In [13]:

```
#Importing Data
import warnings
warnings.filterwarnings('ignore')
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
df = pd.read_csv('musk_csv.csv')
```

In [14]:

```
print(df.shape)
df.head(5)
```

```
(6598, 170)
```

Out[14]:

	ID	molecule_name	conformation_name	f1	f2	f3	f4	f5	f6	f7	...	f158
0	1	MUSK-211	211_1+1	46	-108	-60	-69	-117	49	38	...	-308
1	2	MUSK-211	211_1+10	41	-188	-145	22	-117	-6	57	...	-59
2	3	MUSK-211	211_1+11	46	-194	-145	28	-117	73	57	...	-134
3	4	MUSK-211	211_1+12	41	-188	-145	22	-117	-7	57	...	-60
4	5	MUSK-211	211_1+13	41	-188	-145	22	-117	-7	57	...	-60

5 rows × 170 columns

In [15]:

```
print(df.molecule_name.describe())
print(df.conformation_name.describe())
```

```
count             6598
unique             102
top       NON-MUSK-j146
freq              1044
Name: molecule_name, dtype: object
count         6598
unique        6598
top       j146_4+5
freq             1
Name: conformation_name, dtype: object
```

Processing molecule_name

molecule_name has 102 unique values but the name also itself defines whether the chemical is MUSK or NON-MUSK i.e the classification task.

In [16]:

```
#Cleaning molecule_name
from tqdm import tqdm
import re
processed_molecular_name = []
for sentance in tqdm(df['molecule_name'].values):
    sentance = re.sub(r"-", " ", sentance)
    sentance = re.sub("\S*\d\S*", "", sentance).strip()
    sentance = re.sub("[^a-zA-Z]+", "", sentance)
    sentance = ' '.join(e.lower() for e in sentance.split())
    processed_molecular_name.append(sentance.strip())

#adding processed molecule_name to dataframe
df['molecule_name_processed'] = processed_molecular_name

#Label Encoding molecule_name_processed to convert it into numerical form
from sklearn.preprocessing import LabelEncoder
LE = LabelEncoder()
df['molecule_name_processed'] = LE.fit_transform(df['molecule_name_processed'])
```

```
100%|██████████| 6598/6598 [00:00<00:00, 76756.28
it/s]
```

In [17]:

```
df.head(5)
```

Out[17]:

	ID	molecule_name	conformation_name	f1	f2	f3	f4	f5	f6	f7	...	f159	f
0	1	MUSK-211	211_1+1	46	-108	-60	-69	-117	49	38	...	52	-
1	2	MUSK-211	211_1+10	41	-188	-145	22	-117	-6	57	...	-2	5
2	3	MUSK-211	211_1+11	46	-194	-145	28	-117	73	57	...	-154	5
3	4	MUSK-211	211_1+12	41	-188	-145	22	-117	-7	57	...	-4	5
4	5	MUSK-211	211_1+13	41	-188	-145	22	-117	-7	57	...	-4	5

5 rows × 171 columns

Sliptting Data into train(0.8) and test(0.2)

Note :- molecule_name_processed is dropped from the features as it would easily predict the classes.

In [18]:

```
#Seperating features and classes
x = df.drop(['conformation_name', 'class', 'molecule_name', 'ID','molecule_name_process
ed'], axis = 1)
y = df['class']

#Converting classes vector (integers) to binary class matrix to use it with categorical
_crossentropy.
from keras.utils import to_categorical
y = to_categorical(y)

#Train Test Split
from sklearn.model_selection import train_test_split
x_train, x_test, y_train, Y_test = train_test_split(x, y, test_size = 0.2, random_state
= 0)
print("Shape of Training Set = ", x_train.shape)
```

```
Shape of Training Set =  (5278, 166)
```

Standardizing the features

In [19]:

```
from sklearn.preprocessing import StandardScaler
ss = StandardScaler()
x_train = ss.fit_transform(x_train)
x_test = ss.transform(x_test)
```

MLP Model

1. MLP Model is chosen as its simple, robust and works well for classification tasks.
2. As the data available for training is very less so deeper NN might not work well.
3. Dense layers with 64,32,32 units are used along with relu activation function.
4. To prevent overfitting l2 regularization and Dropout are used.
5. Categorical_crossentropy is used over binary_crossentropy to easily convert probabilistic output to class labels using argmax.

In [21]:

```
from keras.models import Sequential
from keras.layers import Dense, Activation
from keras.layers.normalization import BatchNormalization
from keras.layers import Dropout
from keras import regularizers
import keras

reg = regularizers.l2(0.001)
input_dim = x_train.shape[1]
batch_size = 64
n_epoch = 25
output_dim = 2

model = Sequential()

model.add(Dense(64, activation= 'relu',input_shape=(input_dim,), activity_regularizer=r
eg))
model.add(Dropout(0.20))
model.add(Dense(32, activation= 'relu',activity_regularizer = reg))
model.add(Dense(32, activation= 'relu', activity_regularizer = reg))
model.add(Dense(output_dim, activation = "sigmoid"))
model.summary()
model.compile(optimizer = "adam", loss='categorical_crossentropy', metrics=['accuracy'
])

result = model.fit(x_train,y_train, batch_size=batch_size, epochs=n_epoch, verbose=2, v
alidation_data=(x_test, Y_test))
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #   
=================================================================
dense_9 (Dense)              (None, 64)                10688     
_________________________________________________________________
dropout_3 (Dropout)          (None, 64)                0         
_________________________________________________________________
dense_10 (Dense)             (None, 32)                2080      
_________________________________________________________________
dense_11 (Dense)             (None, 32)                1056      
_________________________________________________________________
dense_12 (Dense)             (None, 2)                 66        
=================================================================
Total params: 13,890
Trainable params: 13,890
Non-trainable params: 0
_________________________________________________________________
Train on 5278 samples, validate on 1320 samples
Epoch 1/25
 - 1s - loss: 1.8836 - acc: 0.7779 - val_loss: 0.9234 - val_acc: 0.8485
Epoch 2/25
 - 0s - loss: 0.7528 - acc: 0.8452 - val_loss: 0.6135 - val_acc: 0.8485
Epoch 3/25
 - 0s - loss: 0.5590 - acc: 0.8452 - val_loss: 0.4936 - val_acc: 0.8485
Epoch 4/25
 - 0s - loss: 0.4567 - acc: 0.8463 - val_loss: 0.4020 - val_acc: 0.8568
Epoch 5/25
 - 0s - loss: 0.3788 - acc: 0.9032 - val_loss: 0.3512 - val_acc: 0.9492
Epoch 6/25
 - 0s - loss: 0.3324 - acc: 0.9416 - val_loss: 0.3048 - val_acc: 0.9538
Epoch 7/25
 - 0s - loss: 0.3003 - acc: 0.9515 - val_loss: 0.2754 - val_acc: 0.9636
Epoch 8/25
 - 0s - loss: 0.2701 - acc: 0.9600 - val_loss: 0.2519 - val_acc: 0.9598
Epoch 9/25
 - 0s - loss: 0.2489 - acc: 0.9665 - val_loss: 0.2334 - val_acc: 0.9712
Epoch 10/25
 - 0s - loss: 0.2371 - acc: 0.9714 - val_loss: 0.2241 - val_acc: 0.9644
Epoch 11/25
 - 0s - loss: 0.2284 - acc: 0.9651 - val_loss: 0.2669 - val_acc: 0.9462
Epoch 12/25
 - 0s - loss: 0.2044 - acc: 0.9740 - val_loss: 0.2162 - val_acc: 0.9614
Epoch 13/25
 - 0s - loss: 0.1929 - acc: 0.9756 - val_loss: 0.1826 - val_acc: 0.9742
Epoch 14/25
 - 0s - loss: 0.1883 - acc: 0.9754 - val_loss: 0.1970 - val_acc: 0.9682
Epoch 15/25
 - 0s - loss: 0.1825 - acc: 0.9756 - val_loss: 0.1644 - val_acc: 0.9811
Epoch 16/25
 - 0s - loss: 0.1734 - acc: 0.9790 - val_loss: 0.1875 - val_acc: 0.9712
Epoch 17/25
 - 0s - loss: 0.1732 - acc: 0.9763 - val_loss: 0.1802 - val_acc: 0.9727
Epoch 18/25
 - 0s - loss: 0.1544 - acc: 0.9831 - val_loss: 0.1503 - val_acc: 0.9833
Epoch 19/25
 - 0s - loss: 0.1595 - acc: 0.9797 - val_loss: 0.1707 - val_acc: 0.9742
Epoch 20/25
 - 0s - loss: 0.1618 - acc: 0.9782 - val_loss: 0.1662 - val_acc: 0.9780
Epoch 21/25
 - 0s - loss: 0.1511 - acc: 0.9799 - val_loss: 0.1652 - val_acc: 0.9750
Epoch 22/25
```

```
 - 0s - loss: 0.1539 - acc: 0.9786 - val_loss: 0.1794 - val_acc: 0.9689
Epoch 23/25
 - 0s - loss: 0.1438 - acc: 0.9812 - val_loss: 0.1393 - val_acc: 0.9750
Epoch 24/25
 - 0s - loss: 0.1375 - acc: 0.9812 - val_loss: 0.1387 - val_acc: 0.9803
Epoch 25/25
 - 0s - loss: 0.1357 - acc: 0.9831 - val_loss: 0.1256 - val_acc: 0.9886
```

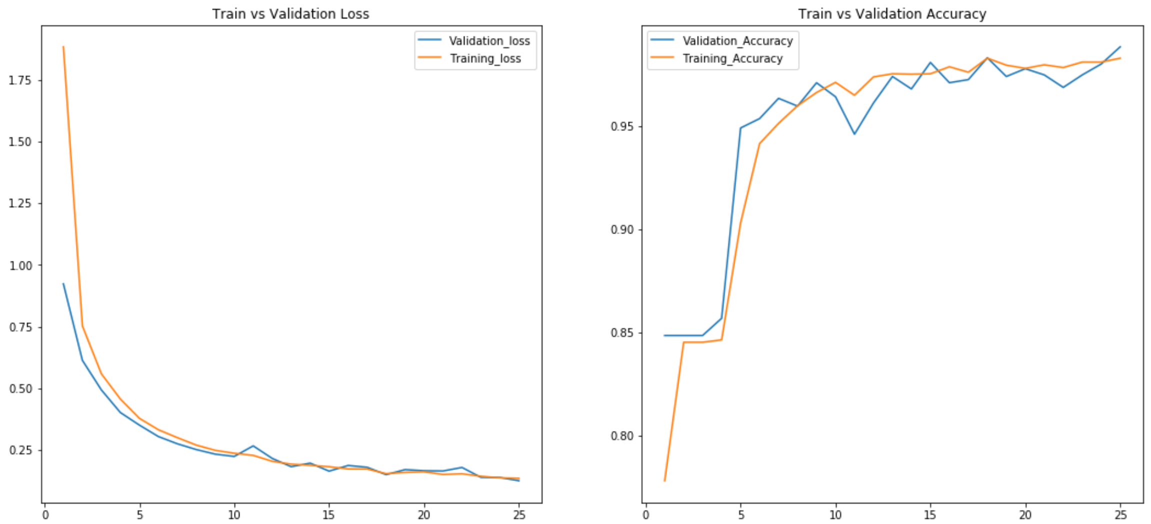
Plotting and printing Metrics

In [22]:

```
test_loss = result.history['val_loss']
train_loss = result.history['loss']
test_acc = result.history['val_acc']
train_acc = result.history['acc']

n_epoch_lst = list(range(1,n_epoch+1))

import matplotlib.pyplot as plt
fig = plt.figure(figsize=(18,8))

#Plotting Train vs Validation loss
ax1 = plt.subplot(121)
ax1.plot(n_epoch_lst,test_loss, label='Validation_loss' )
ax1.plot(n_epoch_lst,train_loss, label='Training_loss')
plt.legend()
plt.title('Train vs Validation Loss')

#Plotting Train vs Validation Accuracy
ax2 = plt.subplot(122)
ax2.plot(n_epoch_lst,test_acc, label='Validation_Accuracy' )
ax2.plot(n_epoch_lst,train_acc, label='Training_Accuracy')
plt.legend()
plt.title('Train vs Validation Accuracy')
plt.plot()
```

Out[22]:

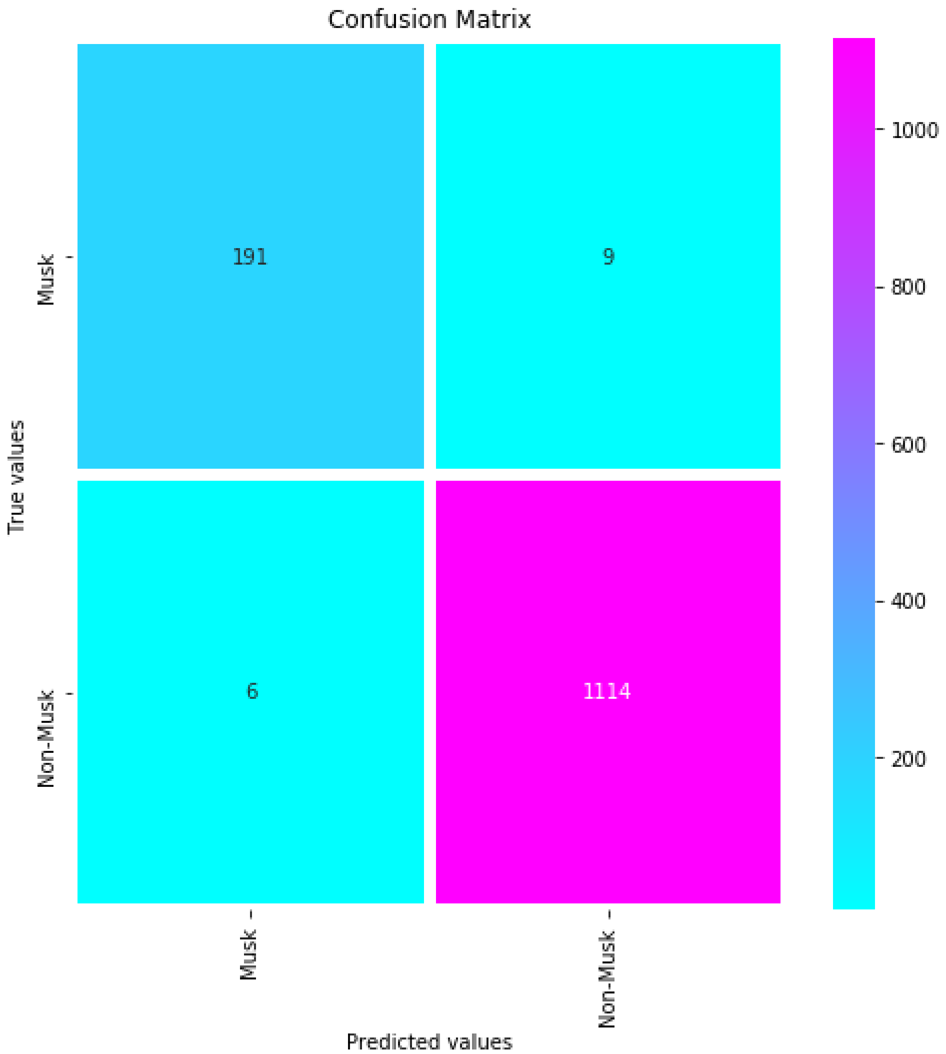
```
[]
```



In [23]:

```
#Printing Training and Validation - Accuracy & Loss
score = model.evaluate(x_test, Y_test, verbose = 0)
print('Validation Loss',score[0])
print('Validation Accuracy',score[1]*100)
print('*'*20)
print('Train loss',train_loss[-1])
print('Train Accuracy',train_acc[-1]*100)

#Predicting classes from validation set
Y_pred = model.predict(x_test)

#Converting Probabilistic prediction Output to Class labels (Musk or Non-Musk)
Activities = {0:'Non-Musk',1:'Musk'}
y_pred = pd.Series([Activities[y] for y in np.argmax(Y_pred, axis=1)])
y_test = pd.Series([Activities[y] for y in np.argmax(Y_test, axis=1)])

#Confusion Matrix
from sklearn.metrics import confusion_matrix
cm=confusion_matrix(y_test, y_pred)
print(cm)
labels=['Musk','Non-Musk']
cm_df = pd.DataFrame(cm,index=labels, columns =labels)

#Confusion Matrix Heatmap
import matplotlib.pyplot as plt
import seaborn as sns
plt.figure(figsize=(8,8))
sns.heatmap(cm_df, annot=True, fmt='d', cmap='cool', linewidth=5)
plt.xlabel('Predicted values')
plt.ylabel('True values')
plt.xticks(rotation=90)
plt.title('Confusion Matrix')
plt.show()
```

```
Validation Loss 0.09127355534018892
Validation Accuracy 98.86363636363636
********************
Train loss 0.13566809801745477
Train Accuracy 98.31375521030694
[[ 191    9]
 [   6 1114]]
```



In [24]:

```
#Using classification report to print other metrics (F1-score, Precision, Recall)
from sklearn import metrics
classificationreport = metrics.classification_report(y_test, y_pred)
print(classificationreport)
```

```
              precision    recall  f1-score   support

        Musk       0.97      0.95      0.96       200
    Non-Musk       0.99      0.99      0.99      1120

   micro avg       0.99      0.99      0.99      1320
   macro avg       0.98      0.97      0.98      1320
weighted avg       0.99      0.99      0.99      1320
```