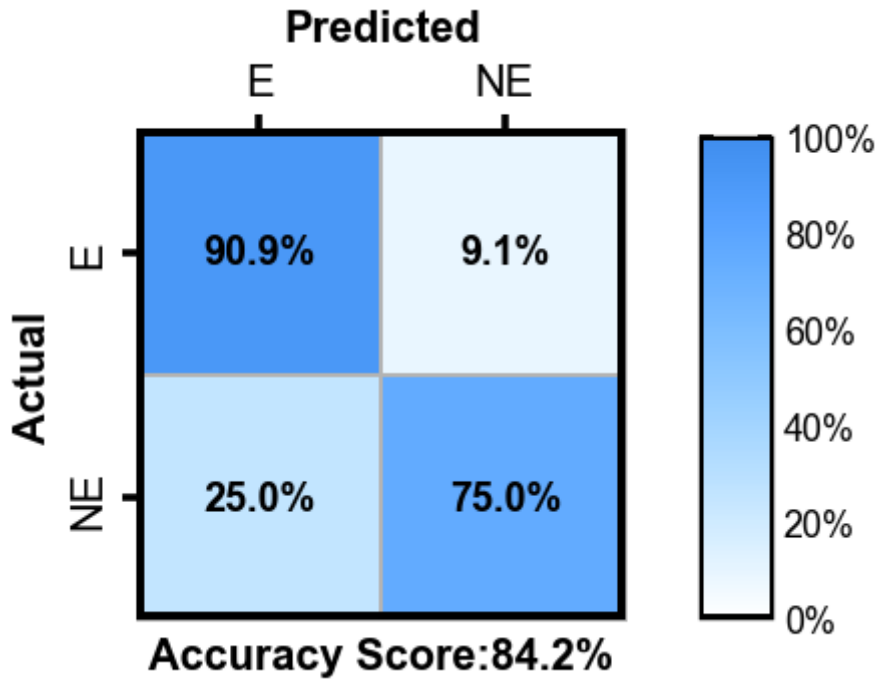
Out[219]: <BarContainer object of 6 artists>



In [322…
```
# test set
final_pred_rf=rfbest[1].predict(X_test)
confmatrf = confusion_matrix(y_test, final_pred_rf)
print(confmatrf)
conf_mat_heatmap(confmatrf, "testrf", save=0, )
```

```
[[10  1]
 [ 2  6]]
```

```
D:\Anaconda\lib\site-packages\ipykernel_launcher.py:44: UserWarning: FixedFormatter should only be used together with FixedLocator
```



SVM

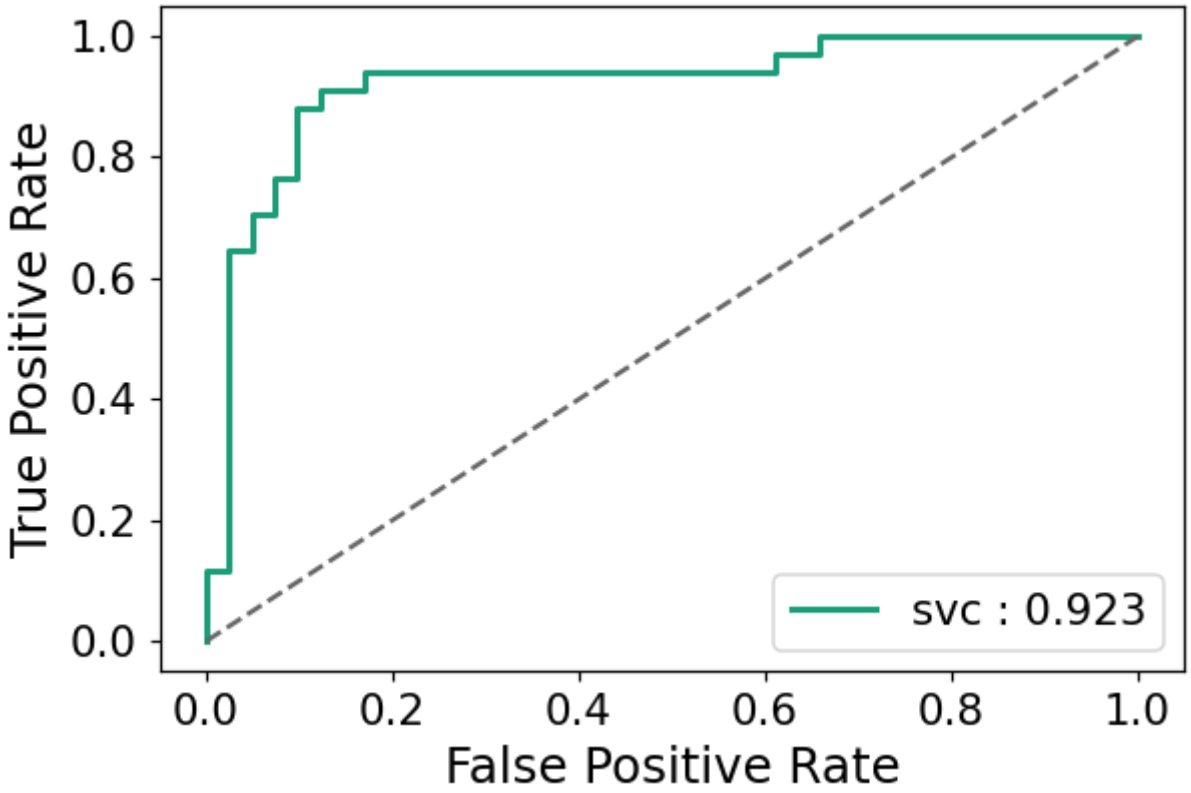
the best: SVC(class_weight='balanced', degree=1, gamma='auto', kernel='linear', probability=True, random_state=42)

In [347…
```
#trainable parameters
svc_clf = SVC(probability=True, random_state=42)
svc_clf.get_params()
```

Out[347]:
```
{'C': 1.0,
 'break_ties': False,
 'cache_size': 200,
 'class_weight': None,
 'coef0': 0.0,
 'decision_function_shape': 'ovr',
 'degree': 3,
 'gamma': 'scale',
 'kernel': 'rbf',
 'max_iter': -1,
 'probability': True,
 'random_state': 42,
 'shrinking': True,
 'tol': 0.001,
 'verbose': False}
```

In [30]:
```
param3 = [{'kernel':["rbf", "poly", "linear"],
           "C":[0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3],
           "degree":[1,2,3,4,5],
           "gamma":["auto", 1/5, 1/6, 1/7, 1/8, 1/9, 1/10, 1/11],
           "class_weight":[None, "balanced"],
          }]
svcbest = GridSearch_result(svc_clf, X_train_3, y_train_3, param3,)
print(svcbest)
ML_result(svcbest[1], X_train_3, y_train_3, "SVM", roc="rf", feedback=1, save_dir=save_dir)
```

```
Run Time:19.477946281433105 s
[{'C': 1.0, 'class_weight': 'balanced', 'degree': 1, 'gamma': 'auto', 'kernel': 'linear'}, SVC(class_weight='balanced', degree=
1, gamma='auto', kernel='linear',
    probability=True, random_state=42)]
```



Out[30]:
```
{'conf_mat': array([[36,  5],
        [ 3, 31]], dtype=int64),
 'accu': 0.8933333333333333,
 'auc': 0.9225251076040172}
```

re-paint

In [ ]:
```
# try to use R in Python
# you can import rpy2 lib to python and run it directly
import rpy2.robjects as robj
# or simply copy ROC_scores to R document, and run it in R
```

In [39]:
```
def repaint_y_score(ML, X, y, roc):
    ML.fit(X, y)
    y_pred = cross_val_predict(ML, X, y, cv=3)
```

```
    conf_mat=confusion_matrix(y, y_pred)
    accu=accuracy_score(y, y_pred)

    if roc =="rf":
        y_probas_forest = cross_val_predict(ML, X, y, cv=3, method="predict_proba")
        y_scores = y_probas_forest[:, 1] # score = proba of positive class
    if roc == "sgd":
        y_scores = cross_val_predict(ML, X, y, cv=3, method="decision_function")
    return {"conf_mat":conf_mat, "accu":accu, "y_scores":y_scores}
```

In [53]:

```
#get ROC_scores
sgd1 = SGDClassifier(alpha=0.0556, eta0=0.261, learning_rate='invscaling', loss='log',
                     n_jobs=-1, penalty='l1', power_t=0.0736, random_state=42)
sgd2 = repaint_y_score(sgd1, X_train, y_train, roc="sgd")
rf1 =  RandomForestClassifier(max_depth=2, max_features=3, min_samples_leaf=6,
                              n_estimators=3, n_jobs=-1, random_state=42)
rf2 = repaint_y_score(rf1, X_train, y_train, roc="rf")
svm1 = SVC(class_weight='balanced', degree=1, gamma='auto', kernel='linear',
           probability=True, random_state=42)
svm2 = repaint_y_score(svm1, X_train, y_train, roc="rf")
print(sgd2)
print(rf2)
print(svm2)
```

{'conf_mat': array([[38, 3],
       [2, 32]], dtype=int64), 'accu': 0.9333333333333333, 'y_scores': array([0.72312367, 0.39980977, -0.70097657, 1.016311
39, -1.6508767 ,
        0.22766929, -0.87385105, -1.42789829, -0.50978383, -2.07784508,
        1.7860608 , 0.66615838, -1.89814115, 0.71511343, -0.75554835,
       -1.34268972, -0.8452248 , -1.22071699, -1.99413643, -0.50116724,
       -1.25784696, 0.02785996, 1.03386372, -0.04932988, 2.39464792,
       -0.35010662, -1.48451378, 0.38752314, 0.85253221, -0.25019795,
        1.61050879, 1.26859713, -1.49846388, 0.92760207, 1.44594676,
       -1.23269654, -1.55030729, 0.02397522, 0.80580694, -0.94629467,
       -0.43557335, -1.02550174, -0.7015419 , -1.4032276 , 1.43682554,
        0.3152954 , 0.0334765 , 0.24907712, -1.51670632, -0.59102003,
       -1.54509993, 0.68436951, 0.08870872, -1.29385309, 0.36073329,
       -0.98084116, 2.67070193, 0.82453423, -1.83546116, 0.40051707,
       -1.25106773, 2.85025618, 1.30083977, 1.48096699, 0.39160998,
       -1.76196663, 2.74453605, -1.06991411, 0.11569793, 0.26265912,
       -1.52903099, -1.68799994, -0.59308524, -0.28614713, -0.93526019])}
{'conf_mat': array([[38, 3],
       [3, 31]], dtype=int64), 'accu': 0.92, 'y_scores': array([0.51851852, 1.   , 0.18518519, 0.85185185, 0.   ,
       0.66666667, 0.18518519, 0.14814815, 0.33333333, 0.   ,
       1.   , 1.   , 0.   , 1.   , 0.33333333,
       0.   , 0.33333333, 0.   , 0.   , 0.33333333,
       0.   , 0.81481481, 1.   , 0.33333333, 1.   ,
       0.15555556, 0.06060606, 0.66666667, 1.   , 0.26666667,
       0.91111111, 0.85555556, 0.11111111, 0.85555556, 0.76666667,
       0.11111111, 0.06060606, 0.82222222, 0.85555556, 0.15555556,
       0.15555556, 0.   , 0.26666667, 0.21616162, 0.85555556,
       0.91111111, 0.43333333, 0.66666667, 0.06060606, 0.1754902 ,
       0.   , 0.58888889, 0.73333333, 0.   , 0.63809524,
       0.16666667, 0.66296296, 0.9462963 , 0.   , 0.65   ,
       0.   , 0.8510582 , 0.9462963 , 0.8510582 , 0.8510582 ,
       0.09215686, 0.8510582 , 0.09215686, 0.65   , 0.9462963 ,
       0.09215686, 0.   , 0.2254902 , 0.46296296, 0.   ])}
{'conf_mat': array([[36, 5],
       [3, 31]], dtype=int64), 'accu': 0.8933333333333333, 'y_scores': array([0.73192432, 0.76413036, 0.34075397, 0.8213859 ,
0.04307162,
       0.48468324, 0.17474068, 0.11217057, 0.35308007, 0.0253678 ,
       0.97074273, 0.84904803, 0.04047694, 0.84985575, 0.20906655,
       0.09035234, 0.19388436, 0.09649599, 0.02994892, 0.34957773,
       0.14341135, 0.607255 , 0.89448447, 0.56872131, 0.98448264,

```
0.42505149, 0.0838077 , 0.69557985, 0.88925073, 0.43041704,
0.94281477, 0.93168635, 0.17524325, 0.87484605, 0.91246575,
0.16216062, 0.07890475, 0.54335175, 0.89917583, 0.20682048,
0.3352367 , 0.15934692, 0.26901561, 0.10937705, 0.92240921,
0.74401725, 0.54629877, 0.59341492, 0.08076453, 0.2492641 ,
0.04833389, 0.76624209, 0.41523756, 0.07273415, 0.56412295,
0.10386977, 0.98327389, 0.8381593 , 0.02823063, 0.67510847,
0.07836242, 0.99515639, 0.89120713, 0.94804383, 0.81173022,
0.03044441, 0.98583329, 0.09231941, 0.44880951, 0.6787739 ,
0.07401733, 0.04691326, 0.25888165, 0.47388505, 0.11976995])}
```

single mode data

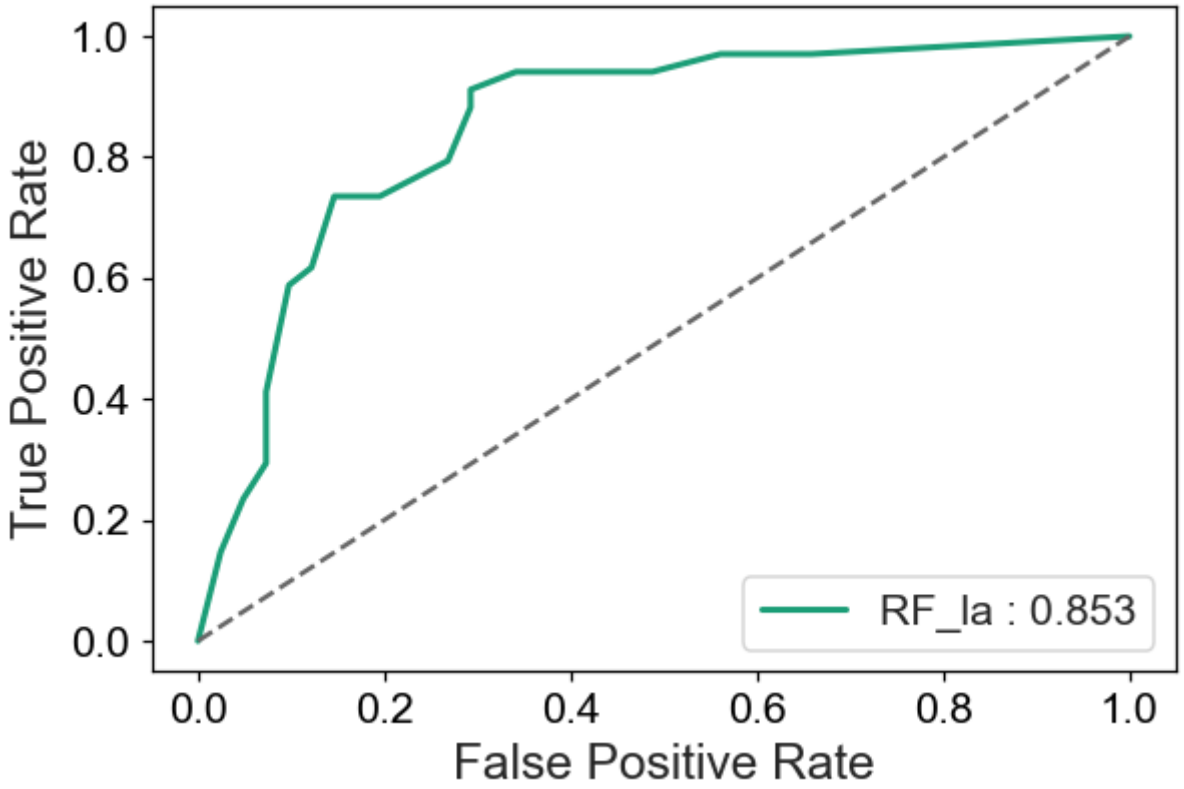
LA

RF

best_RandomForestClassifier(n_estimators=16, n_jobs=-1, random_state=42)

In [67]:
```
forest_la = RandomForestClassifier(random_state=42, n_jobs=-1)
param2 = [{'n_estimators': range(2,20), "max_depth":[None], "max_features":["auto",1,2],
          }]
rfbest_la = GridSearch_result(forest_la, X_train_3[["LAa","LAErr"]], y_train_3, param2,)
print(rfbest_la)
ML_result(rfbest_la[1], X_train_3[["LAa","LAErr"]], y_train_3,"RF_la", roc="rf")
```

```
Run Time:32.22870898246765 s
[{'max_depth': None, 'max_features': 'auto', 'n_estimators': 16}, RandomForestClassifier(n_estimators=16, n_jobs=-1, random_sta
te=42)]
```



Out[67]:
```
{'conf_mat': array([[35,  6],
        [ 9, 25]], dtype=int64),
 'accu': 0.8,
 'auc': 0.8525824964131994}
```

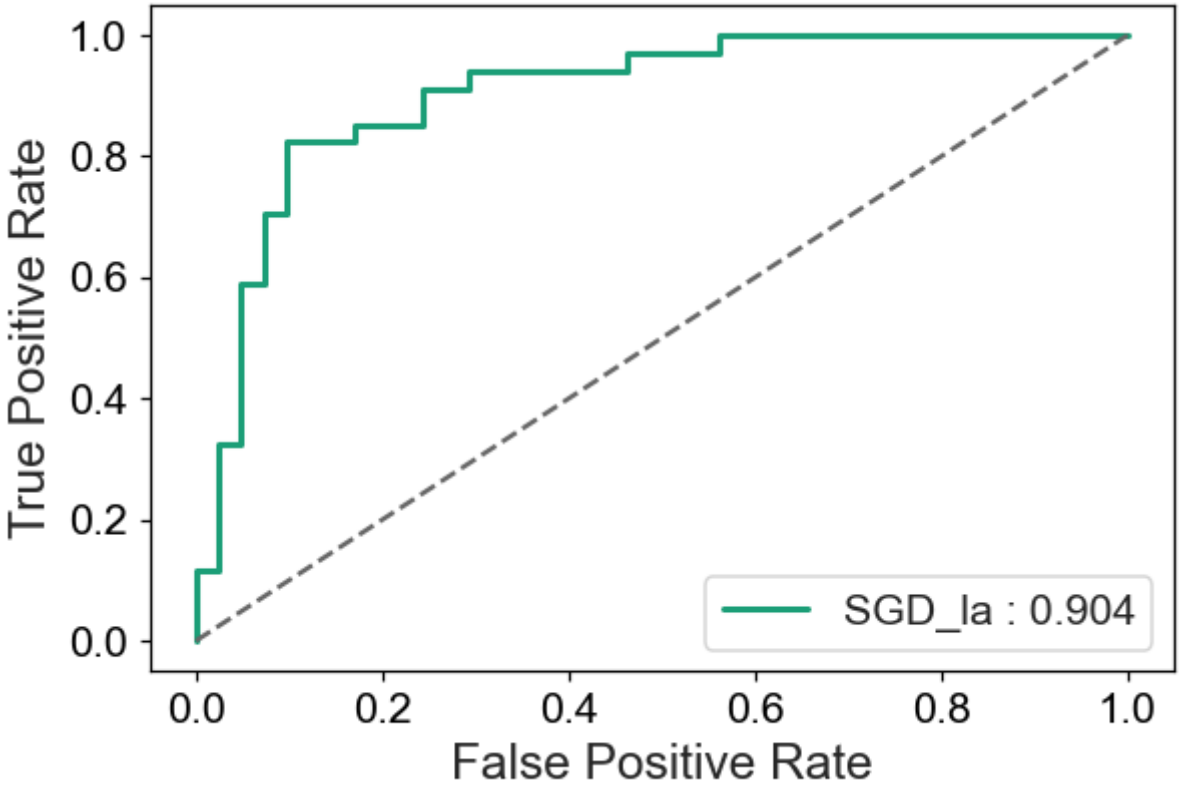
SGD

best_SGDClassifier(eta0=0.07003000000000001, learning_rate='constant', loss='modified_huber', n_jobs=-1, random_state=42)

In [83]:
```
sgd_clf_la = SGDClassifier(random_state=42,n_jobs=-1)
param=[{"learning_rate": ['constant','optimal','invscaling'], 'penalty': ['l2','l1','elasticnet'],
        "eta0":np.linspace(0.0001,0.1,num=21), "loss":["hinge","modified_huber","log"],
         "class_weight":[None,"balanced"]   }]
sgdbest_la = GridSearch_result(sgd_clf_la, X_train_3[["LAa","LAErr"]], y_train_3, param, )
```

```
print(sgdbest_la)
ML_result(sgdbest_la[1], X_train_3[["LAa","LAErr"]], y_train_3, "SGD_la",roc="sgd")
```

```
Run Time:13.13786268234253 s
[{'class_weight': None, 'eta0': 0.07003000000000001, 'learning_rate': 'constant', 'loss': 'modified_huber', 'penalty': 'l2'}, S
GDClassifier(eta0=0.07003000000000001, learning_rate='constant',
              loss='modified_huber', n_jobs=-1, random_state=42)]
```



Out[83]:
```
{'conf_mat': array([[37,  4],
                    [ 7, 27]], dtype=int64),
 'accu': 0.8533333333333334,
 'auc': 0.9038737446197992}
```

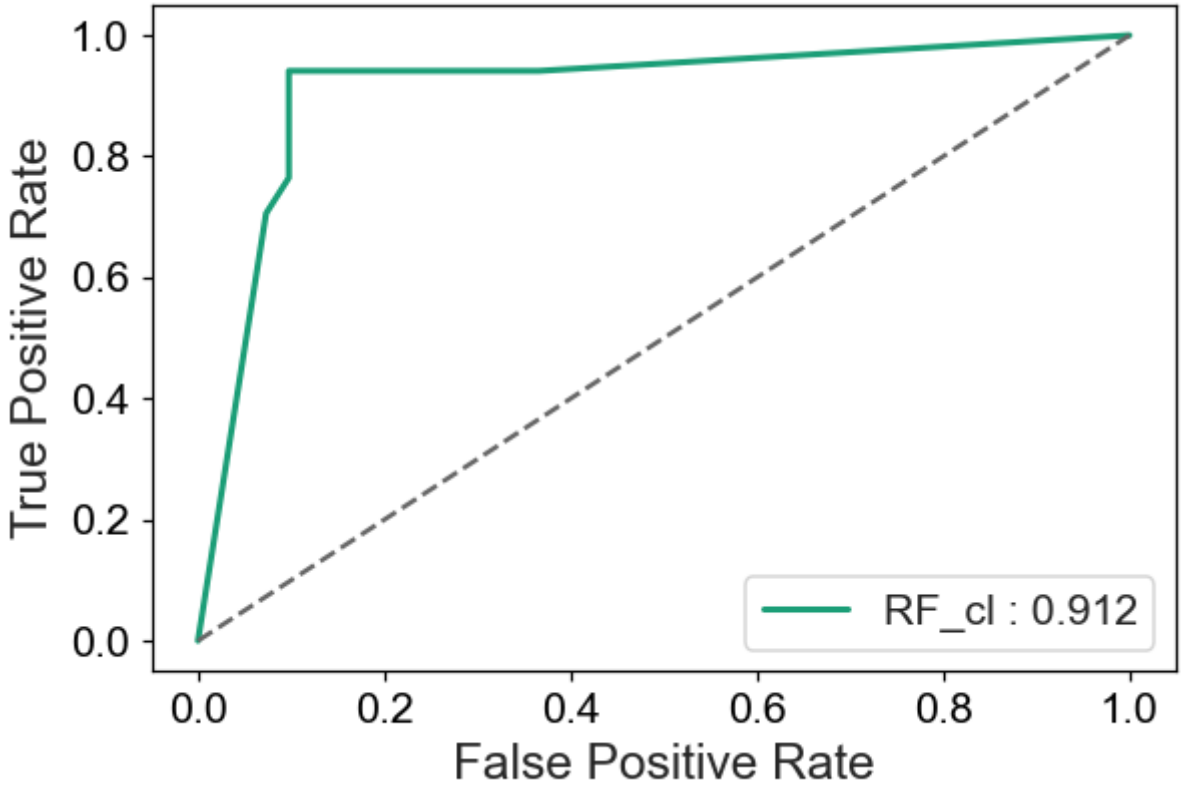
CL

RF

best_RandomForestClassifier(max_features=2, n_estimators=10, n_jobs=-1, random_state=42)

In [70]:
```
forest_cl = RandomForestClassifier(random_state=42, n_jobs=-1)
param2 = [{'n_estimators': range(2,20), "max_depth":[None], "max_features":["auto",1,2],
          }]
rfbest_cl = GridSearch_result(forest_cl, X_train_3[["CLa","CLErr"]], y_train_3, param2,)
print(rfbest_cl)
ML_result(rfbest_cl[1], X_train_3[["CLa","CLErr"]], y_train_3, "RF_cl", roc="rf")
```

```
Run Time:31.991867065429688 s
[{'max_depth': None, 'max_features': 2, 'n_estimators': 10}, RandomForestClassifier(max_features=2, n_estimators=10, n_jobs=-1,
                       random_state=42)]
```



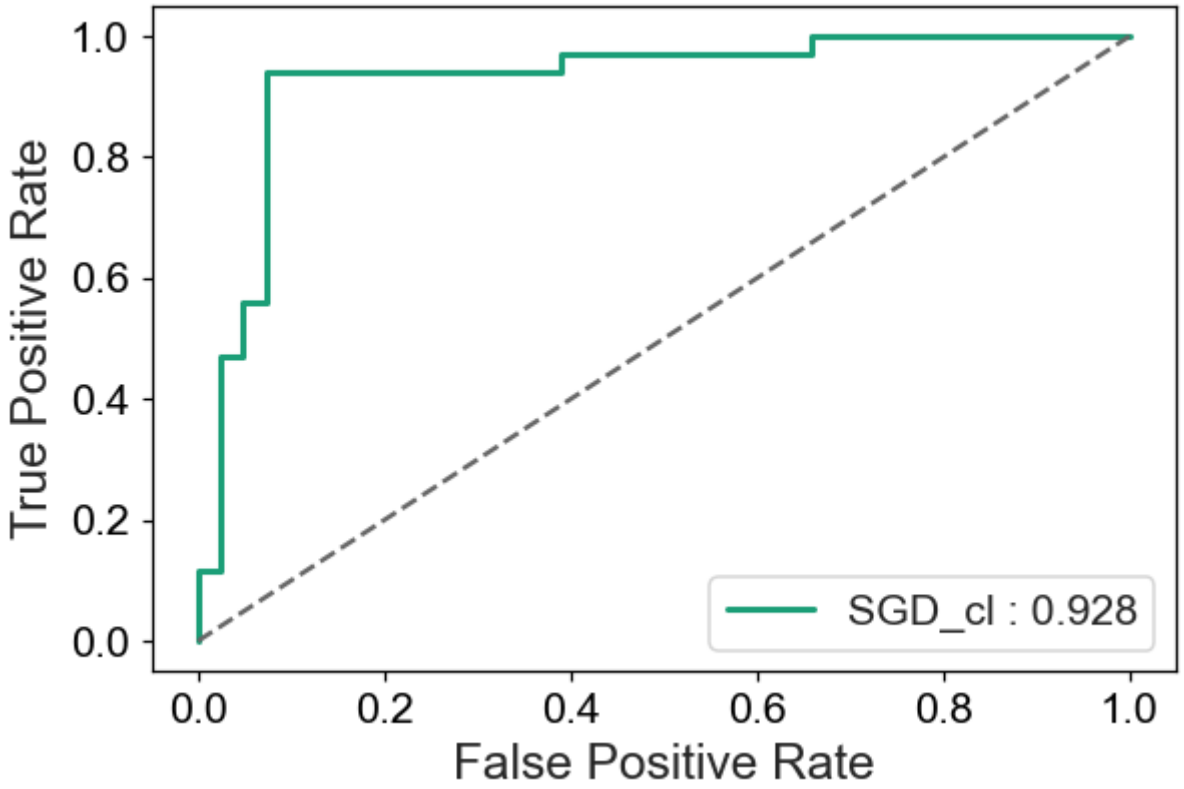
Out[70]:
```
{'conf_mat': array([[37,  4],
        [ 2, 32]], dtype=int64),
 'accu': 0.92,
 'auc': 0.9117647058823529}
```

SGD

best_SGDClassifier(class_weight='balanced', eta0=0.025750000000000002, learning_rate='constant', loss='modified_huber', n_jobs=-1, random_state=42)]

In [84]:
```
sgd_clf_cl = SGDClassifier(random_state=42,n_jobs=-1)
param=[{"learning_rate": ['constant','optimal','invscaling'], 'penalty': ['l2','l1','elasticnet'],
        "eta0":np.linspace(0.001,0.1,num=21), "loss":["hinge","modified_huber","log"],
         "class_weight":[None,"balanced"]   }]
sgdbest_cl = GridSearch_result(sgd_clf_cl, X_train_3[["CLa","CLErr"]], y_train_3, param, )
print(sgdbest_cl)
ML_result(sgdbest_cl[1], X_train_3[["CLa","CLErr"]], y_train_3, "SGD_cl",roc="sgd")
```

```
Run Time:13.701422929763794 s
[{'class_weight': 'balanced', 'eta0': 0.025750000000000002, 'learning_rate': 'constant', 'loss': 'modified_huber', 'penalty':
'l2'}, SGDClassifier(class_weight='balanced', eta0=0.025750000000000002,
              learning_rate='constant', loss='modified_huber', n_jobs=-1,
              random_state=42)]
```



Out[84]:
```
{'conf_mat': array([[38,  3],
       [ 2, 32]], dtype=int64),
 'accu': 0.9333333333333333,
 'auc': 0.9282639885222381}
```

SZ

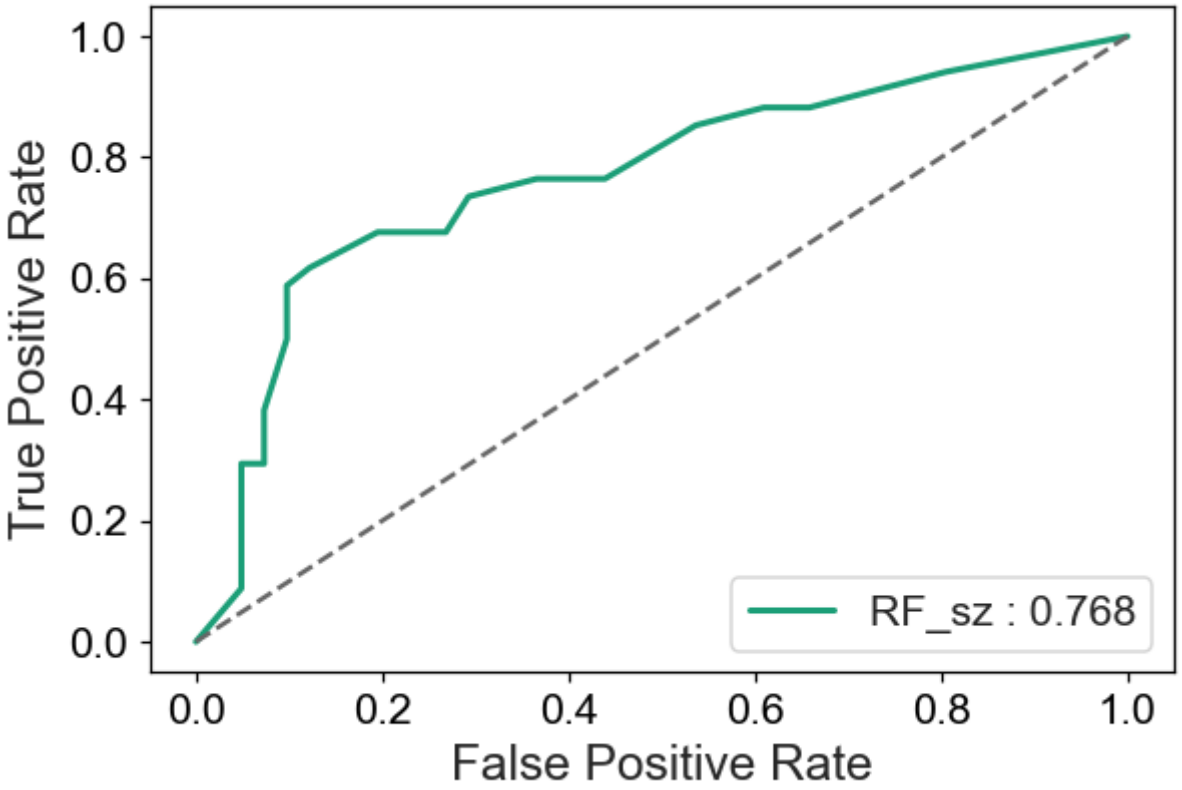
RF

best_RandomForestClassifier(n_estimators=18, n_jobs=-1, random_state=42)

In [93]:
```
forest_sz = RandomForestClassifier(random_state=42, n_jobs=-1)
param2 = [{'n_estimators': range(2,20), "max_depth":[None], "max_features":["auto",1,2],
          }]
```

```
rfbest_sz = GridSearch_result(forest_sz, X_train_3[["SZa","SZErr"]], y_train_3, param2,)
print(rfbest_sz)
ML_result(rfbest_sz[1], X_train_3[["SZa","SZErr"]], y_train_3, "RF_sz", roc="rf")
```

```
Run Time:26.405242681503296 s
[{'max_depth': None, 'max_features': 'auto', 'n_estimators': 18}, RandomForestClassifier(n_estimators=18, n_jobs=-1, random_sta
te=42)]
```



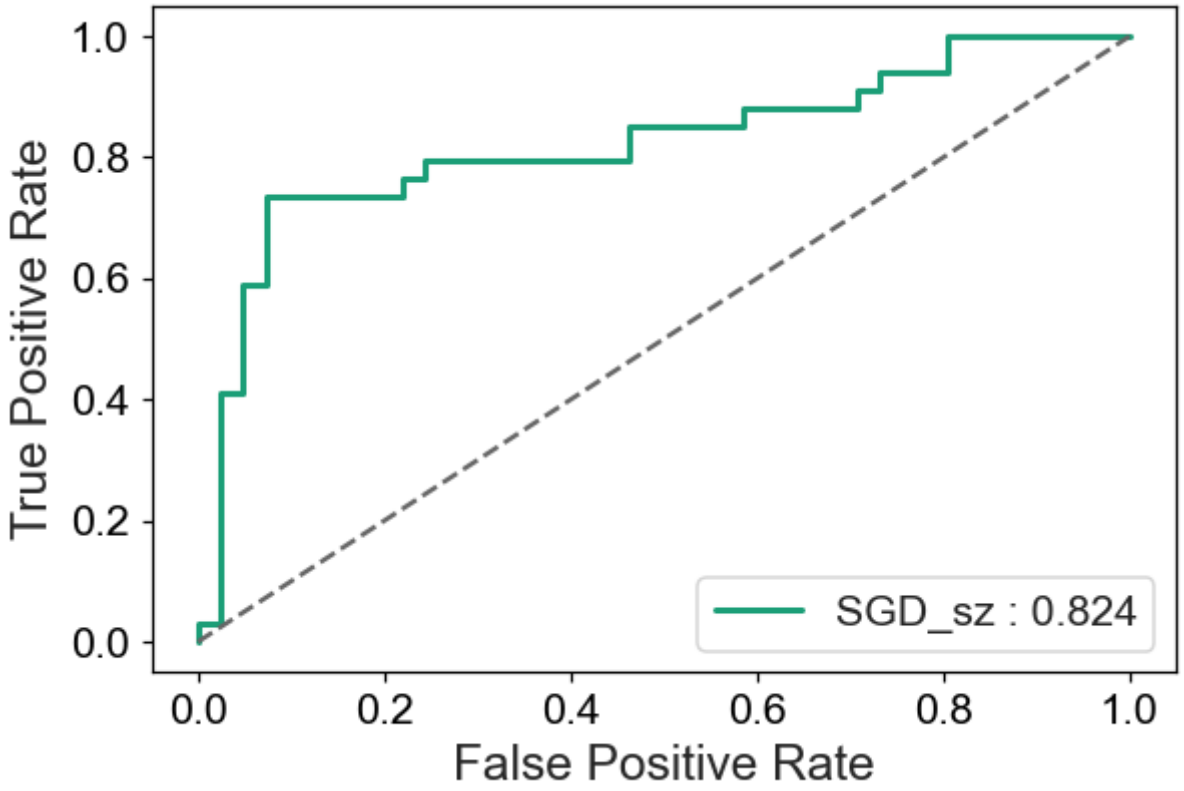
Out[93]:
```
{'conf_mat': array([[36,  5],
       [13, 21]], dtype=int64),
 'accu': 0.76,
 'auc': 0.7679340028694405}
```

SGD

best_SGDClassifier(eta0=0.27999999999999997, learning_rate='constant', n_jobs=-1,
penalty='l1', random_state=42)

In [85]:
```
sgd_clf_sz= SGDClassifier(random_state=42,n_jobs=-1)
param=[{"learning_rate": ['constant','optimal','invscaling'], 'penalty': ['l2','l1','elasticnet'],
        "eta0":np.linspace(0.25,0.35,num=21), "loss":["hinge","modified_huber","log"],
         "class_weight":[None,"balanced"]   }]
sgdbest_sz = GridSearch_result(sgd_clf_sz, X_train_3[["SZa","SZErr"]], y_train_3, param, )
print(sgdbest_sz)
ML_result(sgdbest_sz[1], X_train_3[["SZa","SZErr"]], y_train_3, "SGD_sz", roc="sgd")
```

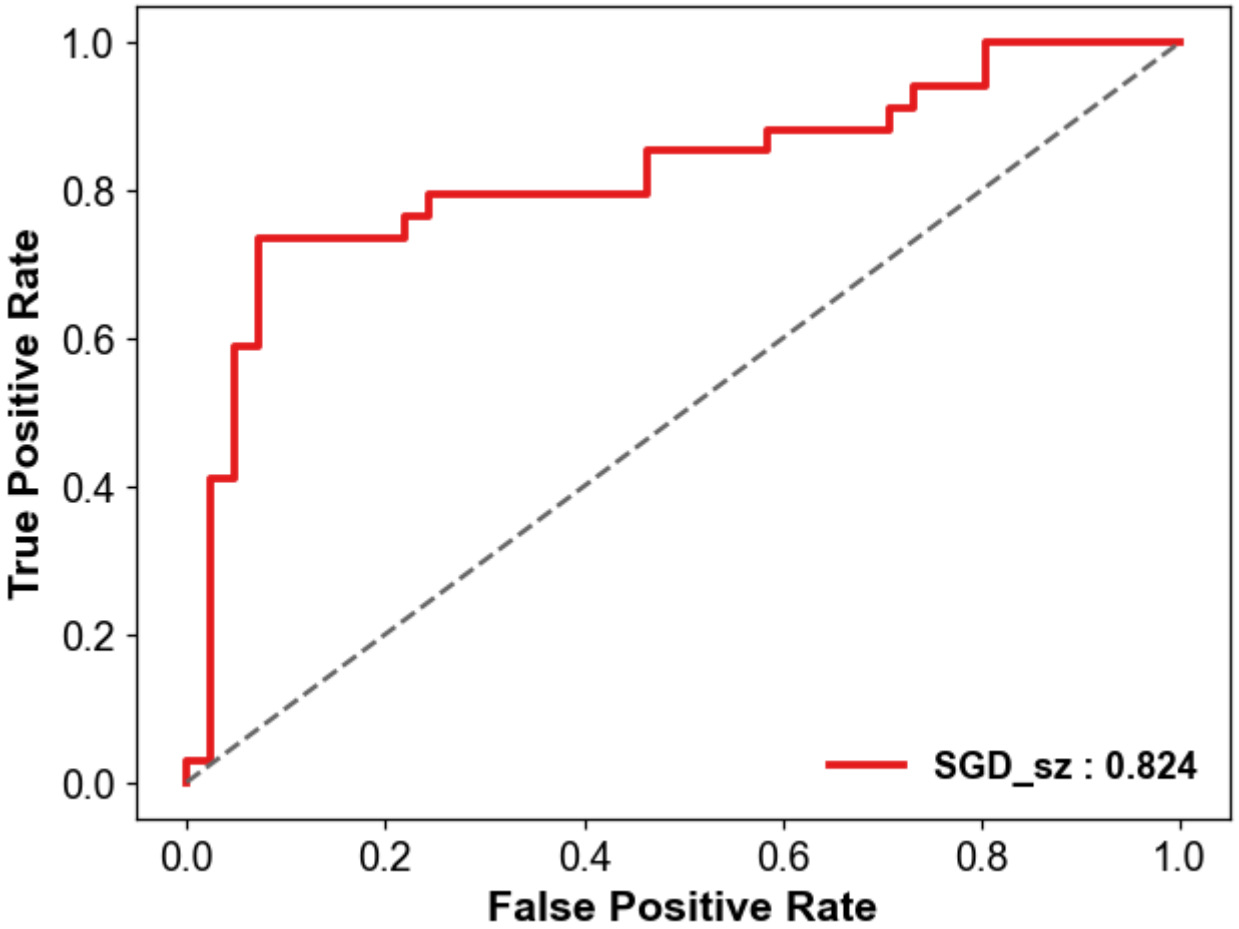
```
Run Time:14.237128734588623 s
[{'class_weight': None, 'eta0': 0.27999999999999997, 'learning_rate': 'constant', 'loss': 'hinge', 'penalty': 'l1'}, SGDClassif
ier(eta0=0.27999999999999997, learning_rate='constant', n_jobs=-1,
              penalty='l1', random_state=42)]
```



Out[85]:
```
{'conf_mat': array([[37,  4],
        [ 9, 25]], dtype=int64),
 'accu': 0.8266666666666667,
 'auc': 0.8235294117647058}
```

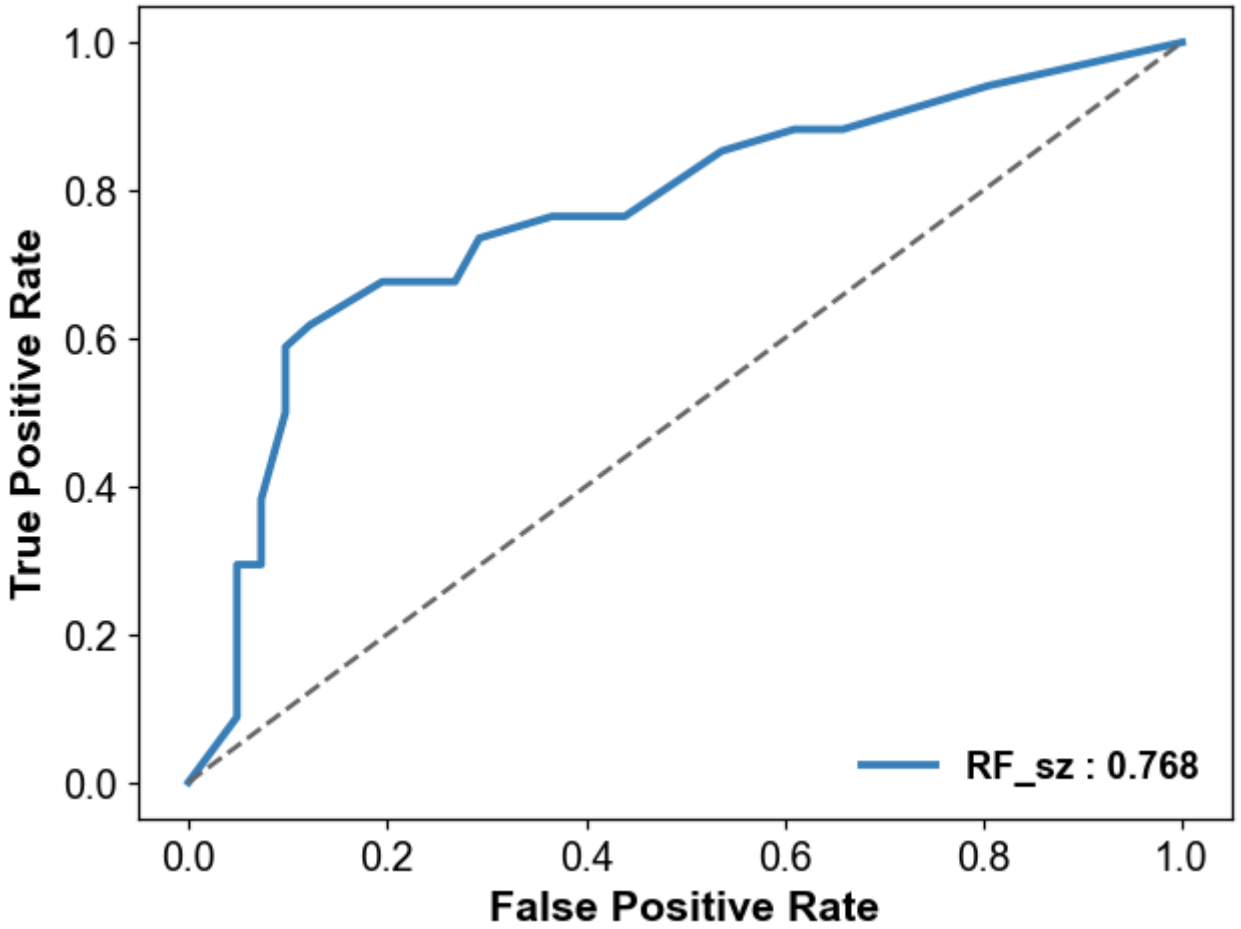
re-paint

In [28]:
```
### SGD re-draw ROC
sgd_clf4 = SGDClassifier(eta0=0.27999999999999997, learning_rate='constant', n_jobs=-1,
              penalty='l1', random_state=42)
ML_result(sgd_clf4, X_train_3[["SZa","SZErr"]], y_train_3, "SGD_sz", roc="sgd",
          save_dir=save_dir, cmap=[sns.color_palette('Set1')[0]],)
```



Out[28]:
```
{'conf_mat': array([[37,  4],
       [ 9, 25]], dtype=int64),
 'accu': 0.8266666666666667,
 'auc': 0.8235294117647058}
```

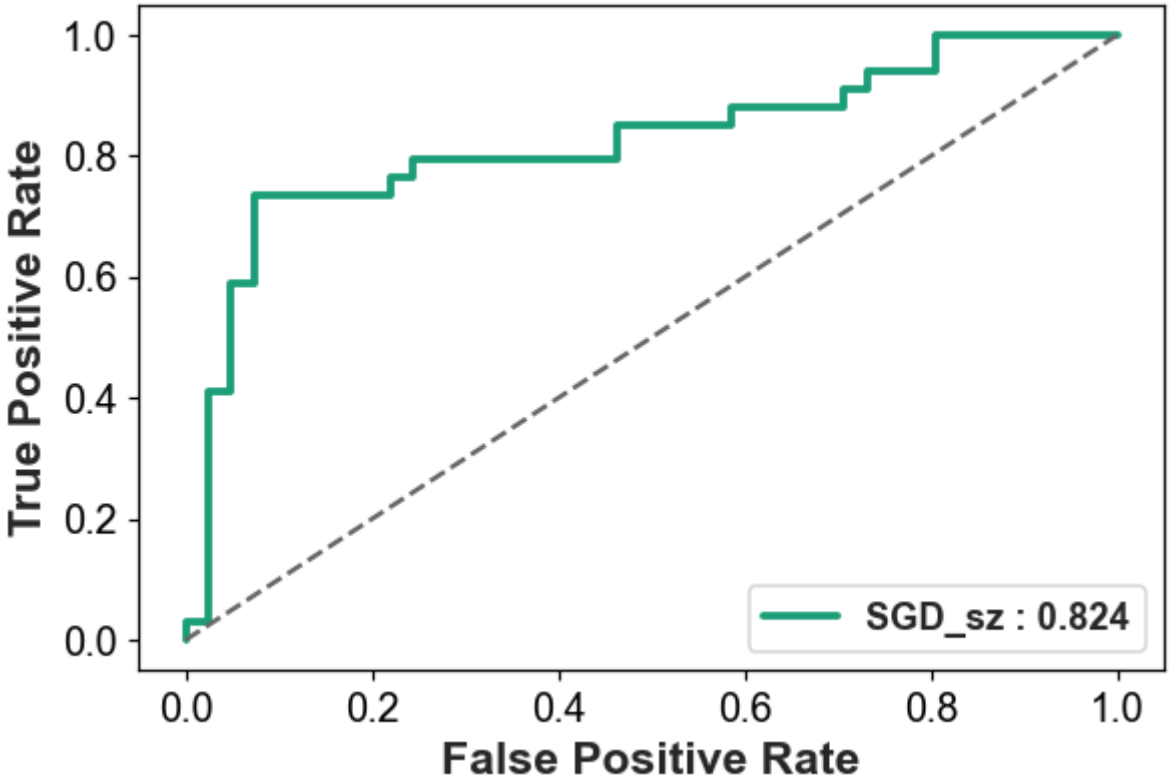
In [29]:
```
### RF re-draw ROC
rfbest = RandomForestClassifier(n_estimators=18, n_jobs=-1, random_state=42)
ML_result(rfbest, X_train_3[["SZa","SZErr"]], y_train_3, "RF_sz", roc="rf",
          save_dir=save_dir, cmap=[sns.color_palette('Set1')[1]],)
```

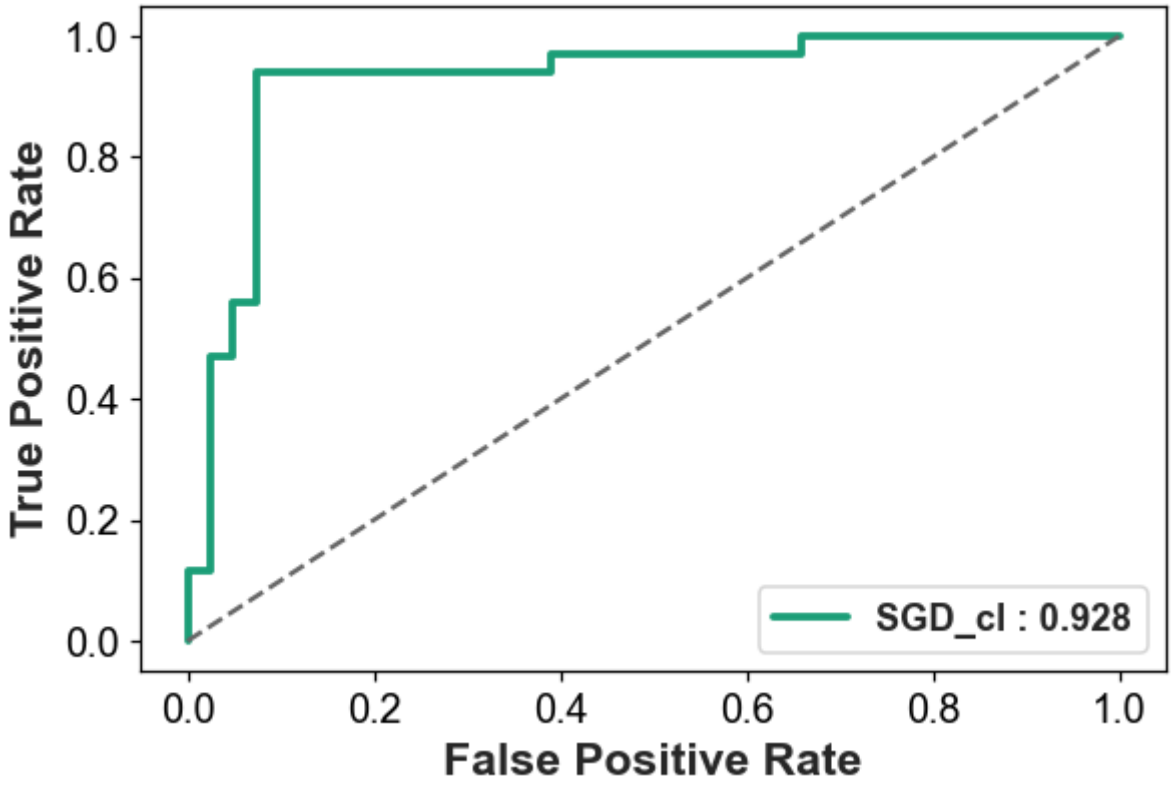


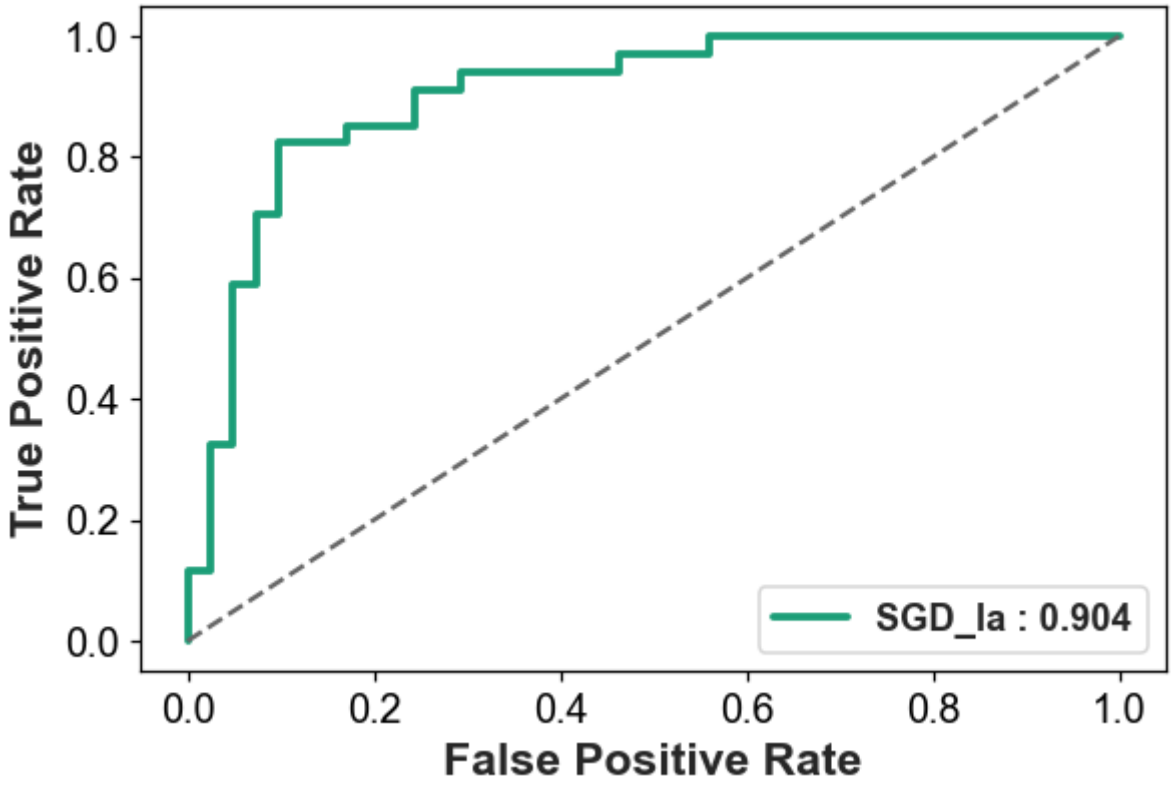
Out[29]:
```
{'conf_mat': array([[36,  5],
        [13, 21]], dtype=int64),
 'accu': 0.76,
 'auc': 0.7679340028694405}
```

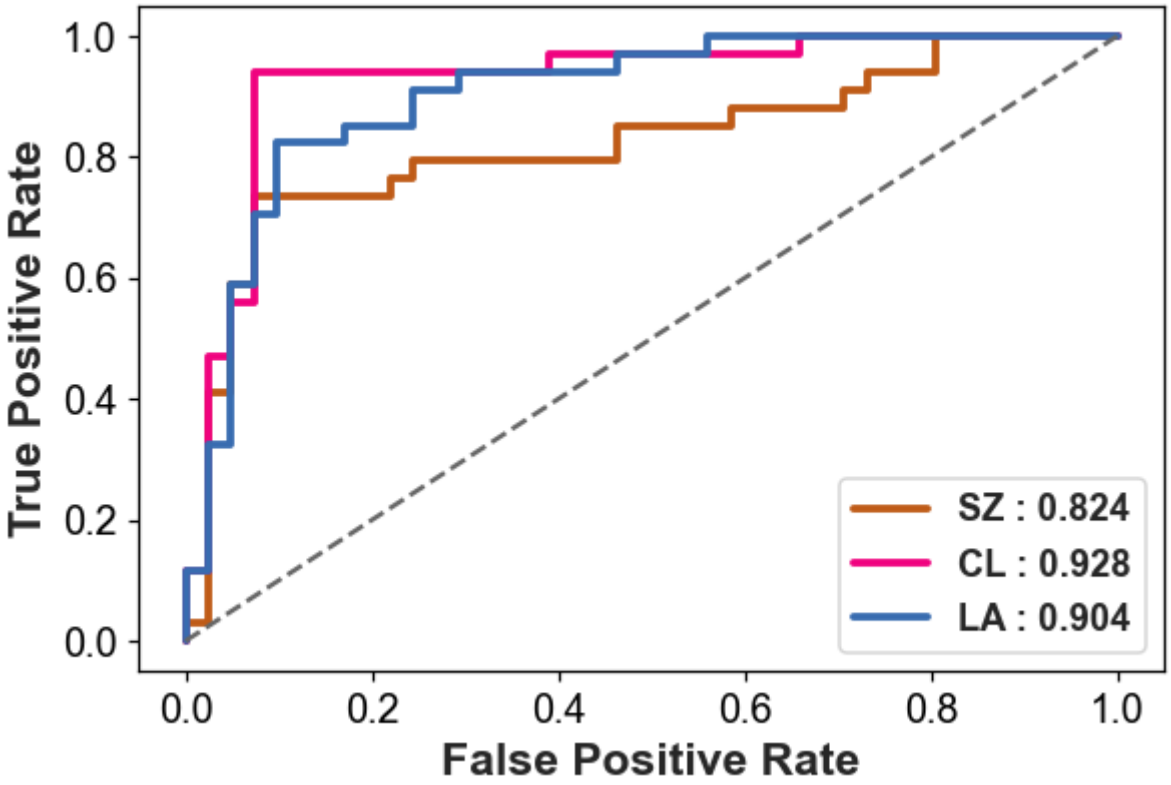
In [307…
```
#re-draw
sz1 = SGDClassifier(eta0=0.28, learning_rate='constant', n_jobs=-1, penalty='l1', random_state=42)
sz2 = ML_result(sz1, X_train[["SZa","SZErr"]], y_train, "SGD_sz",roc="sgd",feedback=1)
cl1 = SGDClassifier(class_weight='balanced', eta0=0.02575, learning_rate='constant', loss='modified_huber', n_jobs=-1, random_
cl2 = ML_result(cl1, X_train[["CLa","CLErr"]], y_train, "SGD_cl",roc="sgd",feedback=1)
la1 = SGDClassifier(eta0=0.07, learning_rate='constant', loss='modified_huber', n_jobs=-1, random_state=42)
la2 = ML_result(la1, X_train[["LAa","LAErr"]], y_train, "SGD_la",roc="sgd",feedback=1)
```

```
plot_roc_curve([sz2["fpr"],cl2["fpr"],la2["fpr"]], [sz2["tpr"],cl2["tpr"],la2["tpr"]],
               label=["SZ","CL","LA"], auc=[sz2["auc"],cl2["auc"],la2["auc"]], cmap=sns.color_palette("Set1"))
```




True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
SGD_cl : 0.928


True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
SGD_la : 0.904



double mode data

LA+SZ

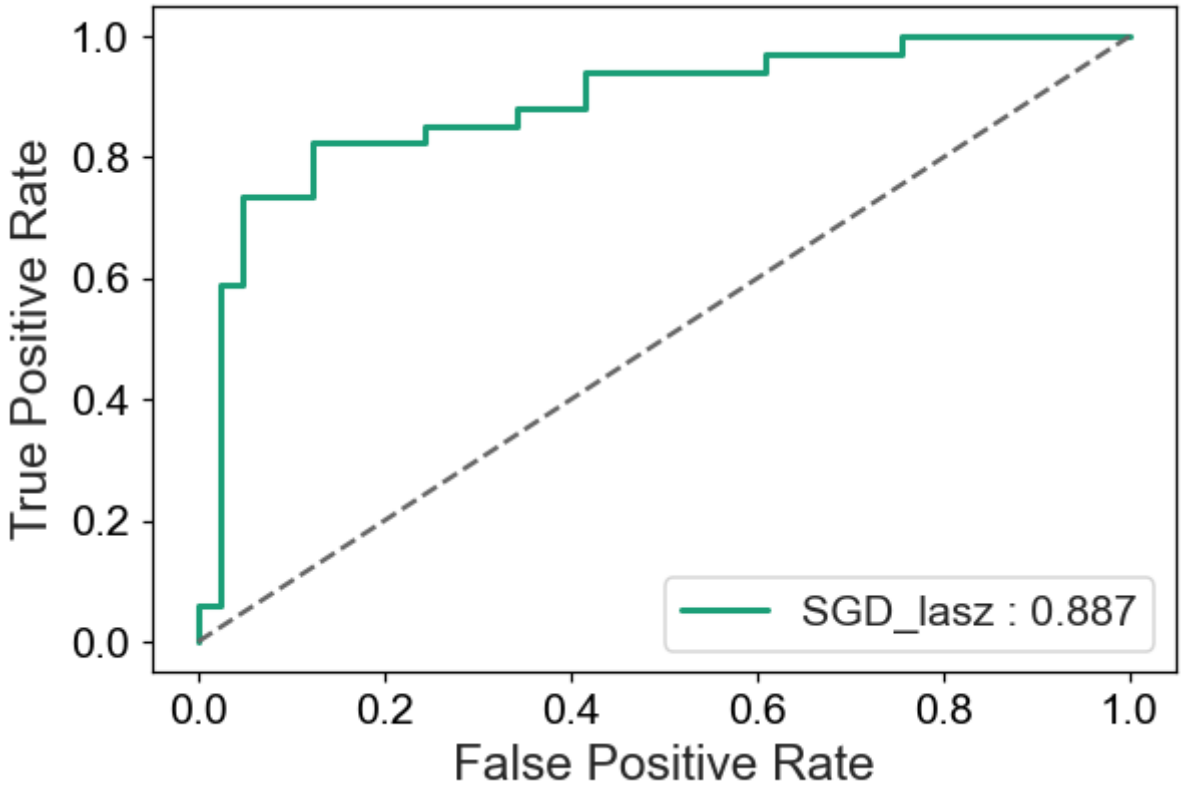
SGD

best_SGDClassifier(eta0=0.15000000000000002, learning_rate='constant', loss='log', n_jobs=-1, random_state=42)

In [86]:
```
index4 = ["LAa","LAErr","SZa","SZErr"]
sgd_clf_lasz = SGDClassifier(random_state=42, n_jobs=-1)

param=[{"learning_rate": ['constant','optimal','invscaling'], 'penalty': ['l2','l1','elasticnet'],
       "eta0":np.linspace(0.1,0.2,num=21), "loss":["hinge","modified_huber","log"],
```

```
        "class_weight":[None,"balanced"]  }]
sgdbest_lasz = GridSearch_result(sgd_clf_lasz, X_train_3[index4], y_train_3, param, )
print(sgdbest_lasz)
ML_result(sgdbest_lasz[1], X_train_3[index4], y_train_3, "SGD_lasz", roc="sgd")
```

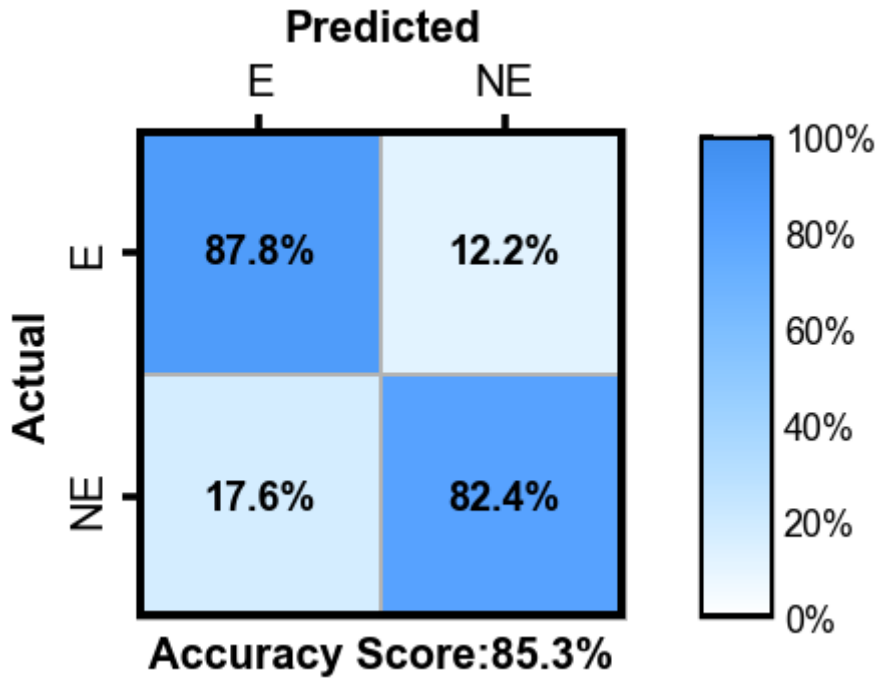
```
Run Time:12.960336446762085 s
[{'class_weight': None, 'eta0': 0.15000000000000002, 'learning_rate': 'constant', 'loss': 'log', 'penalty': 'l2'}, SGDClassifie
r(eta0=0.15000000000000002, learning_rate='constant', loss='log',
              n_jobs=-1, random_state=42)]
```



Out[86]:
```
{'conf_mat': array([[36,  5],
       [ 6, 28]], dtype=int64),
 'accu': 0.8533333333333334,
 'auc': 0.8873744619799139}
```

In [278…
```
conf_mat_heatmap(np.array([[36,  5],  [ 6, 28]]), label="sgd_2a", save=0, )
```

```
D:\Anaconda\lib\site-packages\ipykernel_launcher.py:44: UserWarning: FixedFormatter should only be used together with FixedLoca
tor
```

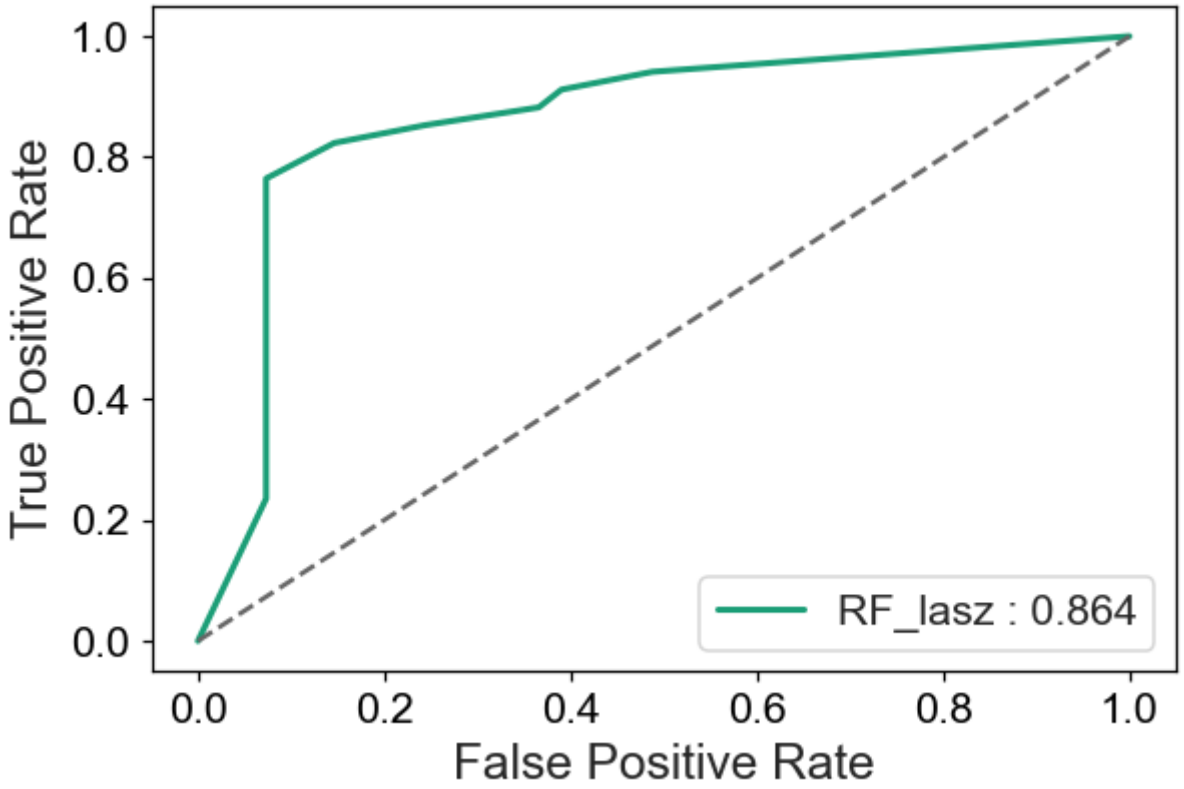


RF

best_RandomForestClassifier(max_features=3, n_estimators=10, n_jobs=-1, random_state=42)]

In [87]:
```
forest_clf_lasz = RandomForestClassifier(random_state=42, n_jobs=-1)
param2 = [{'n_estimators': range(2,20), "max_depth":[None], "max_features":["auto",4,3,2],
          }]
rfbest_lasz = GridSearch_result(forest_clf_lasz, X_train_3[index4], y_train_3, param2,)
print(rfbest_lasz)
ML_result(rfbest_lasz[1], X_train_3[index4], y_train_3,"RF_lasz", roc="rf")
```

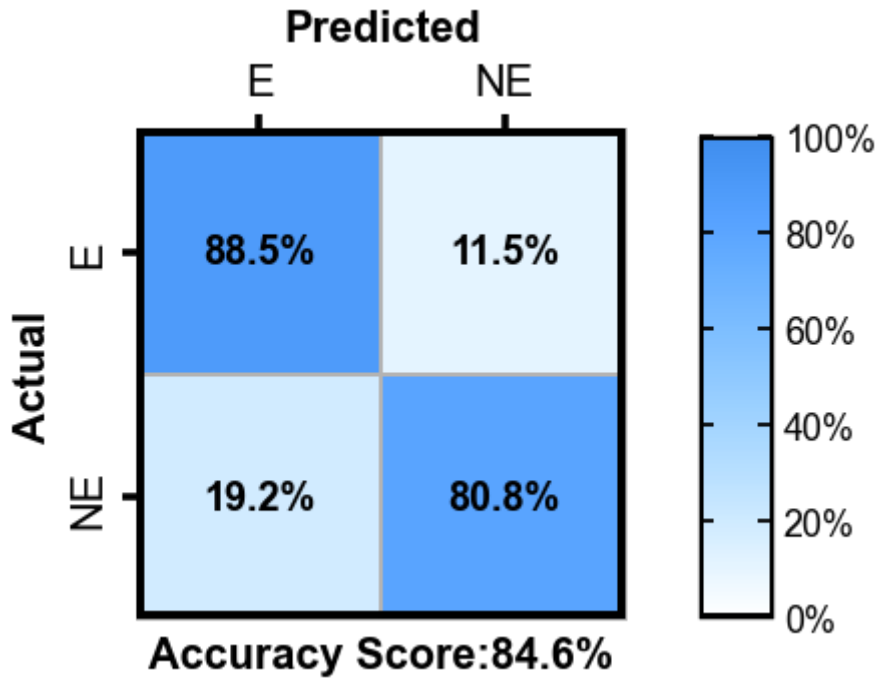
```
Run Time:35.15780067443848 s
[{'max_depth': None, 'max_features': 3, 'n_estimators': 10}, RandomForestClassifier(max_features=3, n_estimators=10, n_jobs=-1,
                       random_state=42)]
```



Out[87]:
```
{'conf_mat': array([[38,  3],
       [ 8, 26]], dtype=int64),
 'accu': 0.8533333333333334,
 'auc': 0.8637015781922526}
```

In [26]:
```
conf_mat_heatmap(np.array([[23,  3], [ 5, 21]]), label="rf_2a", save=0, )
```

```
D:\Anaconda\lib\site-packages\ipykernel_launcher.py:43: UserWarning: FixedFormatter should only be used together with FixedLocator
```

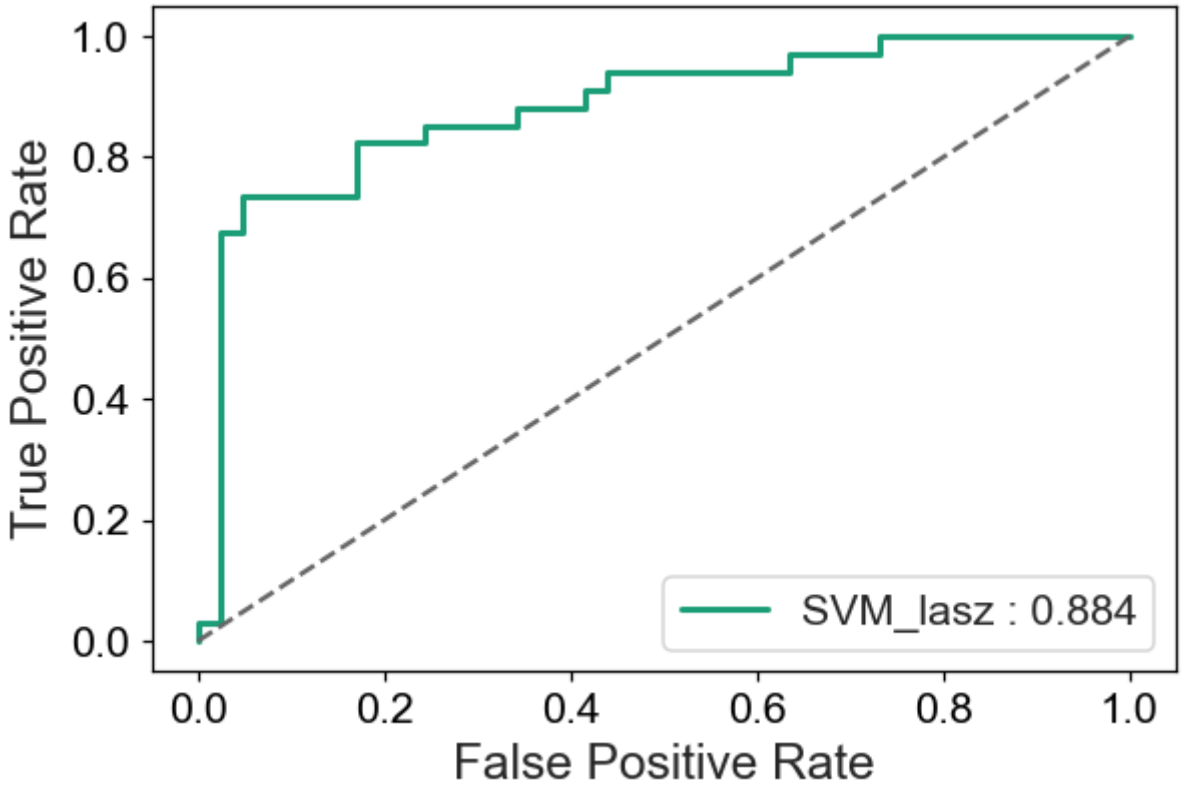


SVM

best_SVC(C=0.8, coef0=0.7, gamma=0.1111111111111111, kernel='poly', probability=True, random_state=42)

In [78]:
```
svc_lasz = SVC(probability=True,random_state=42)
param3 = [{'C':[0.8,0.9,1, 0.7], "class_weight":[None,"balanced"],
           "kernel":['linear',"poly","rbf",],"degree":[1,2,3],"coef0":[0.1,0.4,0.7,1.0]
           "gamma":["auto",1/10,1/9,1/11], }]
svcbest_lasz = GridSearch_result(svc_lasz, X_train_3[index4], y_train_3, param3,)
print(svcbest_lasz)
ML_result(svcbest_lasz[1], X_train_3[index4], y_train_3, "SVM_lasz", roc="rf")
```

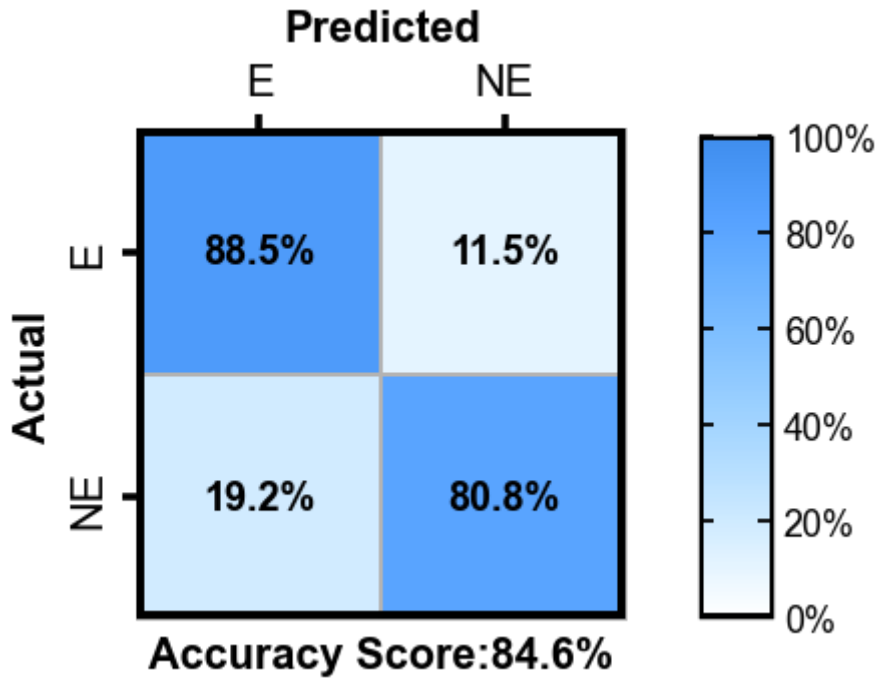
```
Run Time:36.057945251464844 s
[{'C': 0.8, 'class_weight': None, 'coef0': 0.7, 'degree': 3, 'gamma': 0.1111111111111111, 'kernel': 'poly'}, SVC(C=0.8, coef0=
0.7, gamma=0.1111111111111111, kernel='poly', probability=True,
    random_state=42)]
```



Out[78]:
```
{'conf_mat': array([[39,  2],
       [ 9, 25]], dtype=int64),
 'accu': 0.8533333333333334,
 'auc': 0.8837876614060258}
```

In [20]:
```
conf_mat_heatmap(np.array([[23,  3],[ 5, 21]]), label="svm_2a", save=0, )
```

```
D:\Anaconda\lib\site-packages\ipykernel_launcher.py:43: UserWarning: FixedFormatter should only be used together with FixedLocator
```



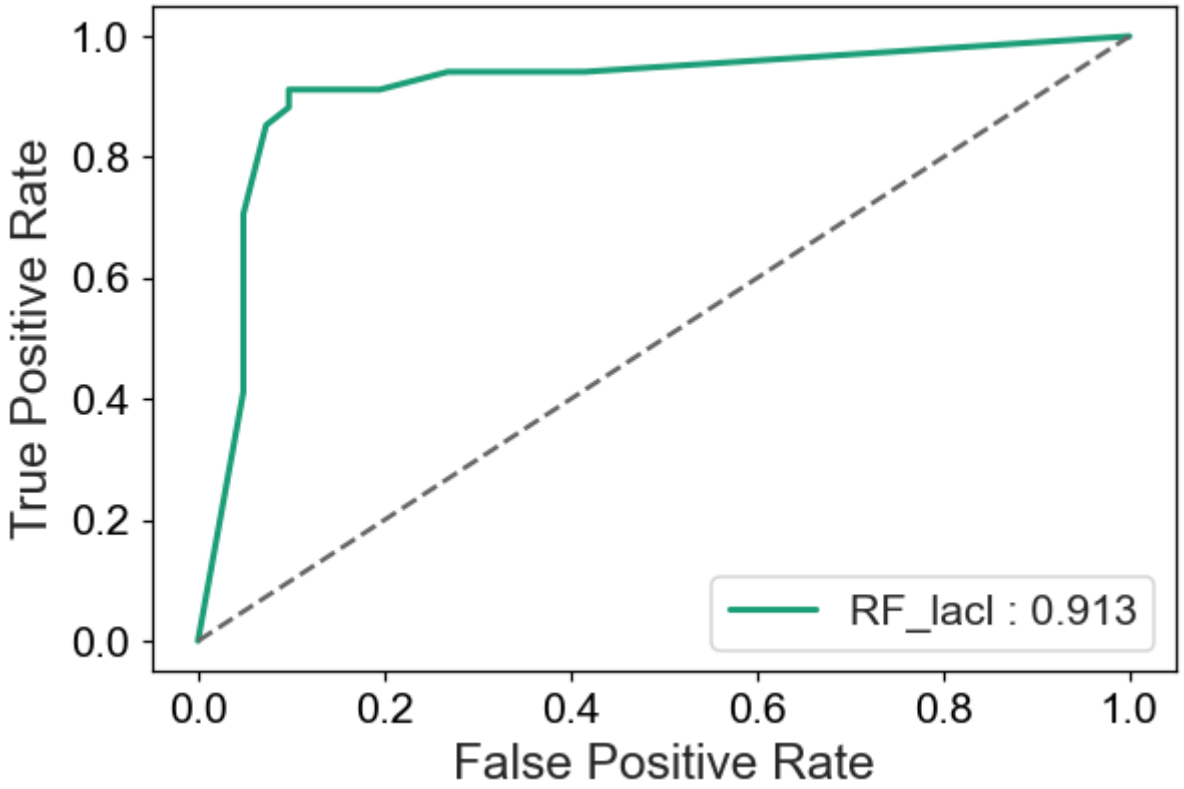
LA+CL

RF

best_RandomForestClassifier(n_estimators=10, n_jobs=-1, random_state=42)]

In [79]:
```
index6=["LAa","LAErr","CLa","CLErr"]
forest_clf_lacl = RandomForestClassifier(n_jobs=-1,random_state=42)
param2 = [{'n_estimators': range(2,20), "max_depth":[None],
           "max_features":["auto",3,4,2], }]
rfbest_lacl = GridSearch_result(forest_clf_lacl, X_train_3[index6], y_train_3, param2,)
print(rfbest_lacl)
ML_result(rfbest_lacl[1], X_train_3[index6], y_train_3,"RF_lacl", roc="rf")
```

```
Run Time:43.674476861953735 s
[{'max_depth': None, 'max_features': 'auto', 'n_estimators': 10}, RandomForestClassifier(n_estimators=10, n_jobs=-1, random_sta
te=42)]
```



Out[79]:
```
{'conf_mat': array([[37,  4],
        [ 3, 31]], dtype=int64),
 'accu': 0.9066666666666666,
 'auc': 0.9128407460545194}
```

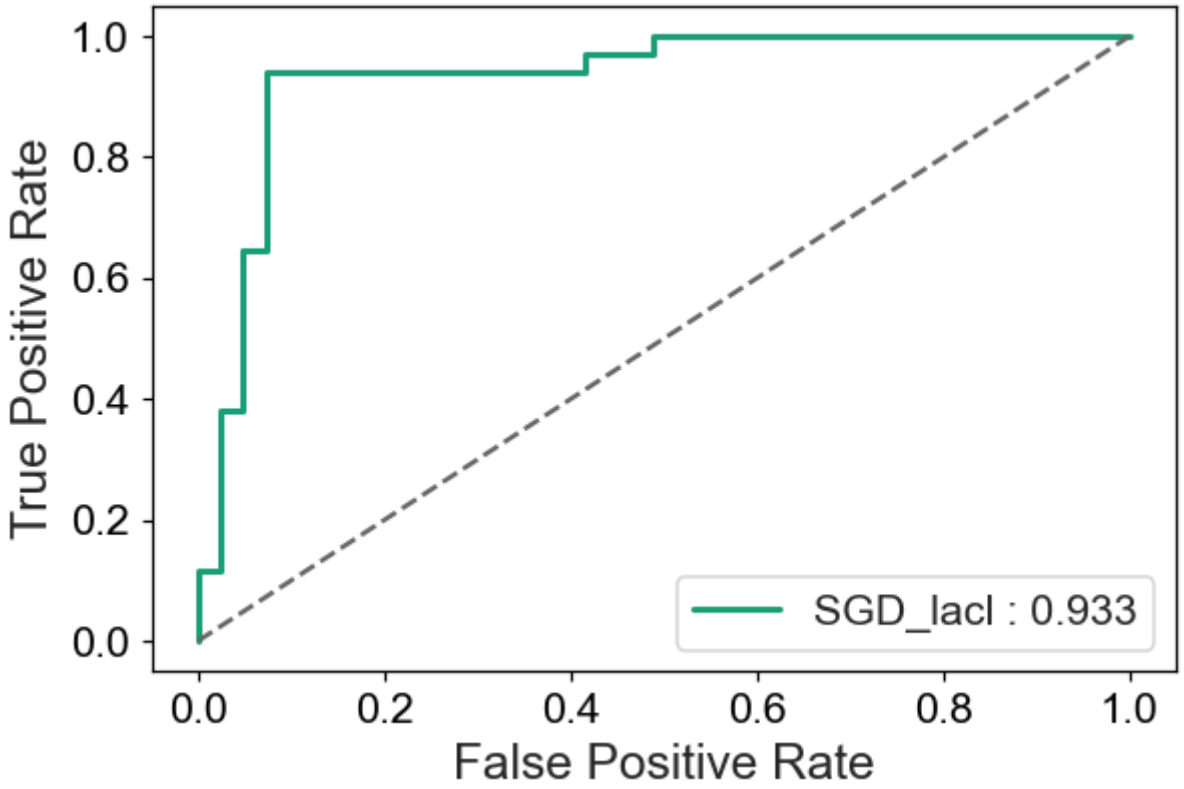
SDG

best_SGDClassifier(eta0=0.9, learning_rate='constant', n_jobs=-1, random_state=42)

In [88]:
```
sgd_clf_lacl = SGDClassifier(random_state=42, n_jobs=-1)
param=[{"learning_rate": ['constant','optimal','invscaling'], 'penalty': ['l2','l1','elasticnet'],
        "eta0":np.linspace(0.8,1.2,num=21), "loss":["hinge","modified_huber","log"],
         "class_weight":[None,"balanced"], }]
sgdbest_lacl = GridSearch_result(sgd_clf_lacl, X_train_3[index6], y_train_#, param, )
```

```
print(sgdbest_lacl)
ML_result(sgdbest_lacl[1], X_train_3[index6], y_train_3, "SGD_lacl", roc="sgd")
```

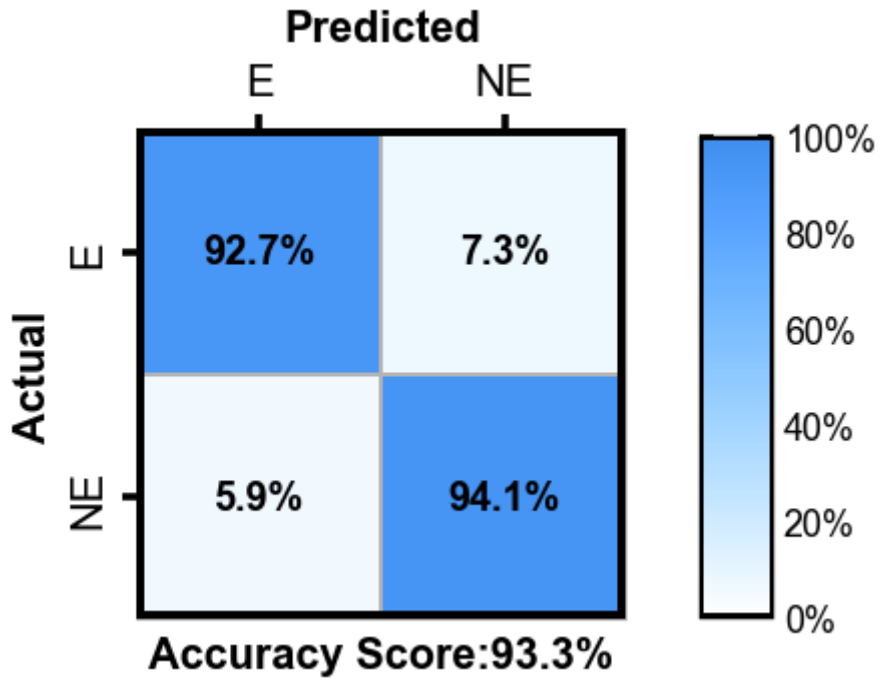
```
Run Time:12.817719221115112 s
[{'class_weight': None, 'eta0': 0.9, 'learning_rate': 'constant', 'loss': 'hinge', 'penalty': 'l2'}, SGDClassifier(eta0=0.9, le
arning_rate='constant', n_jobs=-1, random_state=42)]
```



Out[88]:
```
{'conf_mat': array([[38,  3],
       [ 2, 32]], dtype=int64),
 'accu': 0.9333333333333333,
 'auc': 0.9325681492109039}
```

In [279…
```
conf_mat_heatmap(np.array([[38,  3], [ 2, 32]]), label="sgd_2b", save=0, )
```

```
D:\Anaconda\lib\site-packages\ipykernel_launcher.py:44: UserWarning: FixedFormatter should only be used together with FixedLoca
tor
```



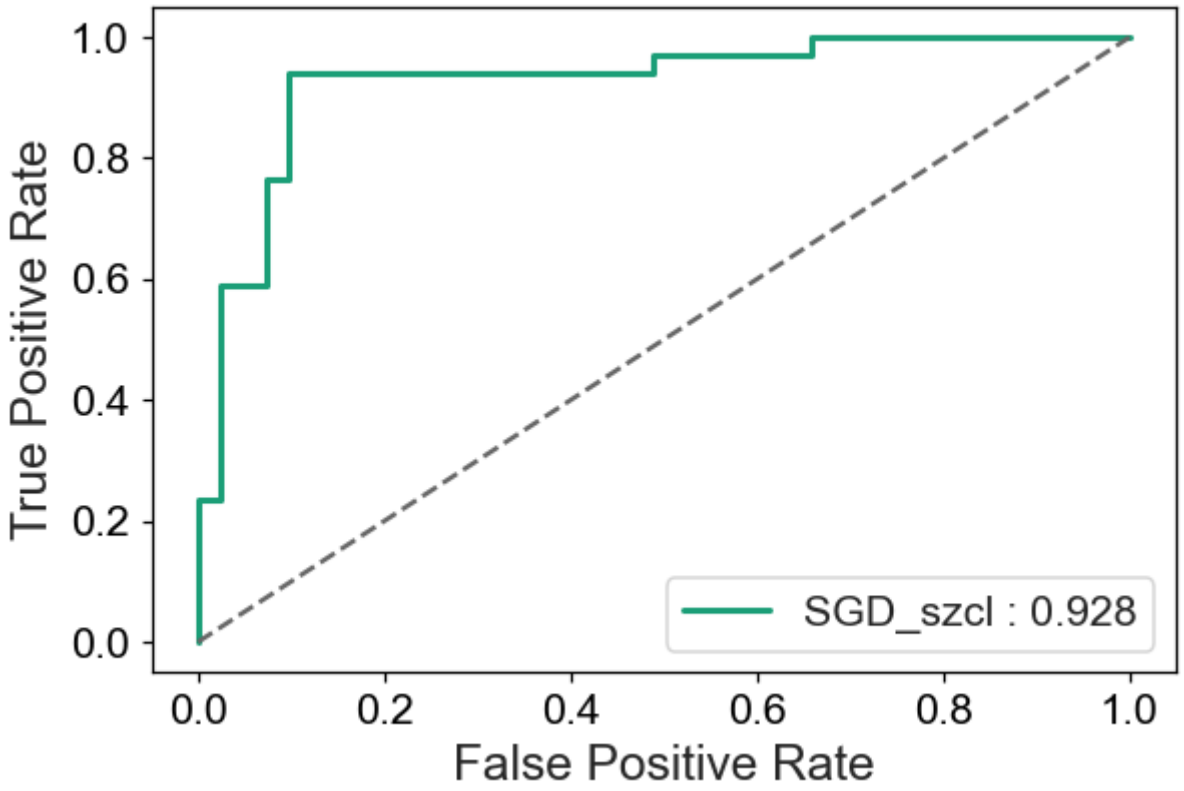
SZ+CL

SGD

SGDClassifier(class_weight='balanced', eta0=0.11, learning_rate='constant', n_jobs=-1, random_state=42)

In [89]:
```
index5 = ["CLa","CLErr","SZa","SZErr"]
sgd_clf_szcl = SGDClassifier(random_state=42,n_jobs=-1)

param=[{"learning_rate": ['constant','optimal','invscaling'], 'penalty': ['l2','l1','elasticnet'],
        "eta0":np.linspace(0.1,0.3,num=21), "loss":["hinge","modified_huber","log"],
         "class_weight":[None,"balanced"],
       }]
sgdbest_szcl = GridSearch_result(sgd_clf_szcl, X_train[index5], y_train, param, )
print(sgdbest_szcl)
ML_result(sgdbest_szcl[1], X_train_3[index5], y_train_3, "SGD_szcl", roc="sgd")
```

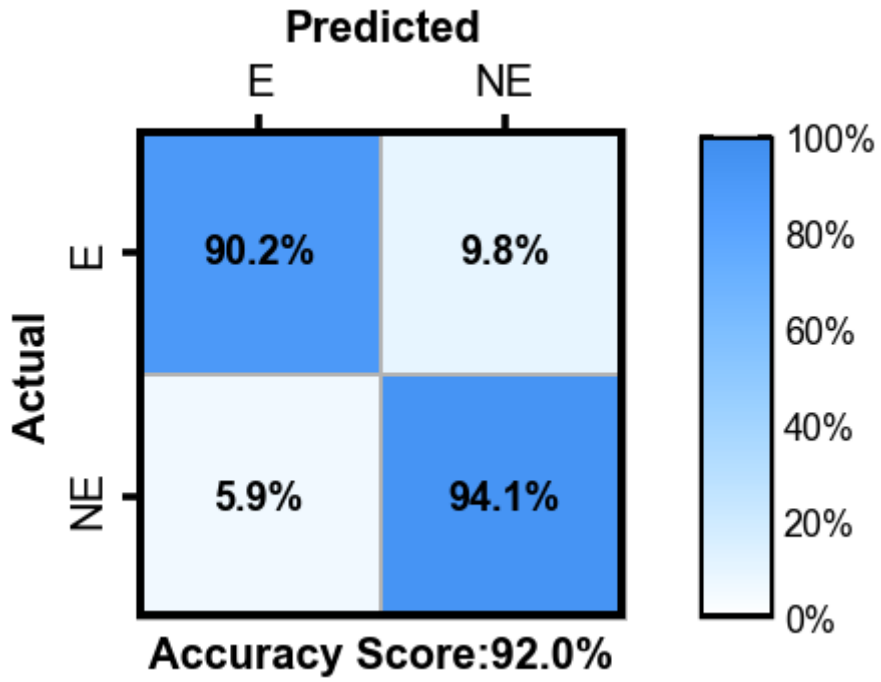
```
Run Time:13.62061357498169 s
[{'class_weight': 'balanced', 'eta0': 0.11, 'learning_rate': 'constant', 'loss': 'hinge', 'penalty': 'l2'}, SGDClassifier(class
_weight='balanced', eta0=0.11, learning_rate='constant',
              n_jobs=-1, random_state=42)]
```



Out[89]:
```
{'conf_mat': array([[37,  4],
       [ 2, 32]], dtype=int64),
 'accu': 0.92,
 'auc': 0.9275466284074606}
```

In [280…
```
conf_mat_heatmap(np.array([[37,  4], [ 2, 32]]), label="sgd_2b", save=0, )
```

```
D:\Anaconda\lib\site-packages\ipykernel_launcher.py:44: UserWarning: FixedFormatter should only be used together with FixedLoca
tor
```

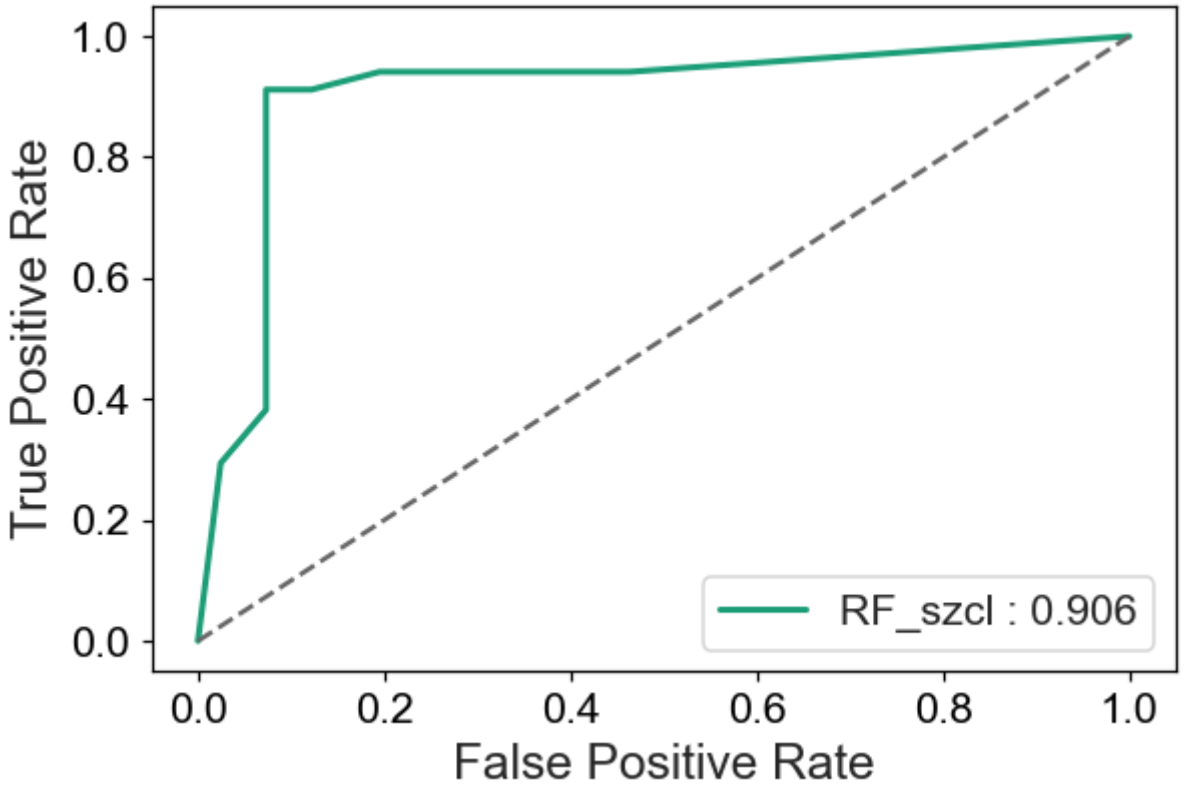


RF

RandomForestClassifier(n_estimators=15, n_jobs=-1, random_state=42)]

In [82]:
```
forest_clf_szcl = RandomForestClassifier(n_jobs=-1,random_state=42)
param2 = [{'n_estimators': range(2,20), "max_depth":[None], "max_features":["auto",3,4,2],  }]
rfbest_szcl = GridSearch_result(forest_clf_szcl, X_train[index5], y_train, param2,)
print(rfbest_szcl)
ML_result(rfbest_szcl[1], X_train_3[index5], y_train_3, "RF_szcl", roc="rf")
```

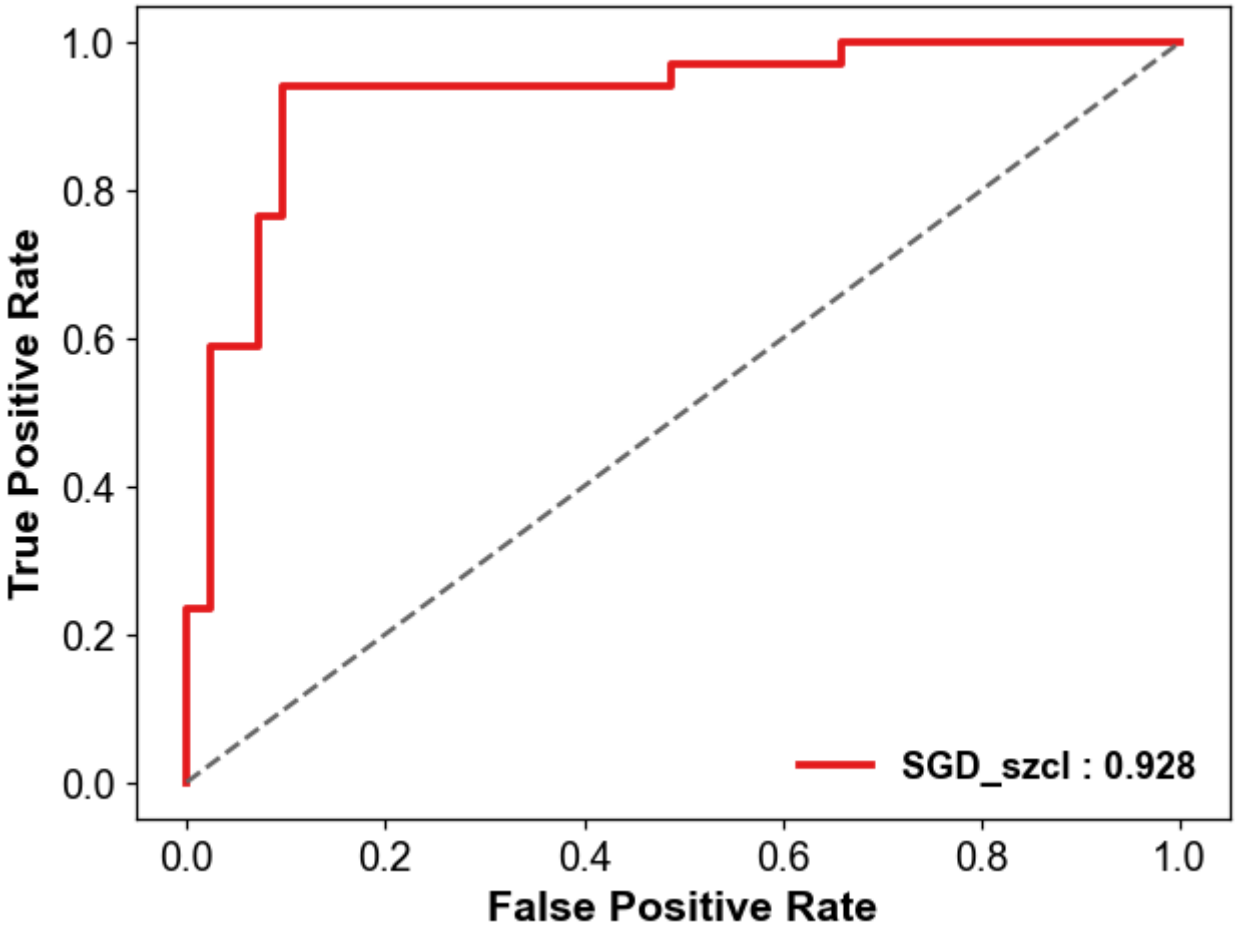
```
Run Time:42.83885598182678 s
[{'max_depth': None, 'max_features': 'auto', 'n_estimators': 15}, RandomForestClassifier(n_estimators=15, n_jobs=-1, random_sta
te=42)]
```



Out[82]:
```
{'conf_mat': array([[38,  3],
       [ 3, 31]], dtype=int64),
 'accu': 0.92,
 'auc': 0.9056671449067433}
```

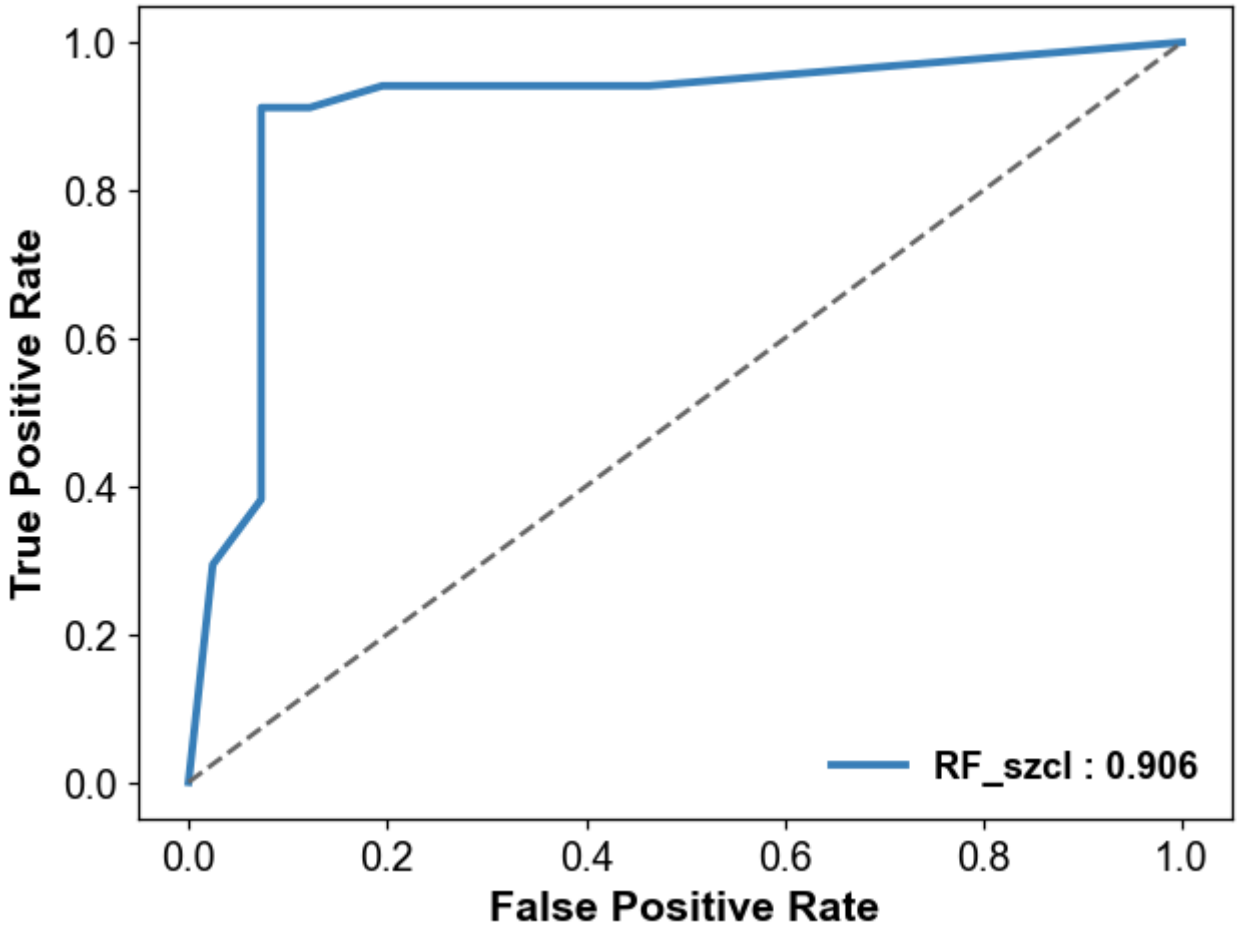
re_draw

In [38]:
```
# SGD re_draw
sgd_clf3 = SGDClassifier(class_weight='balanced', eta0=0.11, learning_rate='constant',
             n_jobs=-1, random_state=42)
index5 = ["CLa","CLErr","SZa","SZErr"]
ML_result(sgd_clf3, X_train_3[index5], y_train_3, "SGD_szcl", roc="sgd",
          save_dir=save_dir, cmap=[sns.color_palette('Set1')[0]],)
```



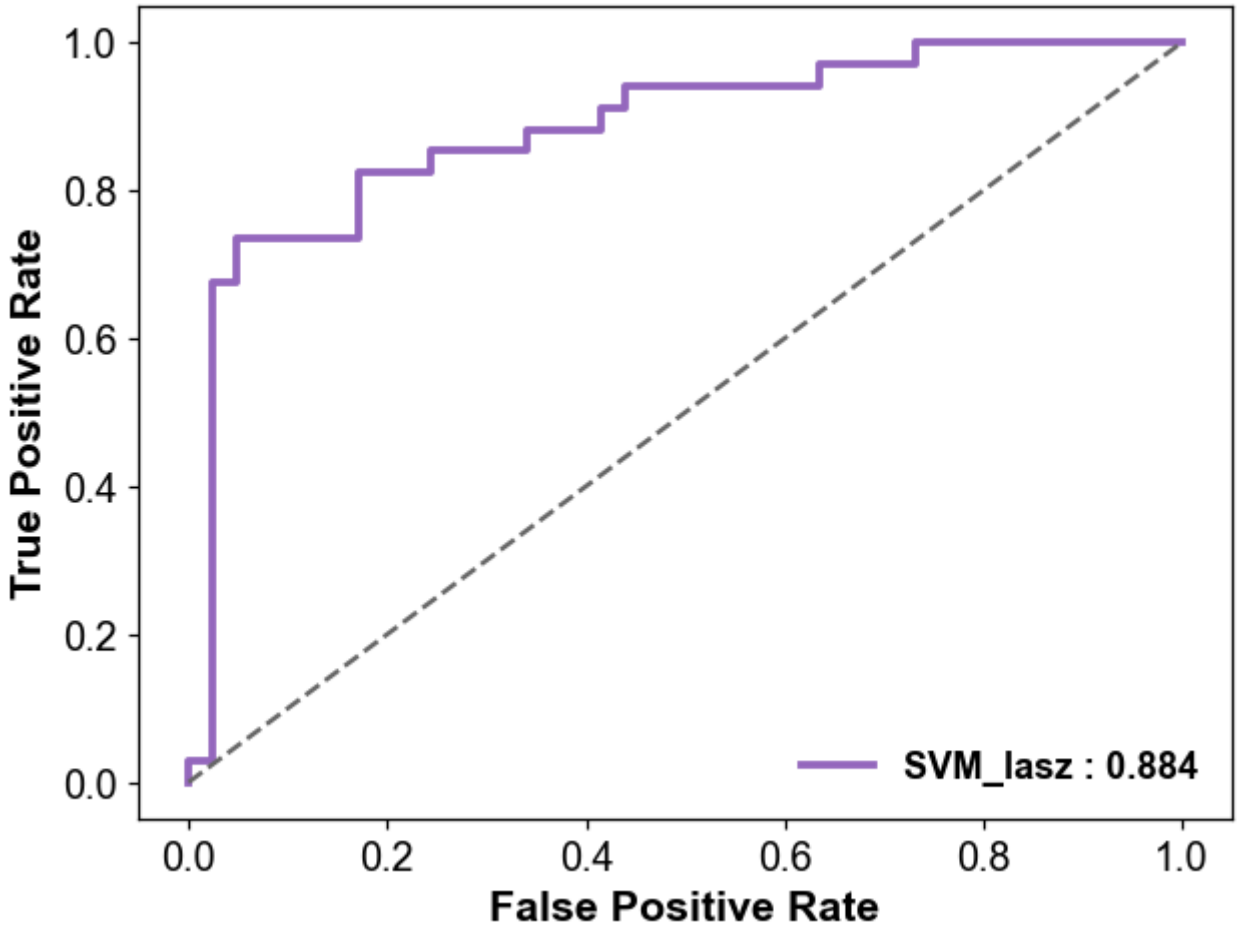
Out[38]:
```
{'conf_mat': array([[37,  4],
       [ 2, 32]], dtype=int64),
 'accu': 0.92,
 'auc': 0.9275466284074606}
```

In [39]:
```
### RF re_draw
rfbest_lasz = RandomForestClassifier(n_estimators=15, n_jobs=-1, random_state=42)
ML_result(rfbest_lasz, X_train_3[index5], y_train_3, "RF_szcl", roc="rf",
          save_dir=save_dir, cmap=[sns.color_palette('Set1')[1]],)
```



Out[39]:
```
{'conf_mat': array([[38,  3],
       [ 3, 31]], dtype=int64),
 'accu': 0.92,
 'auc': 0.9056671449067433}
```

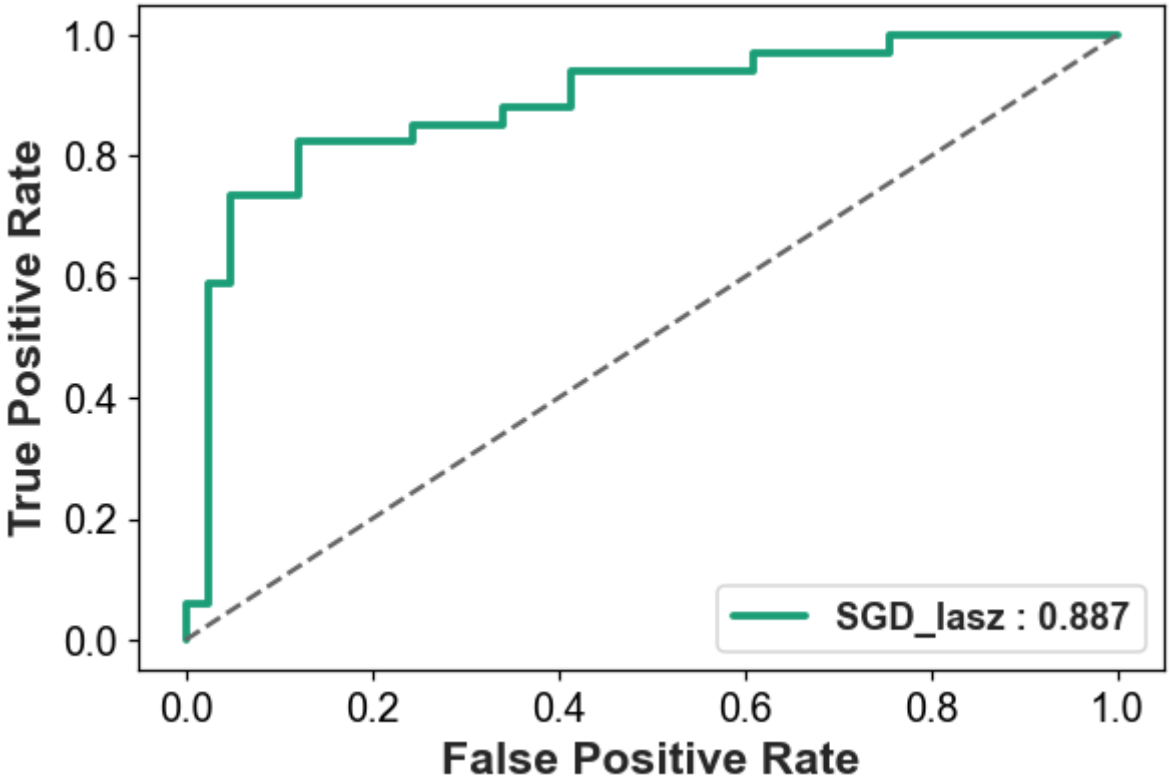
In [34]:
```
### SVM re_draw
svcbest_lasz = SVC(C=0.8, coef0=0.7, gamma=0.1111111111111111, kernel='poly',
                   probability=True, random_state=42)
ML_result(svcbest_lasz, X_train_3[index4], y_train_3, "SVM_lasz", roc="rf",
          save_dir=save_dir, cmap=[plt.get_cmap('tab10')(4)],)
```

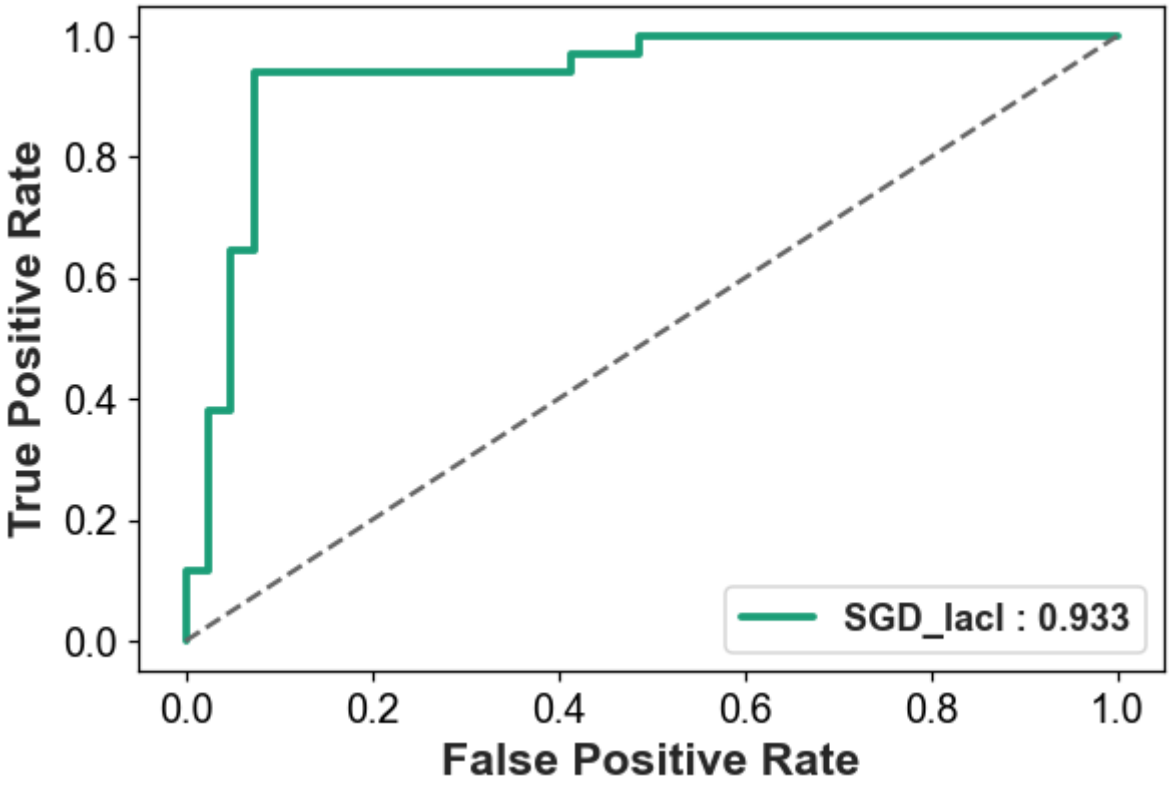


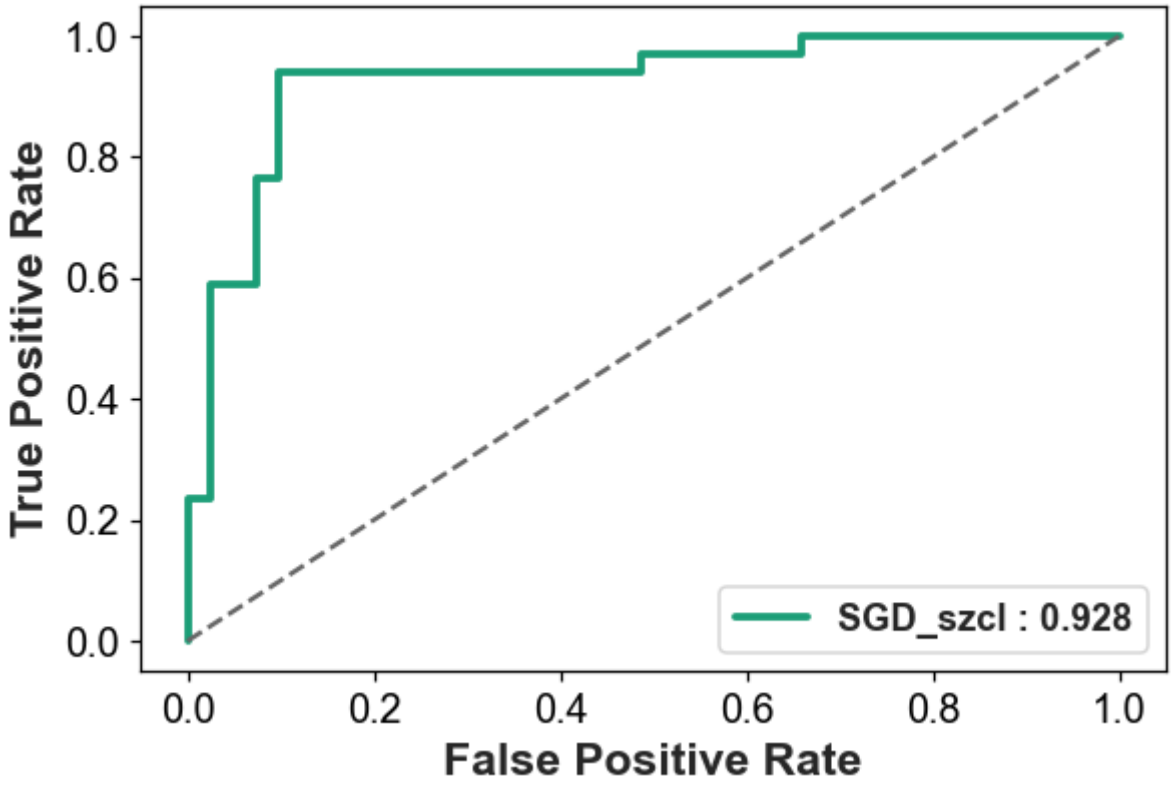
Out[34]:
```
{'conf_mat': array([[39,  2],
        [ 9, 25]], dtype=int64),
 'accu': 0.8533333333333334,
 'auc': 0.8837876614060258}
```

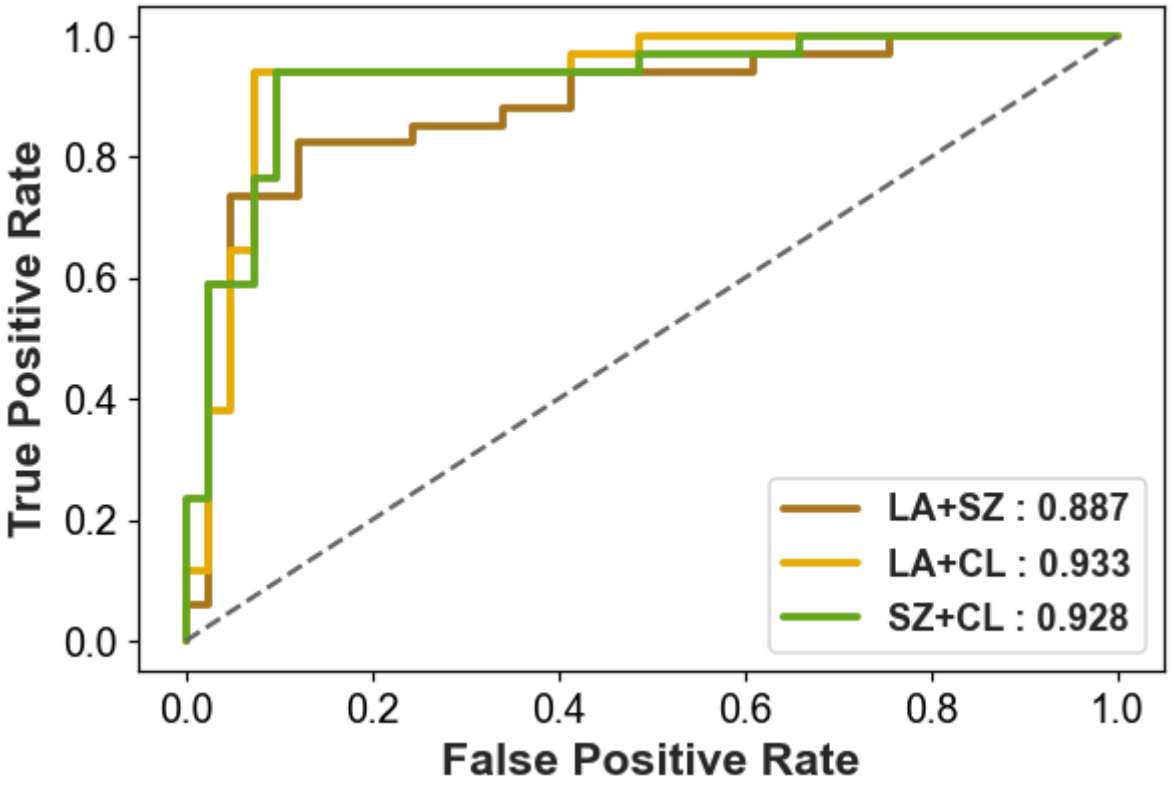
In [308…
```
lasz1 = SGDClassifier(eta0=0.15, learning_rate='constant', loss='log', n_jobs=-1, random_state=42)
lasz2 = ML_result(lasz1, X_train[["LAa","LAErr","SZa","SZErr"]], y_train, "SGD_lasz",roc="sgd",feedback=1)
lacl1 = SGDClassifier(eta0=0.9, learning_rate='constant', n_jobs=-1, random_state=42)
lacl2 = ML_result(lacl1, X_train[["LAa","LAErr","CLa","CLErr"]], y_train, "SGD_lacl",roc="sgd",feedback=1)
szcl1 = SGDClassifier(class_weight='balanced', eta0=0.11, learning_rate='constant', n_jobs=-1, random_state=42)
szcl2 = ML_result(szcl1, X_train[["SZa","SZErr","CLa","CLErr"]], y_train, "SGD_szcl",roc="sgd",feedback=1)
plot_roc_curve([lasz2["fpr"],lacl2["fpr"],szcl2["fpr"]], [lasz2["tpr"],lacl2["tpr"],szcl2["tpr"]],
```

```
                label=["LA+SZ","LA+CL","SZ+CL"], auc=[lasz2["auc"],lacl2["auc"],szcl2["auc"]],
                cmap=sns.color_palette("Dark2_r"))
```




True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
SGD_lacl : 0.933


True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
SGD_szcl : 0.928



on Test Set

In [71]:
```
sgdbest=SGDClassifier(alpha=0.055564444444444444, eta0=0.26126315789473686,
            learning_rate='invscaling', loss='log', n_jobs=-1, penalty='l1',
            power_t=0.07357142857142857, random_state=42)
sgdbest.fit(X_train_3, y_train_3)
```

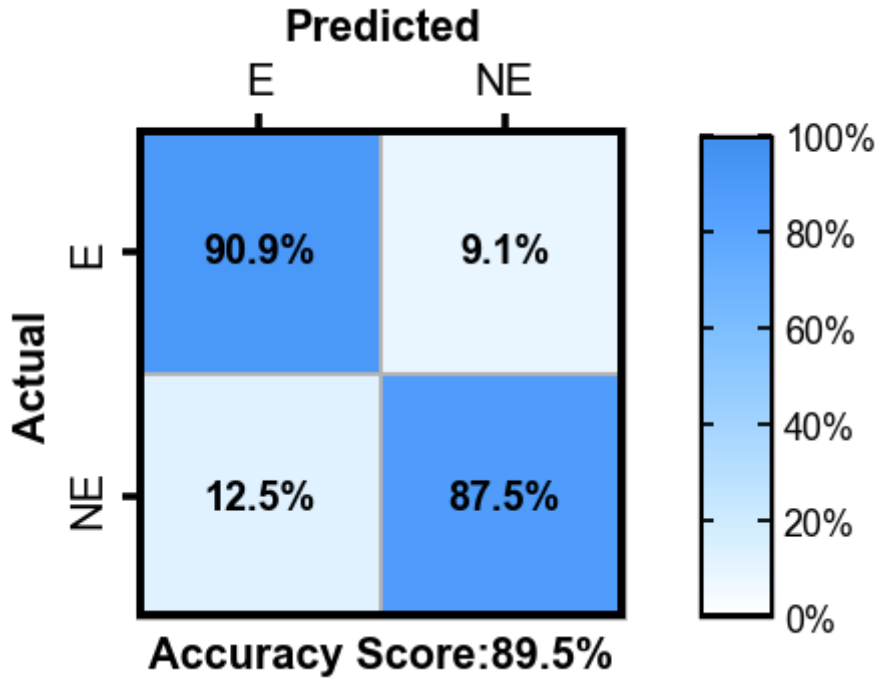
Out[71]:
```
SGDClassifier(alpha=0.055564444444444444, eta0=0.26126315789473686,
              learning_rate='invscaling', loss='log', n_jobs=-1, penalty='l1',
              power_t=0.07357142857142857, random_state=42)
```

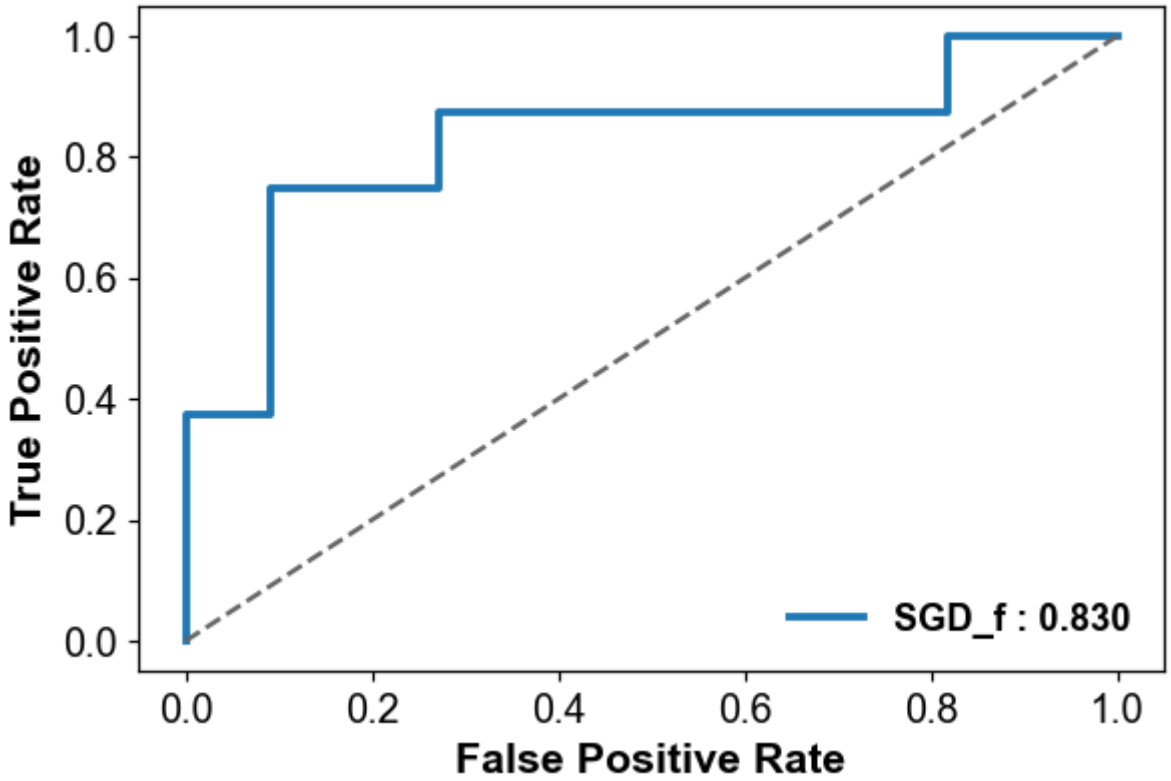
In [74]:
```
final_pred_SGD = sgdbest.predict(X_test)
confmat = confusion_matrix(y_test, final_pred_SGD)
print(confmat)
```

```
conf_mat_heatmap(confmat, rect_set=rect_set, title="test", save_dir=save_dir)

f_test_scores = cross_val_predict(sgdbest[1], X_test, y_test, cv=3, method="decision_function")
fpr1, tpr1, thresholds1 = roc_curve(y_test, f_test_scores)
auc1 = roc_auc_score(y_test, f_test_scores)
plot_roc_curve([fpr1], [tpr1], label=["SGD_f"], auc=[auc1], cmap=None)
```

```
[[10  1]
 [ 1  7]]
```

```
D:\Anaconda\lib\site-packages\ipykernel_launcher.py:44: UserWarning: FixedFormatter should only be used together with FixedLocator
```




True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
SGD_f : 0.830