BinderTutorial_QC

March 6, 2019

1 Binder Tutorial QC Analysis

1.0.1 To begin: Click the top cell and press 'Run' on the toolbar (or shift-enter). Alternatively click Kernel, Restart and Run All.

1.1 Table of Contents:

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1. Import Data

1. Import the pandas python module (https://pandas.pydata.org/).
2. Import the excel sheet "Data" from excel file "data.xlsx" into a data frame called "data".
3. Display the numbe of rows and column.
4. Display the fist 10 rows at the top (head) of the data frame.

```
In [10]: import pandas as pd

         data = pd.read_excel('data.xlsx', sheet_name='Data')

         print("Data Table: {} rows & {} columns".format(*data.shape))
         display(data.head(10))

         peak = pd.read_excel('data.xlsx', sheet_name='Peak')
         print("Peak Table: {} rows & {} columns".format(*peak.shape))
         display(peak.head(10))
```

```
Data Table: 91 rows & 3087 columns


   Order SampleType  QC            M1            M2            M3  \
0      1         QC   1  1.837062e+08  1.296528e+08  3.961182e+07
1      2         QC   1  2.030571e+08  1.178121e+08  6.361418e+07
2      3     Sample   0  1.285728e+08  2.726444e+08  4.611692e+07
3      4     Sample   0  1.491128e+08  1.955086e+08  5.212802e+07
4      5     Sample   0  1.590268e+08  3.780061e+08  4.238071e+07
5      6     Sample   0  1.875314e+08  7.153474e+07  5.007826e+07
6      7         QC   1  1.983585e+08  1.204062e+08  5.190127e+07
```

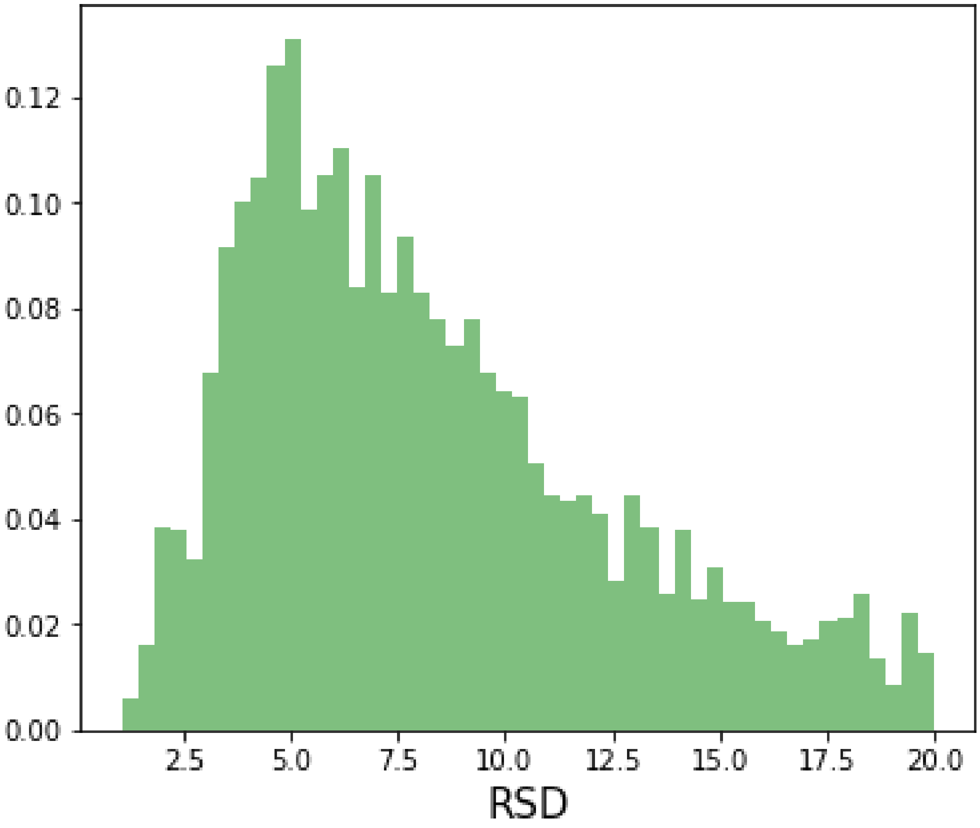
```
7      8     Sample   0  1.460268e+08  2.274148e+08  5.872350e+07
8      9     Sample   0  1.381372e+08  1.269111e+08  5.276344e+07
9     10     Sample   0  1.601298e+08  4.347327e+08  4.883041e+07

             M4            M5            M6            M7      ...        \
0  3.732578e+07  5.339865e+06  1.031822e+08  9.409682e+06      ...
1  6.682747e+07  5.572493e+06  9.366510e+07  9.941482e+06      ...
2  4.717621e+07  3.178726e+06  8.077425e+07  6.924520e+06      ...
3  5.114760e+07  3.428193e+06  8.211311e+07  7.416907e+06      ...
4  4.282051e+07  3.186309e+06  1.000761e+08  7.030797e+06      ...
5  5.036435e+07  4.849348e+06  9.998757e+07  1.039036e+07      ...
6  5.180519e+07  5.348706e+06  8.966852e+07  9.605938e+06      ...
7  5.581725e+07  4.342786e+06  1.059740e+08  1.401639e+07      ...
8  4.936756e+07  3.005090e+06  8.101362e+07  1.484466e+07      ...
9  4.518047e+07  3.326398e+06  7.714394e+07  1.239396e+07      ...

          M3075         M3076         M3077         M3078        M3079  \
0  35153.206002  15735.886504  24928.165047  30134.444665  3035.247672
1  36701.059662  15590.522963  24776.756320  30250.013996  3052.288747
2  43120.310719  16378.981747  28627.451582  31297.776297  1738.358685
3  44663.545552  17429.459487  25703.703594  26399.809078   846.020446
4  41770.351723  18467.519040  27371.393974  28374.785933  1959.397898
5  41616.726360  11426.528395  23313.373795  28582.727888   872.115128
6  32839.675140  16262.163327  21298.643088  28065.010551  3277.276918
7  35339.968664  25426.050392  51819.646796  21762.932664  1822.815140
8  33766.256647  15963.341703  50651.507533  18503.876558   843.925809
9  31442.161072  22600.725041  51901.700174  16804.403434  1522.101762

          M3080         M3081        M3082         M3083         M3084
0  18271.101975  20981.783849  3523.418763  23752.440055  17161.698785
1  22116.296519  24543.382677  3389.677457  24262.317947  18949.290754
2  17695.679626  16703.470005  1113.489872  29717.457693  14683.792853
3  15306.546820  15198.095655  1137.752119  26610.868749  11913.223789
4  14904.243032  15625.089253  1101.738536  26496.665356  12750.259715
5  15301.063816  14321.556052  1030.238432  32587.650554  18655.811727
6  20071.616958  18198.098904  3047.831055  24997.154651  14494.628663
7  23457.954245  23651.858710  1210.741328  22834.426860  15771.899526
8  16572.962662  16625.898352  1186.166100  25623.108950  13811.758227
9  19948.743747  22690.058851  1229.664436  22637.770945  15009.816887

[10 rows x 3087 columns]


Peak Table: 3084 rows & 6 columns


   Idx Name  Mol_Weight  RT_minutes        RSD  D_Ratio
0    1   M1   113.05902       1.276   5.012937     0.28
```

```
1     2   M2   203.11564       0.950   9.557013     0.19
2     3   M3   161.10514       1.428  16.085023     0.26
3     4   M4   129.07893       1.400  18.035797     0.49
4     5   M5   161.10510       1.272  19.515359     0.40
5     6   M6   225.94404       5.923   6.510319     0.33
6     7   M7   194.08026       1.169   2.890900     0.03
7     8   M8   115.06345       7.067   4.733385     0.16
8     9   M9   131.09461       6.220   6.138996     0.33
9    10  M10   117.07900       6.971   4.783892     0.32
```

2. Visualisation

Note: Each cell in the Visualisation Section can be run in any order (provided data is imported in Section 1). ### 2.1. Histagram of RSD

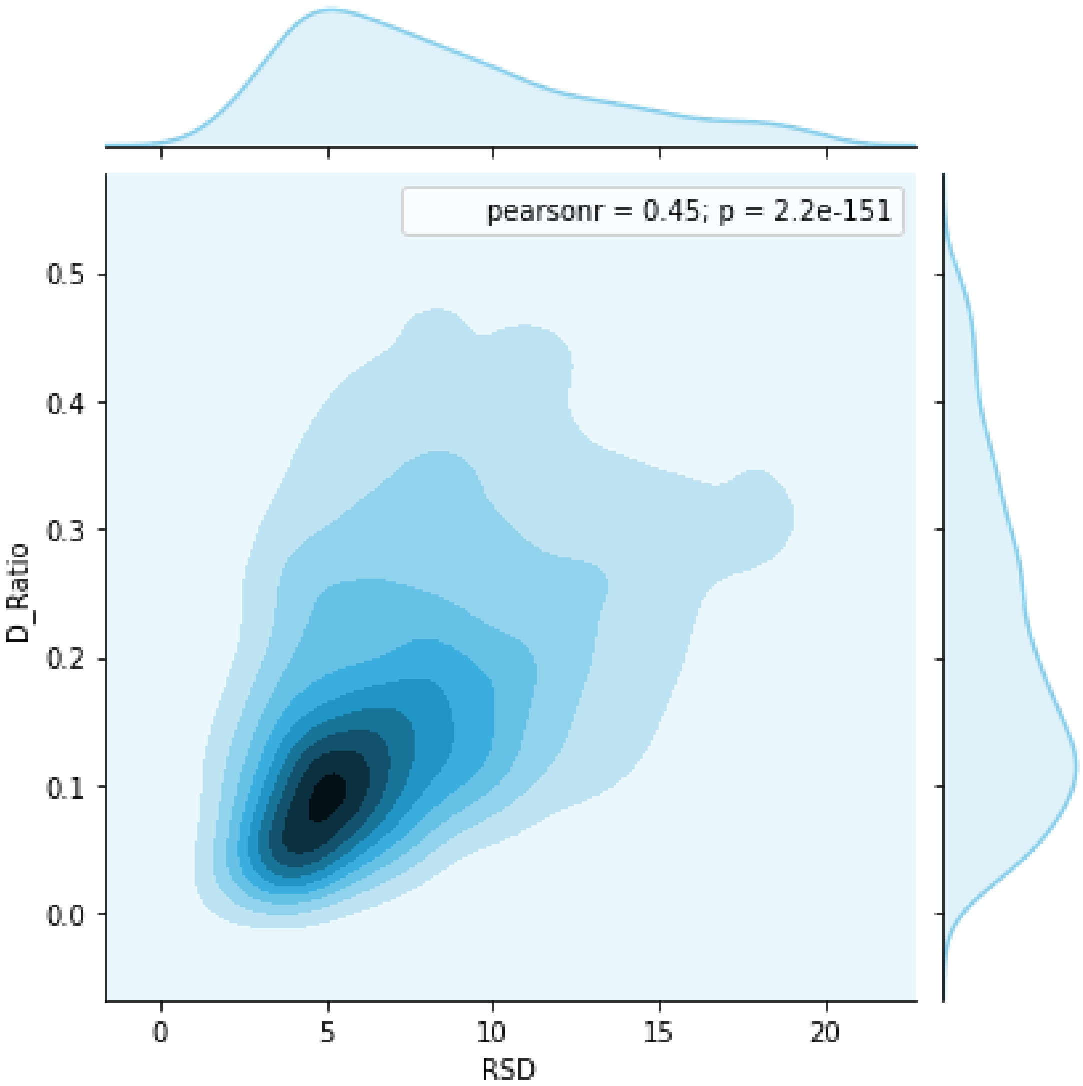
```
In [7]: import matplotlib.pyplot as plt
        %matplotlib inline

        fig = plt.figure(figsize=(6,5))
        plt.hist(peak.RSD, 50, density=True, facecolor='g', alpha=0.5)
        plt.xlabel('RSD', fontsize=15)
        plt.show()
```



2.2. Jointplot of RSD vs. D-Ratio

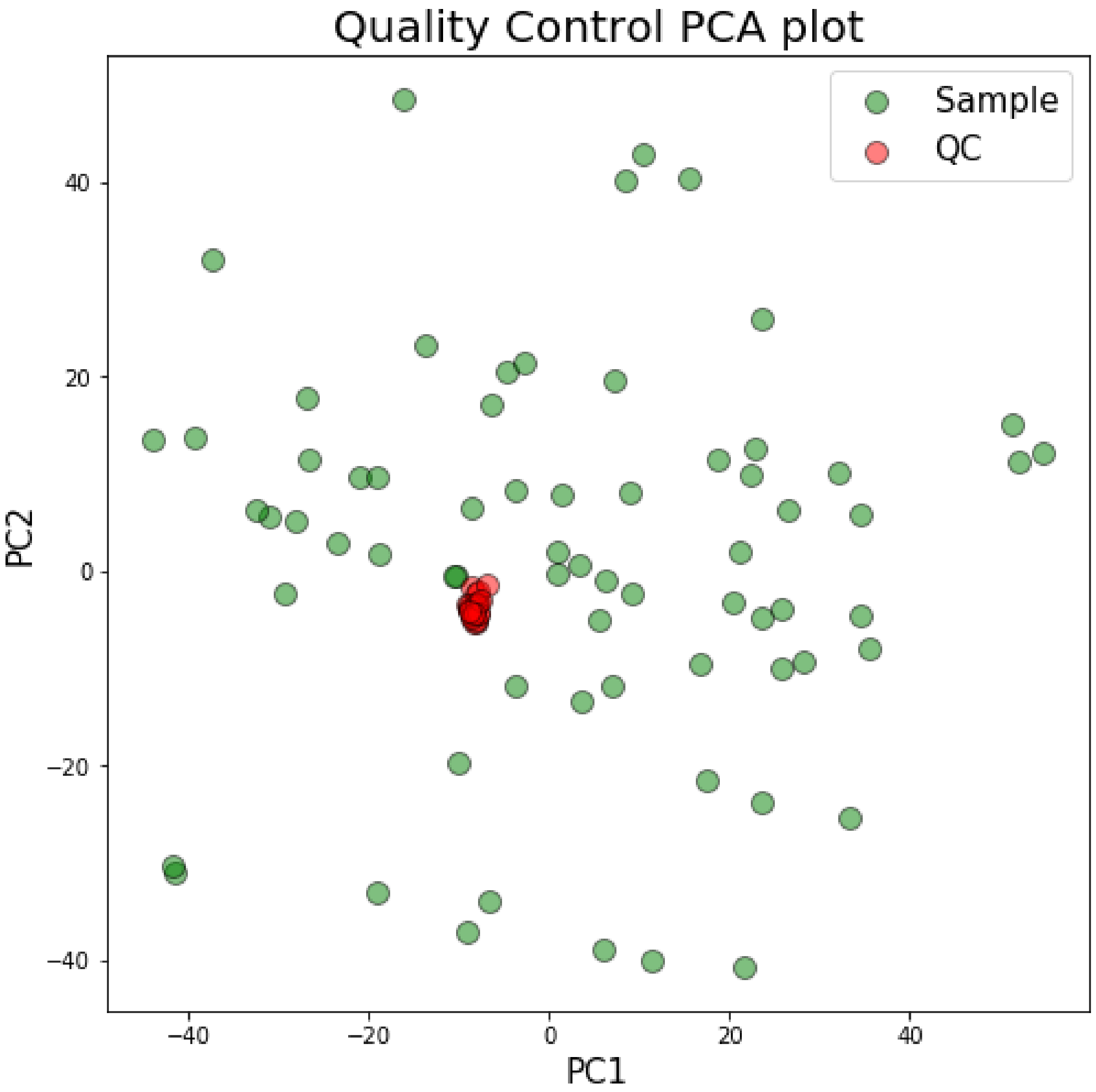
```
In [11]: import seaborn as sns

         sns.jointplot(x=peak.RSD, y=peak.D_Ratio, kind='kde', color="skyblue")
```

```
Out[11]: <seaborn.axisgrid.JointGrid at 0x12a5c2eb8>
```



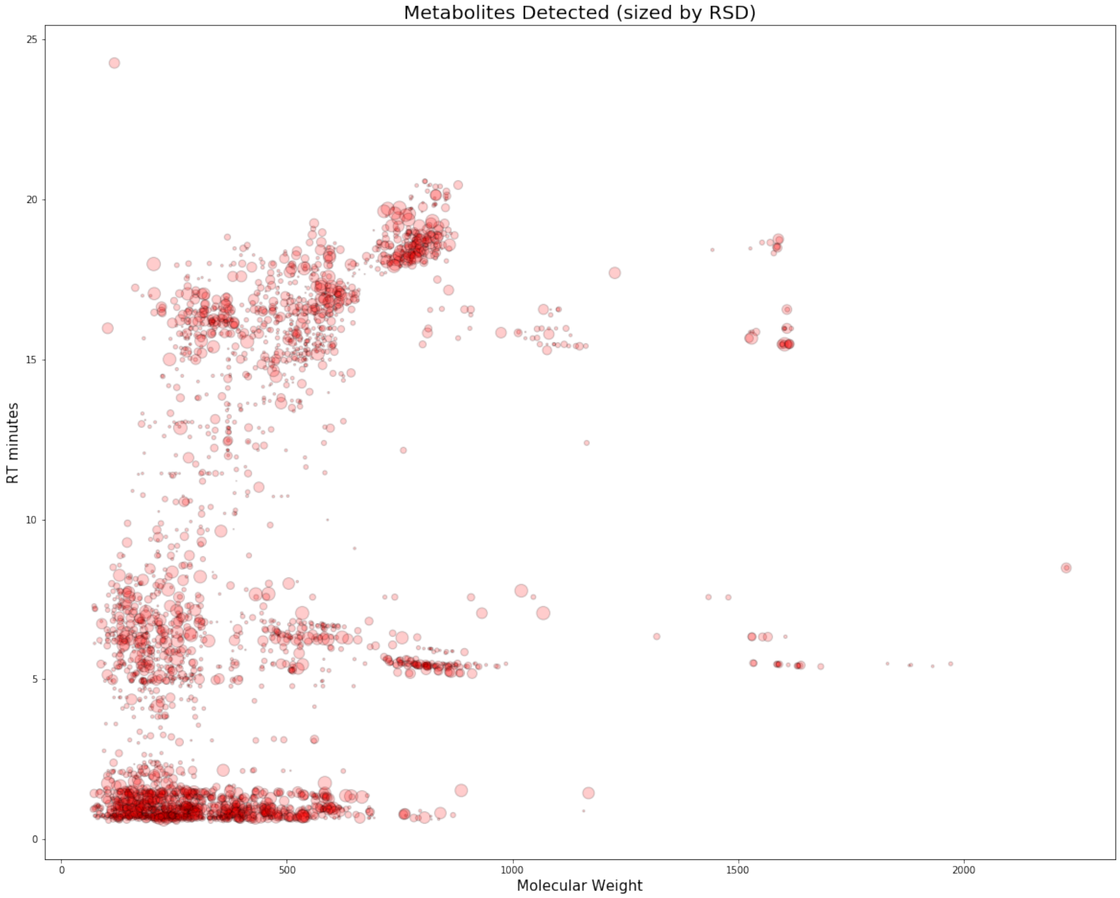
2.3. PCA score plot of QC vs. Sample

```
In [8]: import numpy as np
        from sklearn.decomposition import PCA
        from sklearn.preprocessing import StandardScaler

        import matplotlib.pyplot as plt
        from matplotlib.colors import ListedColormap

        names = peak['Name']
        x = data[names].values
        x = np.log(x)
        x = StandardScaler().fit_transform(x)

        pca = PCA(n_components=2)
        scores = pca.fit_transform(x)
        label = data['SampleType']

        Sample_scores = scores[label == 'Sample',:]
        QC_scores = scores[label == 'QC',:]

        fig = plt.figure(figsize=(8,8))

        h1 = plt.scatter(Sample_scores[:,0],Sample_scores[:,1],edgecolors='Black', facecolors=
        h2 = plt.scatter(QC_scores[:,0],QC_scores[:,1], edgecolors='Black', facecolors='Red',s=

        plt.legend((h1,h2),('Sample','QC'),fontsize=15)

        plt.xlabel('PC1', fontsize=15)
        plt.ylabel('PC2', fontsize=15)
        plt.title('Quality Control PCA plot',fontsize=20)

        plt.show()
```



2.4. Scatter plot of Molecular Weights vs. RT Time (sized by RSD)

```
In [9]: fig = plt.figure(figsize=(20,16))
        plt.scatter(peak.Mol_Weight,peak.RT_minutes, s = peak.RSD**2/2,alpha=0.2, edgecolors =
        plt.xlabel('Molecular Weight', fontsize=15)
        plt.ylabel('RT minutes', fontsize=15)
        plt.title('Metabolites Detected (sized by RSD)',fontsize=20)
        plt.show()
```


Metabolites Detected (sized by RSD)
RT minutes
Molecular Weight
0
5
10
15
20
25
0
500
1000
1500
2000

```
In [ ]:
```