Air Quality

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1 IBM Supervised Learning: Regression peer- reviewed Project

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1.1 Introduction

Air pollution will endanger human health and life in big cities, especially to the elderly and children. This is not an individual problem of one person but a global problem. Therefore, many countries in the world made air pollution monitoring and control stations in many cities to observe air pollutants such as NO2, CO, SO2, PM2.5, and PM10 to alert the citizens about pollution index which exceeds the quality threshold.

Particulate Matter PM 2.5 is a fine atmospheric pollutant that has a diameter of fewer than 2.5 micrometers. Particulate Matter PM10 is a coarse particulate that is 10 micrometers or less in diameter. Carbon Monoxide CO is a product of combustion of fuel such as coal, wood, or natural gas. Vehicular emission contributes to the majority of carbon monoxide let into our atmosphere. Nitrogen dioxide or nitrogen oxide expelled from high-temperature combustion: sulfur dioxide SO2 and Sulphur Oxides SO produced by volcanoes and in industrial processes. Petroleum and Coal often contain sulfur compounds, and their combustion generates sulfur dioxide. Air pollution is caused by the presence of poison gases and substances; therefore, it is impacted by the meteorological factors of a particular place, such as temperature, humidity, rain, and wind.

In this project, the regression analysis technique is used to evaluate the relationship between these factors and **predict** nitrogen oxides NOx based on other parameters; **main objective of the analysis is to focus on prediction.**

1.2 Dataset description

The dataset contains 9358 instances of hourly averaged responses from an array of 5 metal oxide chemical sensors embedded in an Air Quality Chemical Multisensor Device. The device was located on the field in a significantly polluted area, at road level, within an Italian city. Data were recorded from March 2004 to February 2005 (one year) representing the longest freely available recordings of on field deployed air quality chemical sensor devices responses. Ground Truth hourly averaged concentrations for CO, Non Metanic Hydrocarbons, Benzene, Total Nitrogen Oxides (NOx) and Nitrogen Dioxide (NO2) and were provided by a co-located reference certified analyzer.

Dataset attribute information:

- Date (DD/MM/YYYY)
- Time (HH.MM.SS)
- True hourly averaged concentration CO in mg/m^3 (reference analyzer)

- PT08.S1 (tin oxide) hourly averaged sensor response (nominally CO targeted)
- True hourly averaged overall Non Metanic HydroCarbons concentration in microg/m^3 (reference analyzer)
- True hourly averaged Benzene concentration in microg/m^3 (reference analyzer)
- PT08.S2 (titania) hourly averaged sensor response (nominally NMHC targeted)
- True hourly averaged NOx concentration in ppb (reference analyzer)
- PT08.S3 (tungsten oxide) hourly averaged sensor response (nominally NOx targeted)
- True hourly averaged NO2 concentration in microg/m^3 (reference analyzer)
- PT08.S4 (tungsten oxide) hourly averaged sensor response (nominally NO2 targeted)
- PT08.S5 (indium oxide) hourly averaged sensor response (nominally O3 targeted)
- Temperature in Â°C
- Relative Humidity (%)
- AH Absolute Humidity

This dataset is from the UCI machine learning repository and contains hourly averaged responses from an air quality multi-sensor device that was located in a significantly polluted area at road level in an undisclosed Italian city. This data was collected over the course of approx one year (from March 2004 - February 2005)

For reference: https://archive.ics.uci.edu/ml/datasets/Air+Quality#

Note: Evidences of cross-sensitivities as well as both concept and sensor drifts are present as described in De Vito et al., Sens. And Act. B, Vol. 129,2,2008 (citation required) eventually affecting sensors concentration estimation capabilities. **Missing values are tagged with -200 value.**

[1]:
```
# importing dependencies

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import warnings, pprint

from sklearn import metrics
from sklearn.preprocessing import MinMaxScaler
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.preprocessing import StandardScaler, PolynomialFeatures
from sklearn.model_selection import KFold, cross_val_predict, train_test_split
from sklearn.linear_model import LinearRegression, Lasso, Ridge, RidgeCV,␣
↪LassoCV, ElasticNetCV
from sklearn.pipeline import Pipeline

%matplotlib inline

print("All relevant modules were imported.")
```

```
All relevant modules were imported.
```

1.3 Data cleaning and feature engineering.

[2]:
```
airq = pd.read_csv('AirQualityUCI.csv', sep=',', delimiter=";",decimal=",")
```

[3]:
```
airq.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 9471 entries, 0 to 9470
Data columns (total 17 columns):
 #   Column         Non-Null Count  Dtype
---  ------         --------------  -----
 0   Date           9357 non-null   object
 1   Time           9357 non-null   object
 2   CO(GT)         9357 non-null   float64
 3   PT08.S1(CO)    9357 non-null   float64
 4   NMHC(GT)       9357 non-null   float64
 5   C6H6(GT)       9357 non-null   float64
 6   PT08.S2(NMHC)  9357 non-null   float64
 7   NOx(GT)        9357 non-null   float64
 8   PT08.S3(NOx)   9357 non-null   float64
 9   NO2(GT)        9357 non-null   float64
 10  PT08.S4(NO2)   9357 non-null   float64
 11  PT08.S5(O3)    9357 non-null   float64
 12  T              9357 non-null   float64
 13  RH             9357 non-null   float64
 14  AH             9357 non-null   float64
 15  Unnamed: 15    0 non-null      float64
 16  Unnamed: 16    0 non-null      float64
dtypes: float64(15), object(2)
memory usage: 1.2+ MB
```

[4]:
```
airq.columns
```

[4]:
```
Index(['Date', 'Time', 'CO(GT)', 'PT08.S1(CO)', 'NMHC(GT)', 'C6H6(GT)',
       'PT08.S2(NMHC)', 'NOx(GT)', 'PT08.S3(NOx)', 'NO2(GT)', 'PT08.S4(NO2)',
       'PT08.S5(O3)', 'T', 'RH', 'AH', 'Unnamed: 15', 'Unnamed: 16'],
      dtype='object')
```

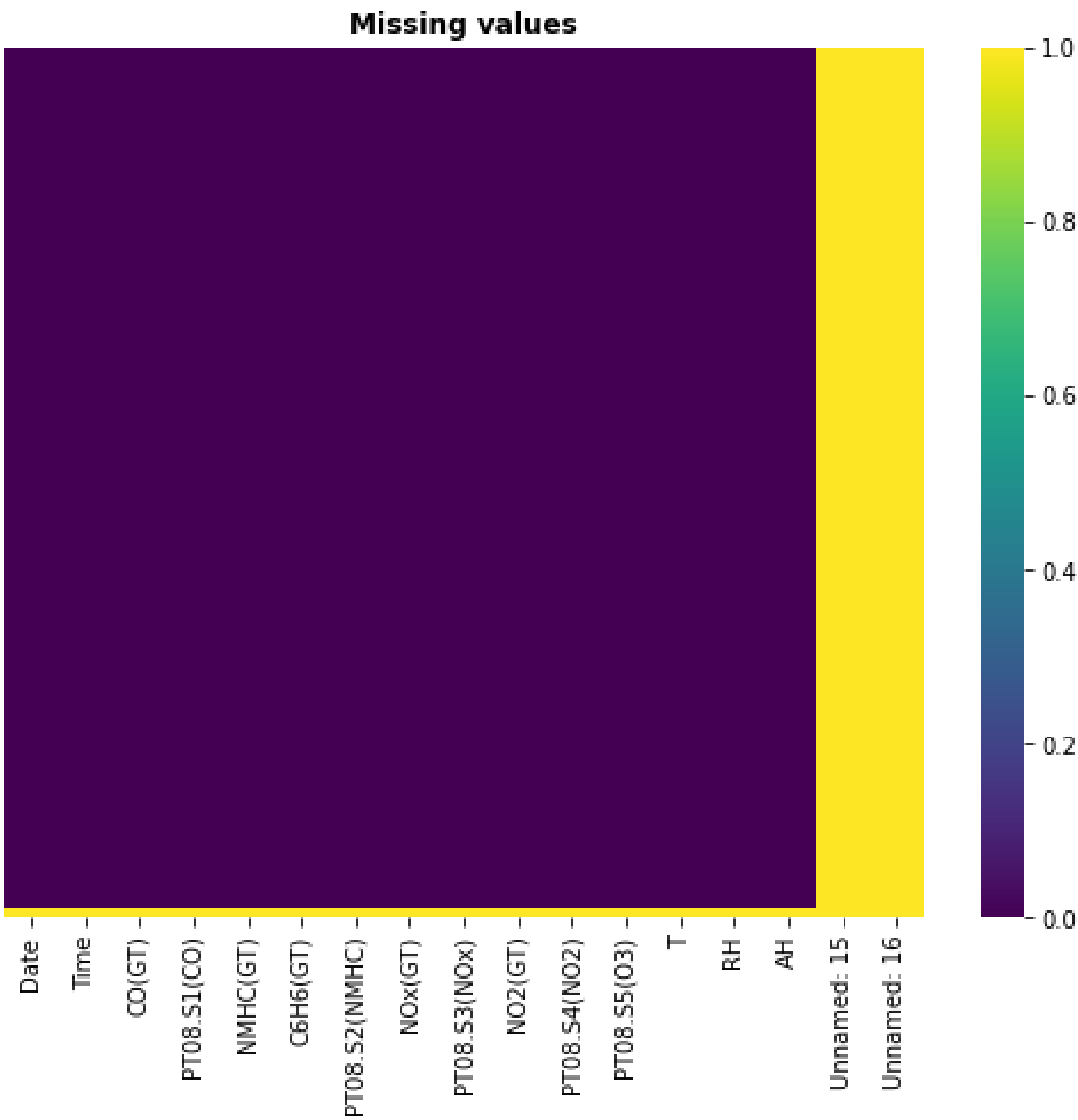
[5]:
```
airq.describe()
```

[5]:
```
            CO(GT)  PT08.S1(CO)     NMHC(GT)     C6H6(GT)  PT08.S2(NMHC)  \
count  9357.000000  9357.000000  9357.000000  9357.000000    9357.000000
mean    -34.207524  1048.990061  -159.090093     1.865683     894.595276
std      77.657170   329.832710   139.789093    41.380206     342.333252
min    -200.000000  -200.000000  -200.000000  -200.000000    -200.000000
25%       0.600000   921.000000  -200.000000     4.000000     711.000000
50%       1.500000  1053.000000  -200.000000     7.900000     895.000000
75%       2.600000  1221.000000  -200.000000    13.600000    1105.000000
```

```
max       11.900000  2040.000000  1189.000000    63.700000    2214.000000

            NOx(GT)  PT08.S3(NOx)      NO2(GT)  PT08.S4(NO2)  PT08.S5(O3)  \
count  9357.000000   9357.000000  9357.000000   9357.000000  9357.000000
mean    168.616971    794.990168    58.148873   1391.479641   975.072032
std     257.433866    321.993552   126.940455    467.210125   456.938184
min    -200.000000   -200.000000  -200.000000   -200.000000  -200.000000
25%      50.000000    637.000000    53.000000   1185.000000   700.000000
50%     141.000000    794.000000    96.000000   1446.000000   942.000000
75%     284.000000    960.000000   133.000000   1662.000000  1255.000000
max    1479.000000   2683.000000   340.000000   2775.000000  2523.000000

                 T           RH           AH  Unnamed: 15  Unnamed: 16
count  9357.000000  9357.000000  9357.000000          0.0          0.0
mean      9.778305    39.485380    -6.837604          NaN          NaN
std      43.203623    51.216145    38.976670          NaN          NaN
min    -200.000000  -200.000000  -200.000000          NaN          NaN
25%      10.900000    34.100000     0.692300          NaN          NaN
50%      17.200000    48.600000     0.976800          NaN          NaN
75%      24.100000    61.900000     1.296200          NaN          NaN
max      44.600000    88.700000     2.231000          NaN          NaN
```

[6]:

```
plt.figure(figsize=(9,7))
plt.title('Missing values', fontweight='bold')

ax = sns.heatmap(airq.isnull(),yticklabels=False,cbar='viridis',cmap='viridis')

plt.show()
```



[7]:
```
airq.isnull().sum()
```

[7]:
```
Date             114
Time             114
CO(GT)           114
PT08.S1(CO)      114
NMHC(GT)         114
C6H6(GT)         114
PT08.S2(NMHC)    114
NOx(GT)          114
PT08.S3(NOx)     114
NO2(GT)          114
```

```
PT08.S4(NO2)      114
PT08.S5(O3)       114
T                 114
RH                114
AH                114
Unnamed: 15      9471
Unnamed: 16      9471
dtype: int64
```

[8]:
```
airq = airq.drop(["Unnamed: 15","Unnamed: 16"], axis=1)
```

[9]:
```
airq.dropna(inplace=True)
```

[10]:
```
airq.set_index("Date", inplace=True)
```

[11]:
```
airq.index = pd.to_datetime(airq.index)
```

[12]:
```
type(airq.index)
```

[12]:
```
pandas.core.indexes.datetimes.DatetimeIndex
```

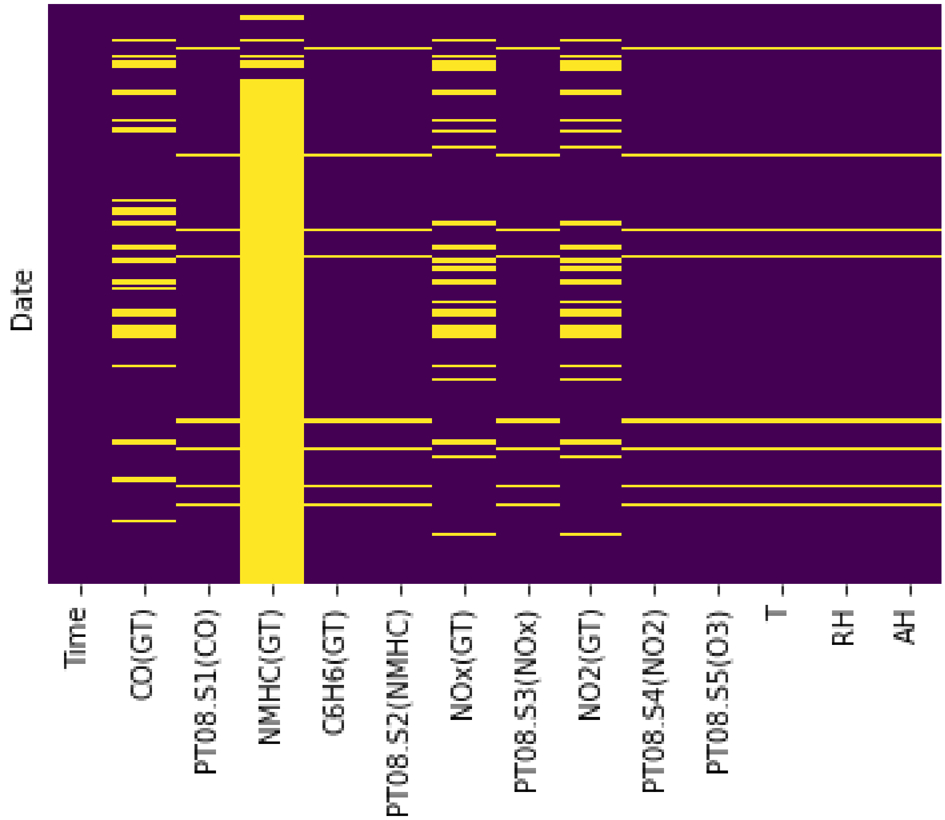
[13]:
```
airq['Time'] = pd.to_datetime(airq['Time'],format= '%H.%M.%S').dt.hour
```

[14]:
```
airq.apply(lambda x : x == -200).sum()
```

[14]:
```
Time                0
CO(GT)           1683
PT08.S1(CO)       366
NMHC(GT)         8443
C6H6(GT)          366
PT08.S2(NMHC)     366
NOx(GT)          1639
PT08.S3(NOx)      366
NO2(GT)          1642
PT08.S4(NO2)      366
PT08.S5(O3)       366
T                 366
RH                366
AH                366
dtype: int64
```

[15]:
```
sns.heatmap(airq.isin([-200]),yticklabels=False,cbar=False,cmap='viridis')
```

[15]:
```
<AxesSubplot:ylabel='Date'>
```

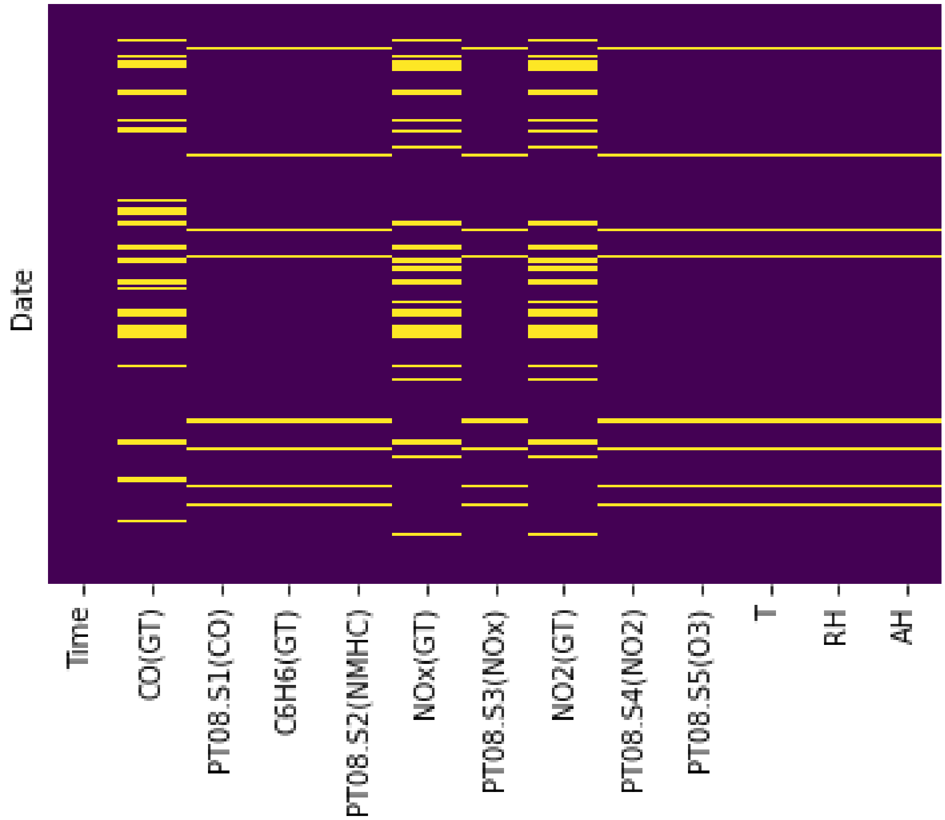


The NHMC(GT) column is missing many values, more than 85% values are NaN; 8443 out of 9357. Thus this column can be removed from the dataset as these values are very less likely to be of any significant importance in this dataset.

[16]:
```
airq.drop('NMHC(GT)', axis=1, inplace=True)
```

[17]:
```
sns.heatmap(airq.isin([-200]),yticklabels=False,cbar=False,cmap='viridis')
```

[17]:
```
<AxesSubplot:ylabel='Date'>
```



[18]:
```
airq.isin([-200]).sum()
```

[18]:
```
Time                0
CO(GT)           1683
PT08.S1(CO)       366
C6H6(GT)          366
PT08.S2(NMHC)     366
NOx(GT)          1639
PT08.S3(NOx)      366
NO2(GT)          1642
PT08.S4(NO2)      366
PT08.S5(O3)       366
T                 366
RH                366
AH                366
dtype: int64
```

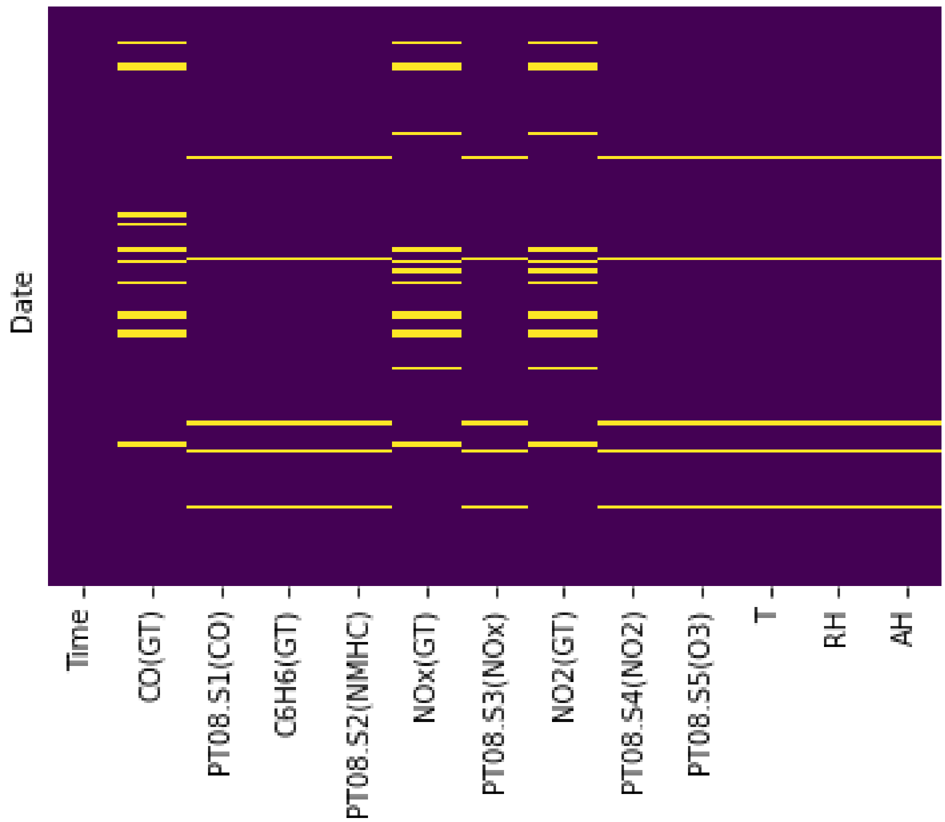
[19]:
```
airq.replace(to_replace= -200, value= np.NaN, inplace= True)
```

[20]:
```python
# Fill NaN values with average of particular date

def remove_outlier(col):
    airq[col] = airq.groupby('Date')[col].transform(lambda x: x.fillna(x.
 ↪mean()))
```

[21]:
```python
col_list = airq.columns[1:]

for i in col_list:
    remove_outlier(i)
```

[22]:
```python
sns.heatmap(airq.isna(),yticklabels=False,cbar=False,cmap='viridis')
```

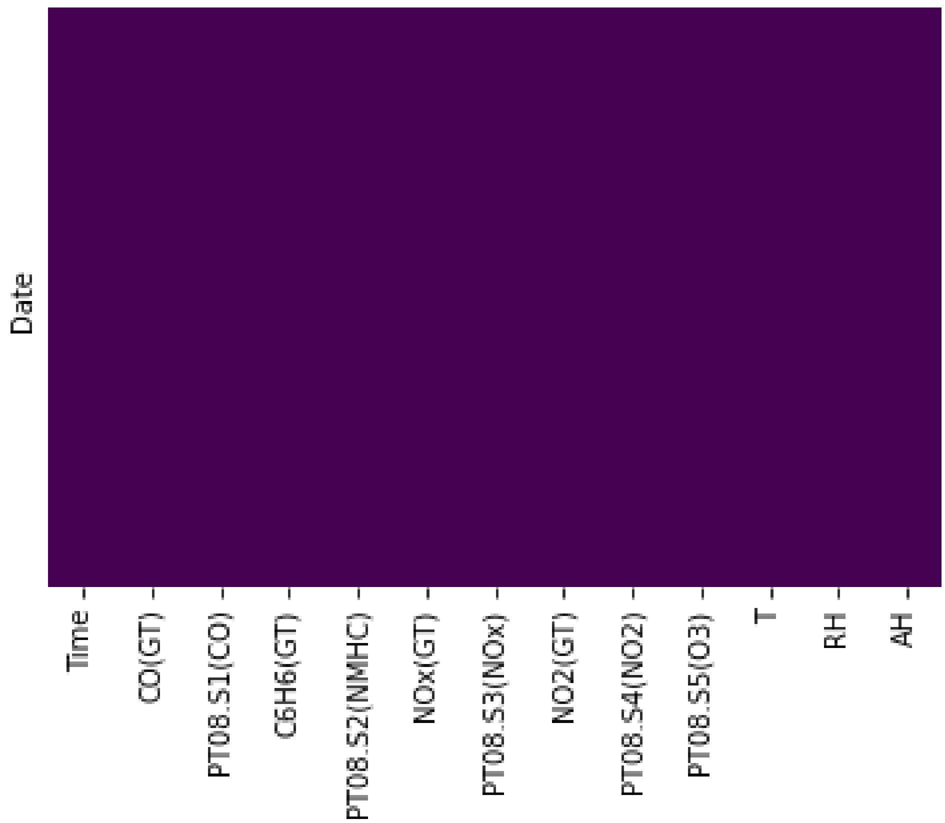
[22]: <AxesSubplot:ylabel='Date'>



[23]:
```python
# forward fill method for removing the leftover nan values

airq.fillna(method='ffill', inplace= True)
```

[24]:
```python
sns.heatmap(airq.isna(),yticklabels=False,cbar=False,cmap='viridis')
```

[24]: <AxesSubplot:ylabel='Date'>



[25]:
```
airq.isnull().any()
```

[25]:
```
Time             False
CO(GT)           False
PT08.S1(CO)      False
C6H6(GT)         False
PT08.S2(NMHC)    False
NOx(GT)          False
PT08.S3(NOx)     False
NO2(GT)          False
PT08.S4(NO2)     False
PT08.S5(O3)      False
T                False
RH               False
AH               False
dtype: bool
```

1.4 EXPLORATORY DATA ANALYSIS

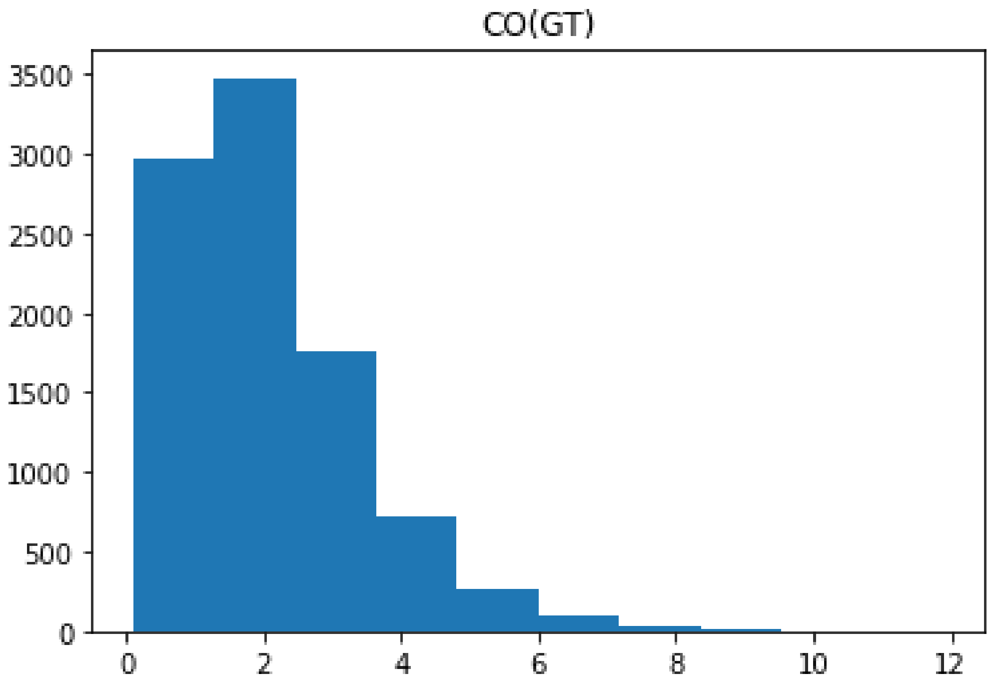
[26]:
```python
airq.dtypes.value_counts()
```

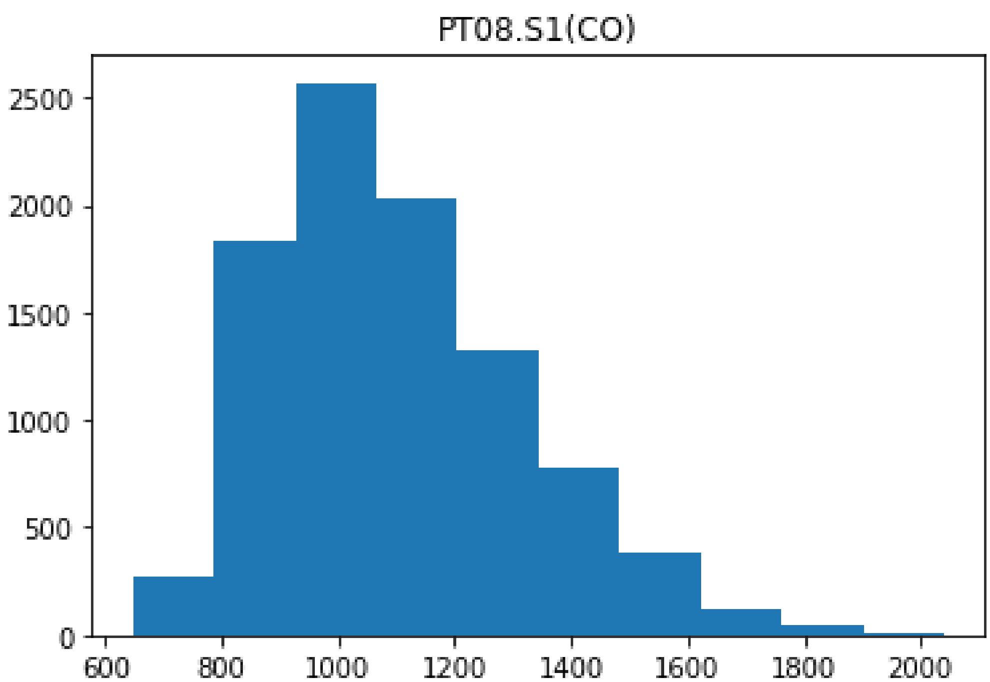
[26]:
```
float64    12
int64       1
dtype: int64
```

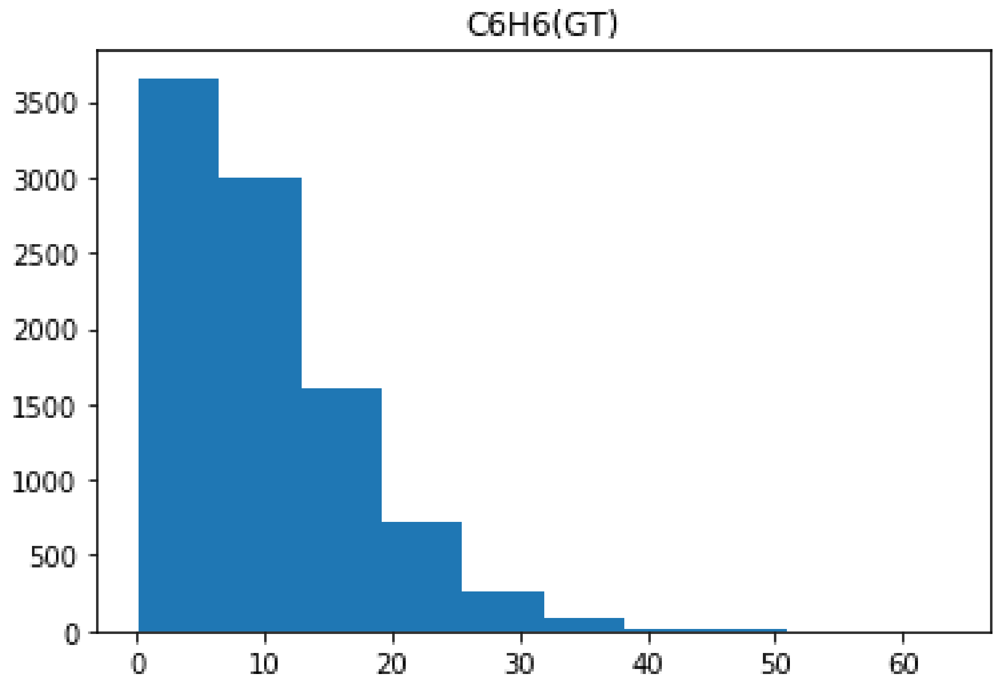
[27]:
```python
columns = list(airq.columns)

columns[1:]
```

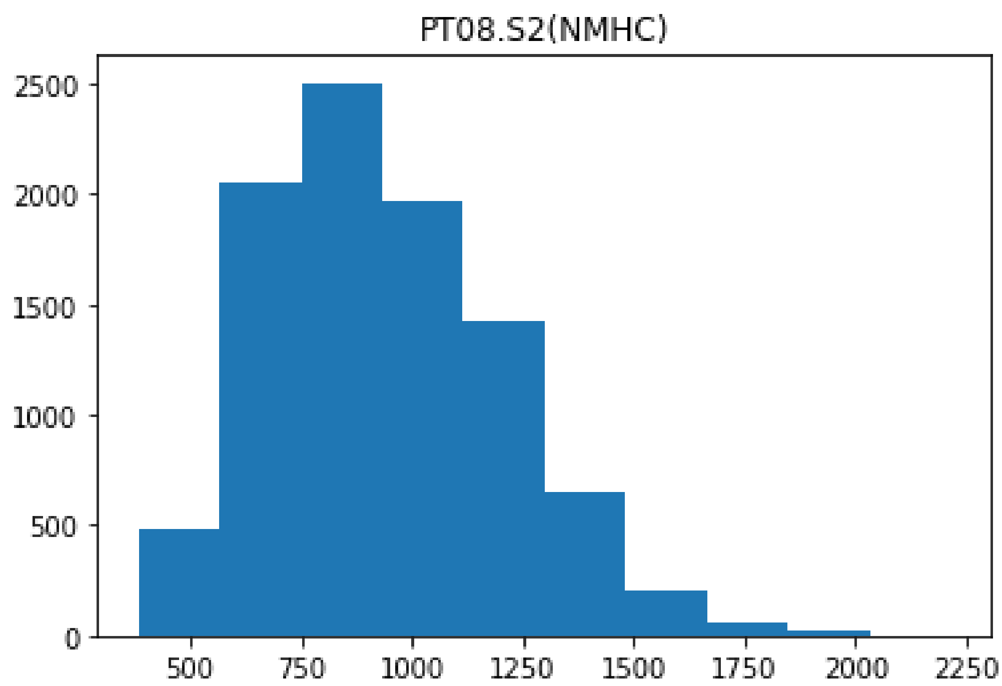
[27]:
```
['CO(GT)',
 'PT08.S1(CO)',
 'C6H6(GT)',
 'PT08.S2(NMHC)',
 'NOx(GT)',
 'PT08.S3(NOx)',
 'NO2(GT)',
 'PT08.S4(NO2)',
 'PT08.S5(O3)',
 'T',
 'RH',
 'AH']
```

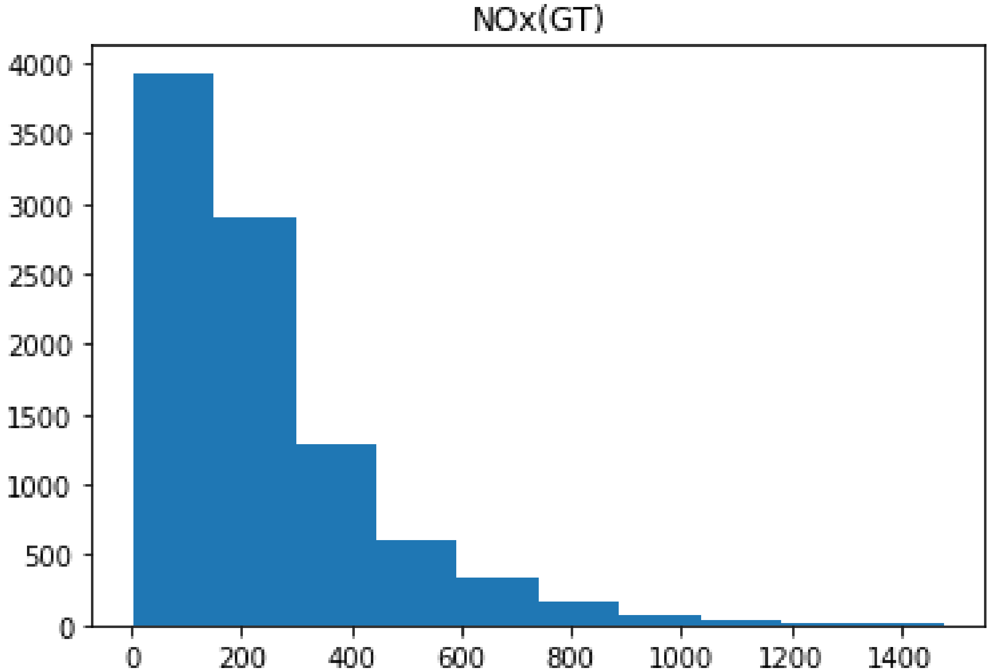
[28]:
```python
for col in columns[1:]:
    plt.hist(airq[col])
    plt.title(col)
    plt.show()
```

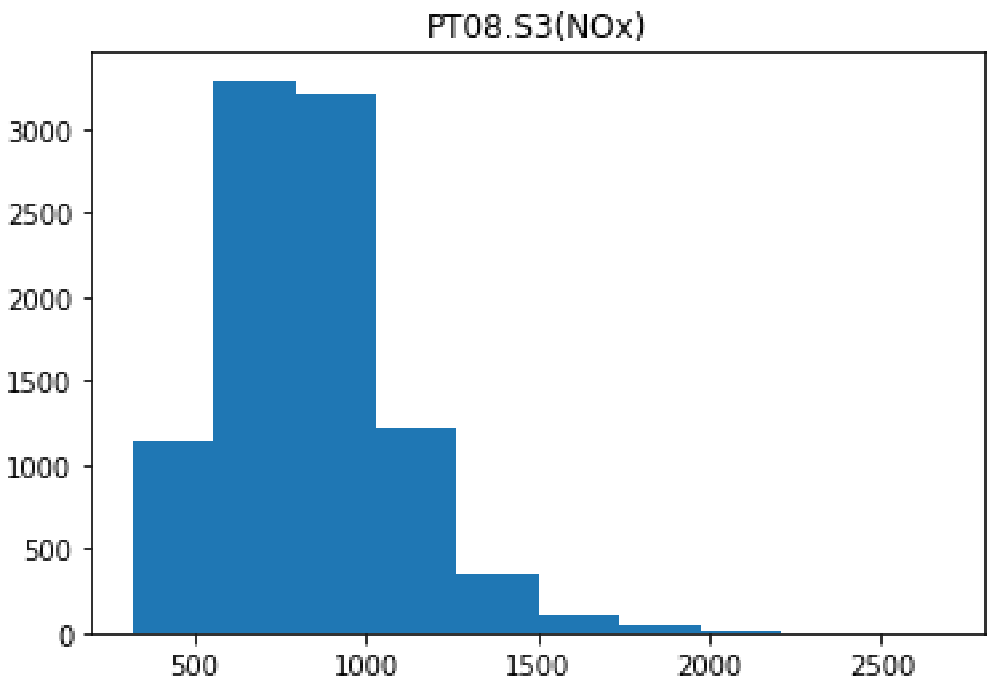

CO(GT)
3500
3000
2500
2000
1500
1000
500
0
0
2
4
6
8
10
12

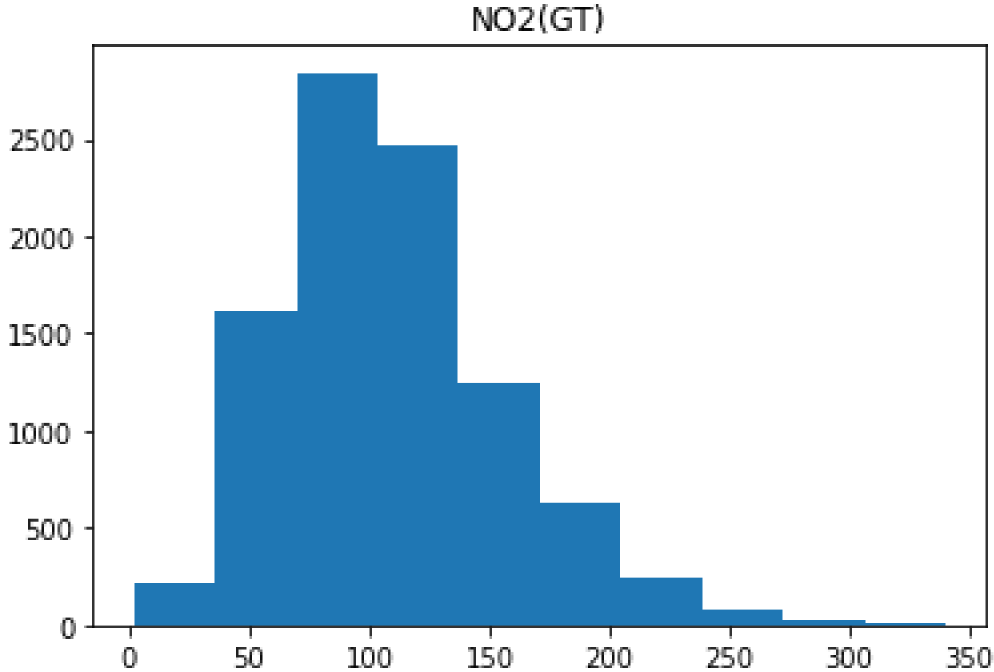

PT08.S1(CO)
2500
2000
1500
1000
500
0
600
800
1000
1200
1400
1600
1800
2000

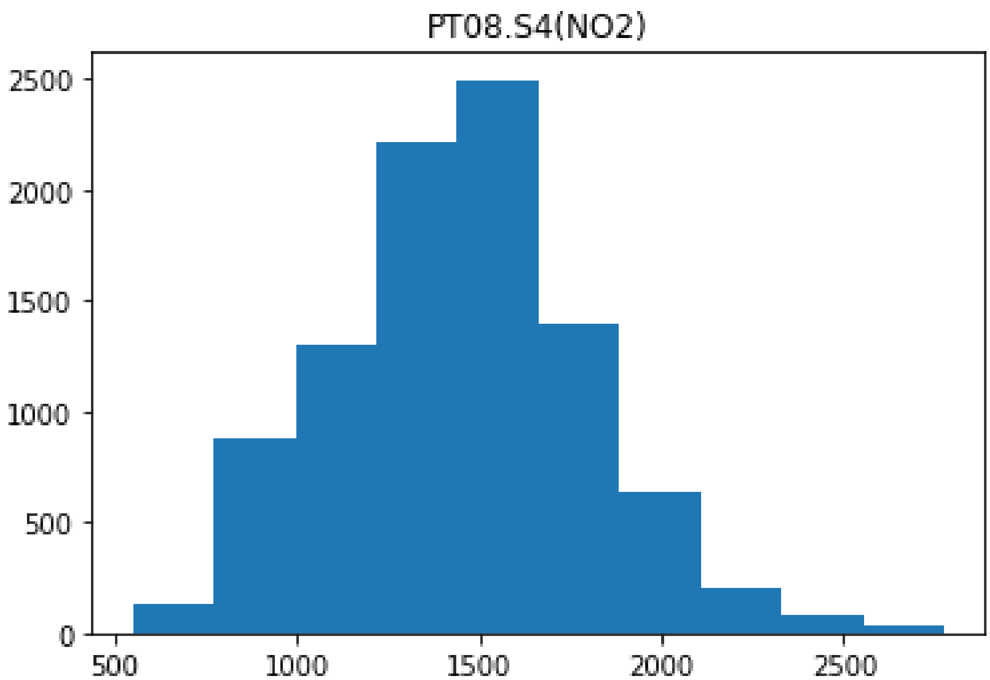

C6H6(GT)
3500
3000
2500
2000
1500
1000
500
0
0
10
20
30
40
50
60

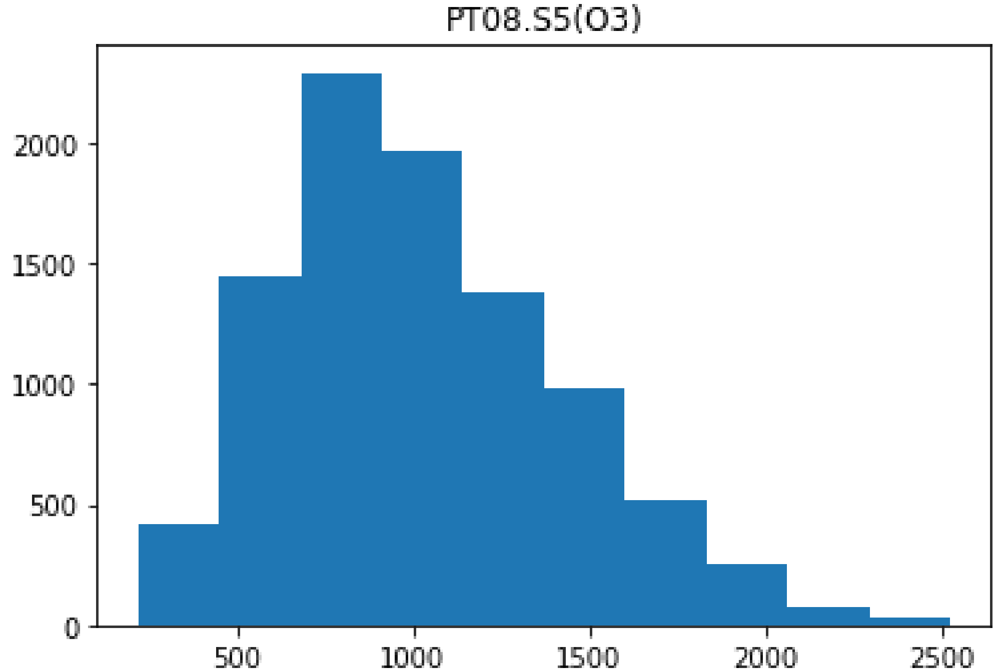

PT08.S2(NMHC)
2500
2000
1500
1000
500
0
500
750
1000
1250
1500
1750
2000
2250

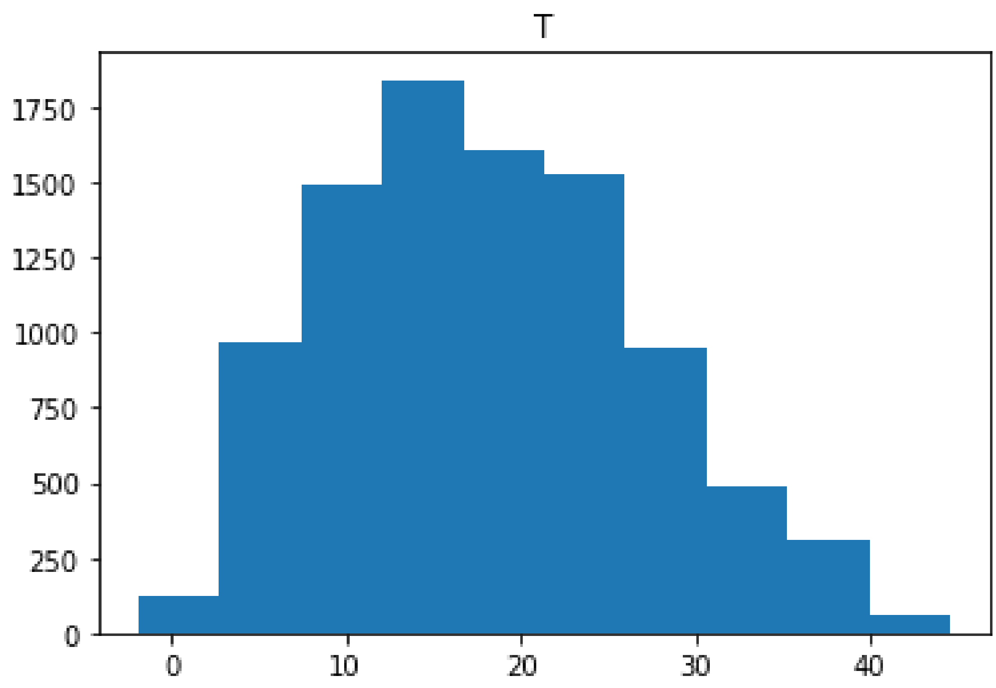

NOx(GT)
4000
3500
3000
2500
2000
1500
1000
500
0
0
200
400
600
800
1000
1200
1400

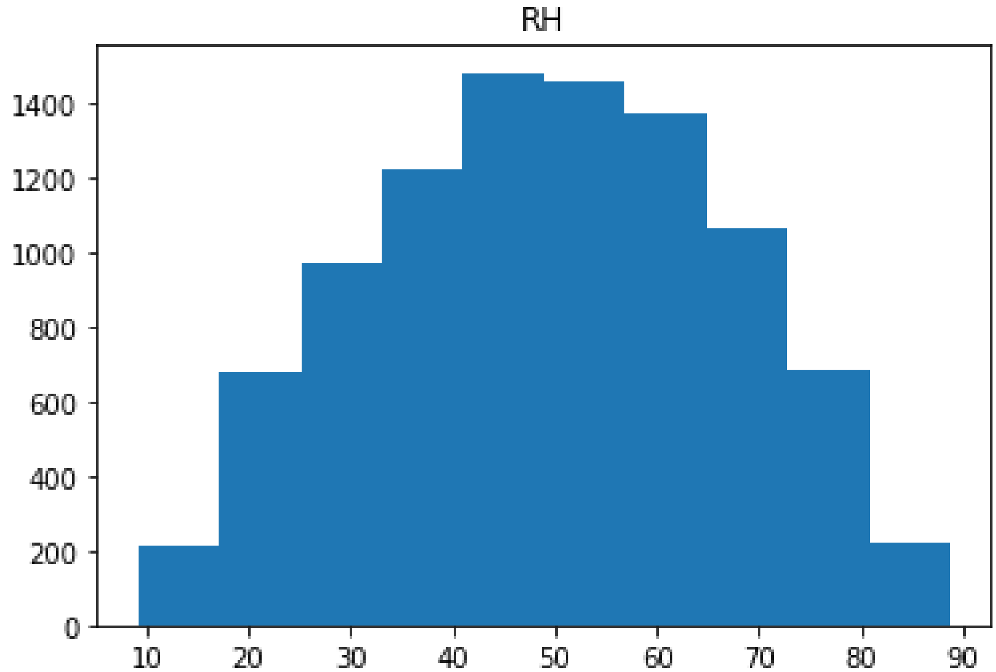

PT08.S3(NOx)
3000
2500
2000
1500
1000
500
0
500
1000
1500
2000
2500

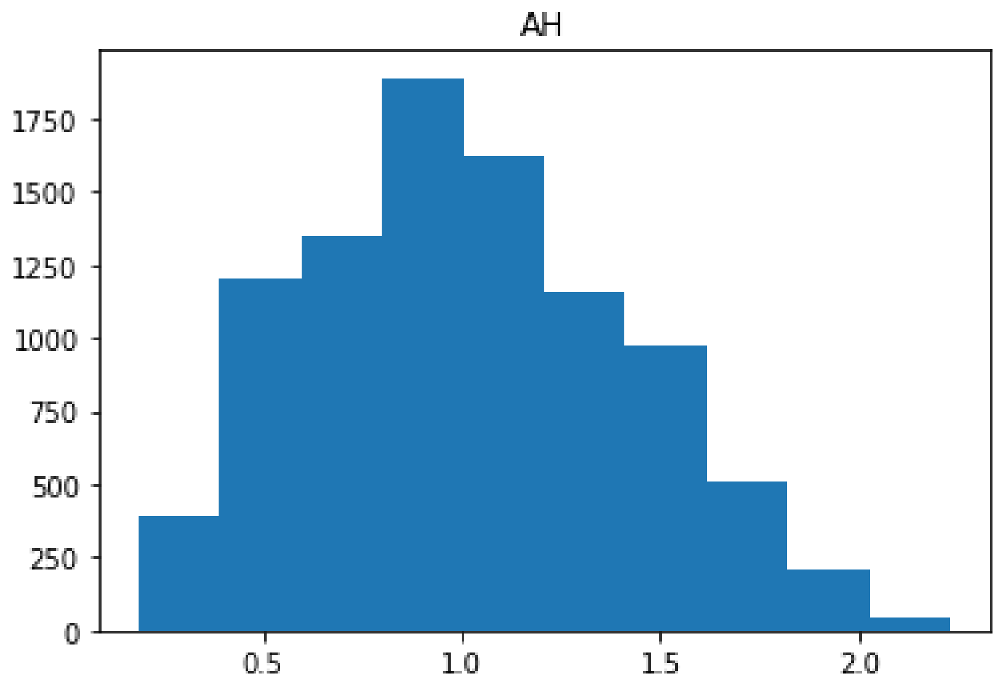

NO2(GT)
2500
2000
1500
1000
500
0
0
50
100
150
200
250
300
350


PT08.S4(NO2)
2500
2000
1500
1000
500
0
500
1000
1500
2000
2500


PT08.S5(O3)
2000
1500
1000
500
0
500
1000
1500
2000
2500


T
1750
1500
1250
1000
750
500
250
0
0
10
20
30
40


RH
1400
1200
1000
800
600
400
200
0
10
20
30
40
50
60
70
80
90

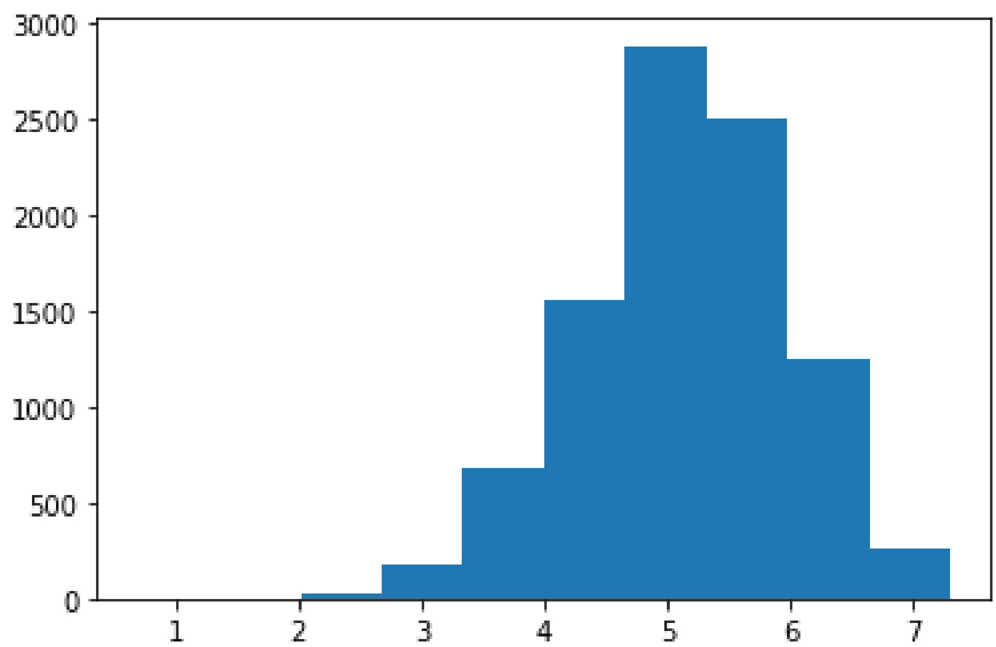

AH
1750
1500
1250
1000
750
500
250
0
0.5
1.0
1.5
2.0

[29]:

```
# Log-transform the skewed features

plt.hist(airq['NOx(GT)'].apply(lambda x: np.log(x)))
```

[29]:

```
(array([1.000e+00, 3.000e+00, 2.300e+01, 1.850e+02, 6.860e+02, 1.556e+03,
        2.882e+03, 2.504e+03, 1.255e+03, 2.620e+02]),
 array([0.69314718, 1.35374461, 2.01434204, 2.67493947, 3.33553689,
        3.99613432, 4.65673175, 5.31732918, 5.97792661, 6.63852403,
        7.29912146]),
 <BarContainer object of 10 artists>)
```

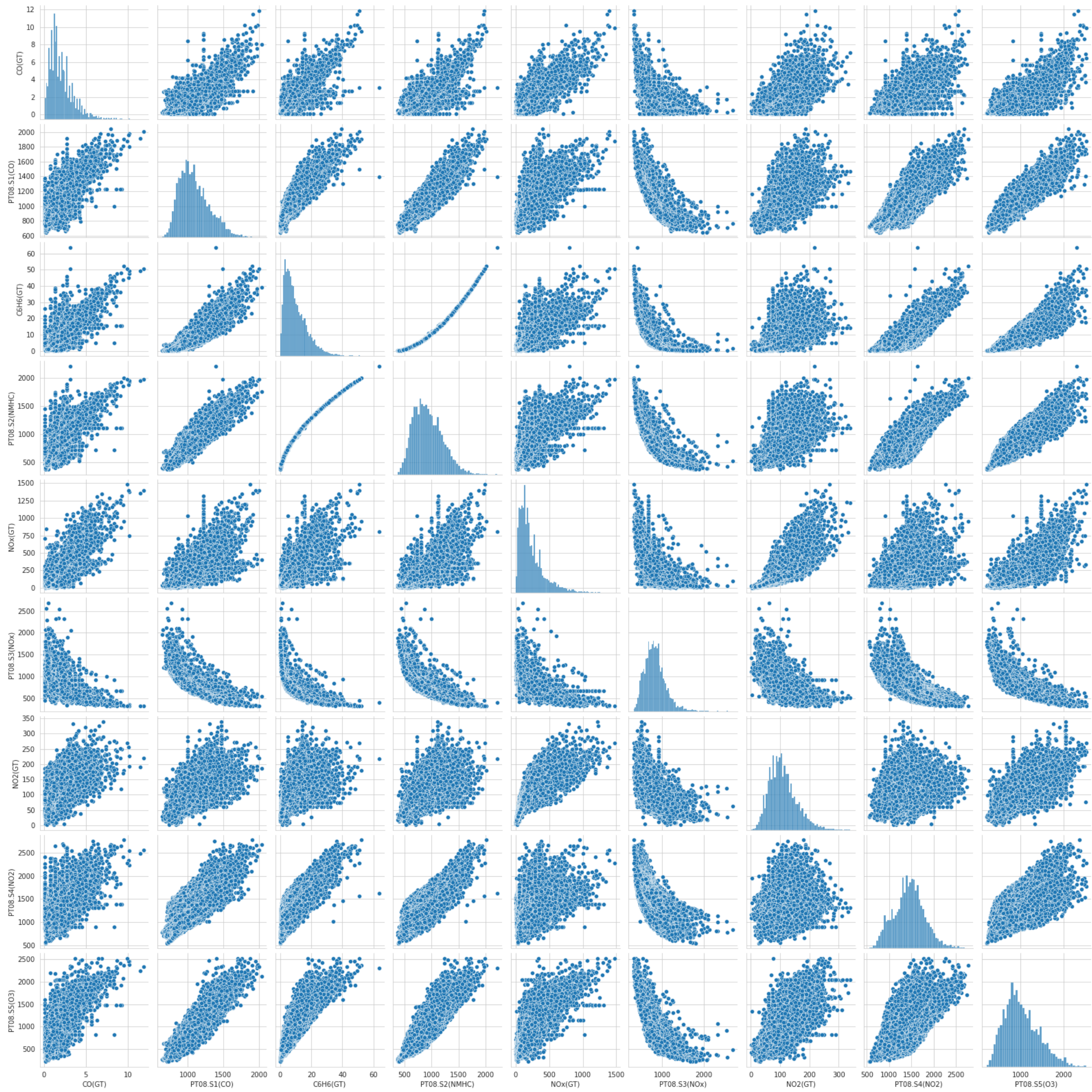


[30]:

```
sns.set_style('whitegrid')
eda_air = airq.drop(['Time','RH','AH','T'], axis=1)
sns.pairplot(eda_air)
```

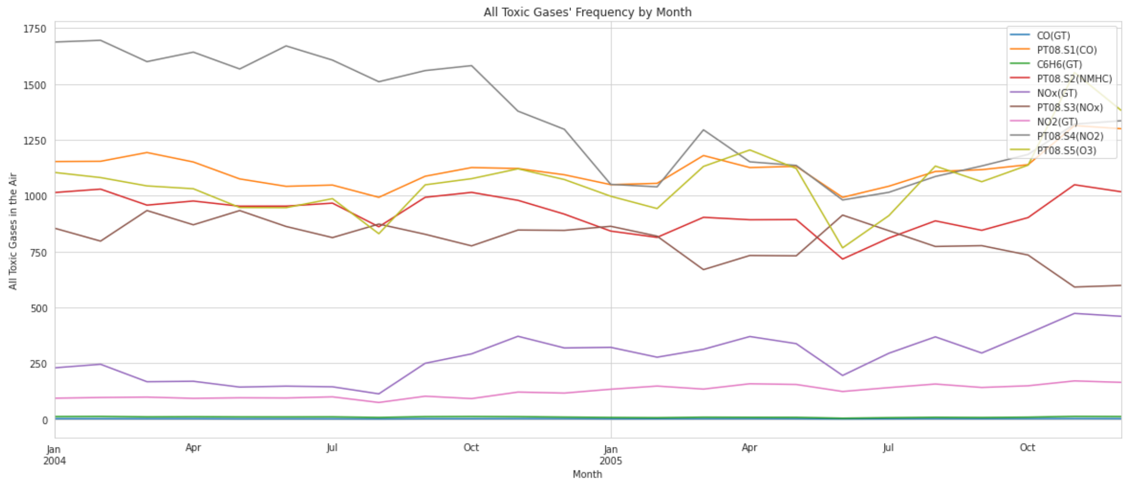
[30]:

```
<seaborn.axisgrid.PairGrid at 0x7fbcce527b20>
```



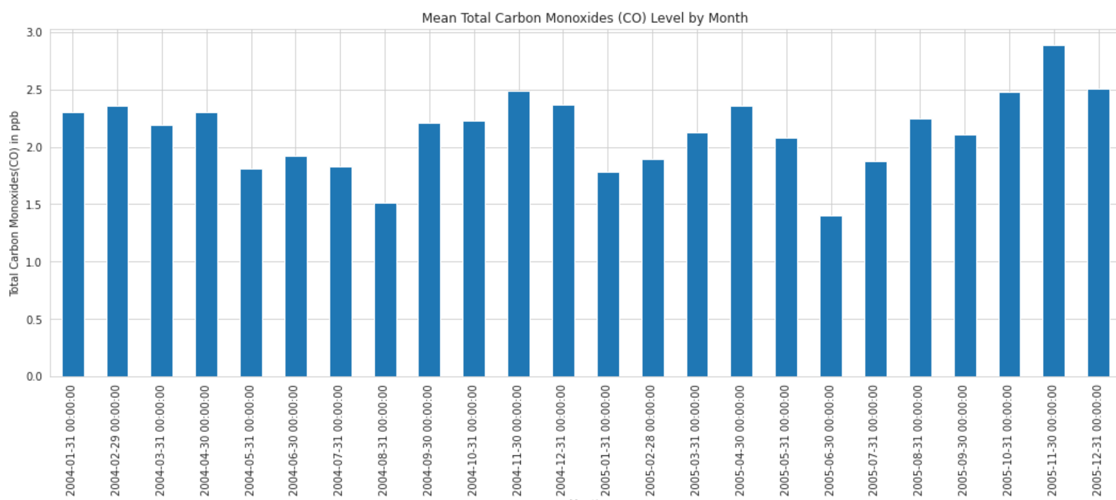
[31]:

```
airq.drop(['Time','RH','AH','T'], axis=1).resample('M').mean().plot(figsize =(20,8))
plt.legend(loc=1)
plt.xlabel('Month')
plt.ylabel('All Toxic Gases in the Air')
plt.title("All Toxic Gases' Frequency by Month");
```



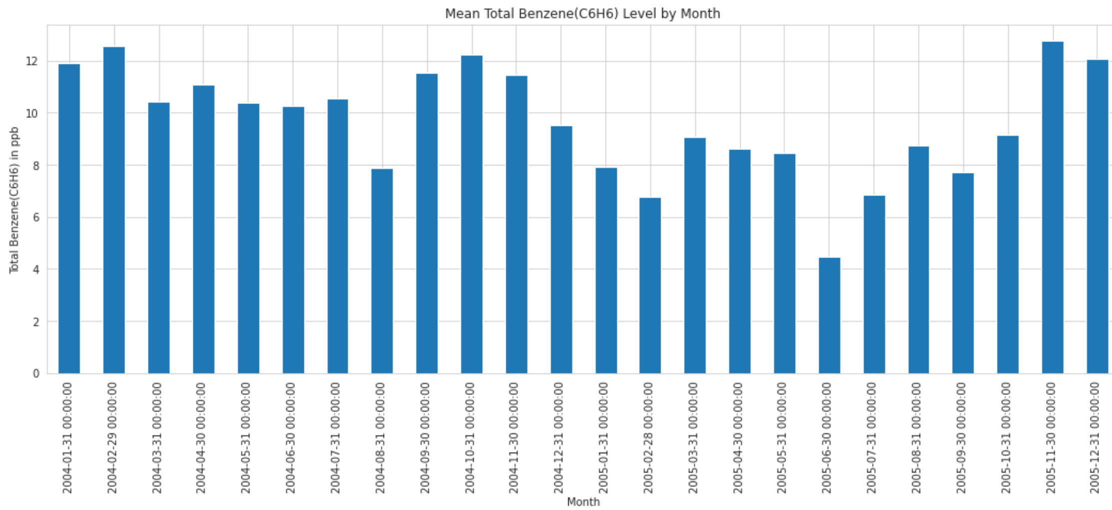

```
[32]: airq['CO(GT)'].resample('M').mean().plot(kind='bar', figsize=(18,6))
      plt.xlabel('Month')
      plt.ylabel('Total Carbon Monoxides(CO) in ppb')    # Parts per billion (ppb)
      plt.title("Mean Total Carbon Monoxides (CO) Level by Month")
```

```
[32]: Text(0.5, 1.0, 'Mean Total Carbon Monoxides (CO) Level by Month')
```



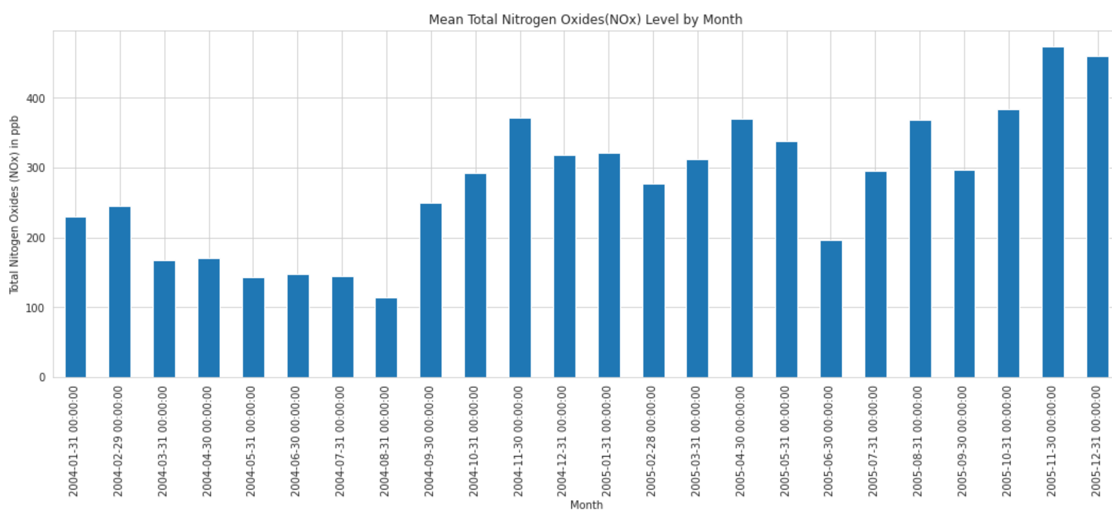

```
[33]: airq['C6H6(GT)'].resample('M').mean().plot(kind='bar', figsize=(18,6))
      plt.xlabel('Month')
      plt.ylabel('Total Benzene(C6H6) in ppb')    # Parts per billion (ppb)
      plt.title("Mean Total Benzene(C6H6) Level by Month")
```

```
[33]: Text(0.5, 1.0, 'Mean Total Benzene(C6H6) Level by Month')
```



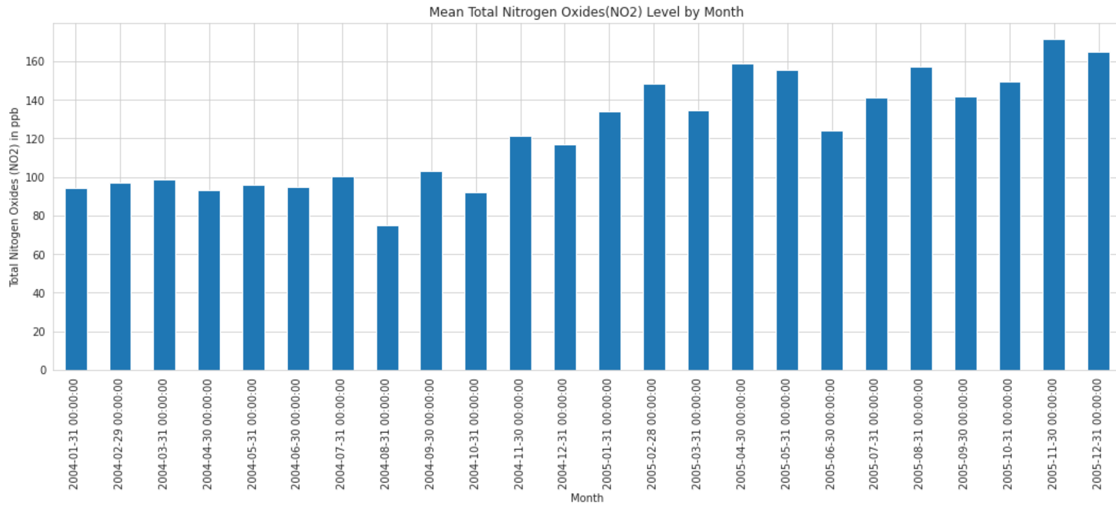
[34]:
```python
airq['NOx(GT)'].resample('M').mean().plot(kind='bar', figsize=(18,6))
plt.xlabel('Month')
plt.ylabel('Total Nitogen Oxides (NOx) in ppb')   # Parts per billion (ppb)
plt.title("Mean Total Nitrogen Oxides(NOx) Level by Month")
```

[34]: Text(0.5, 1.0, 'Mean Total Nitrogen Oxides(NOx) Level by Month')



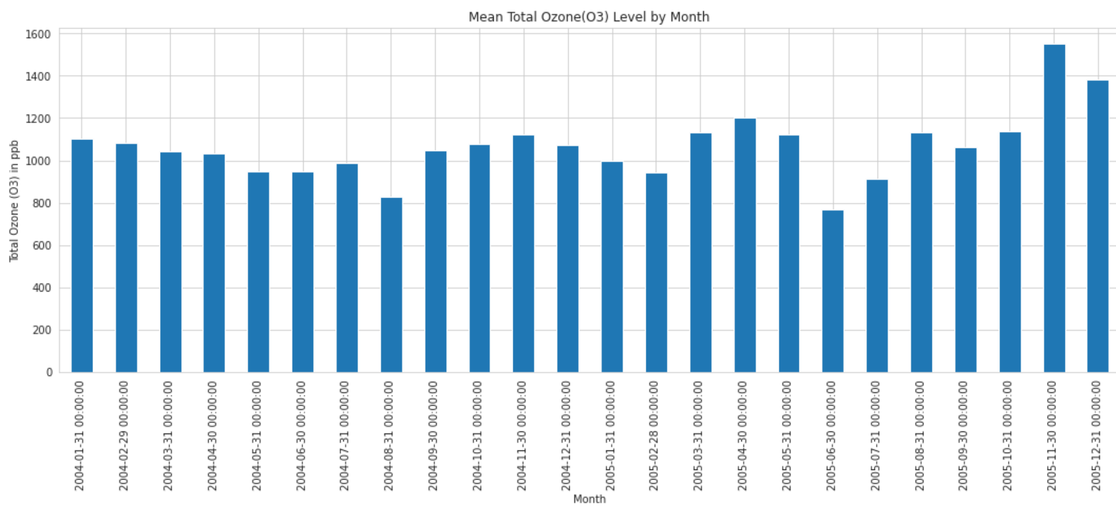
[35]:
```python
airq['NO2(GT)'].resample('M').mean().plot(kind='bar', figsize=(18,6))
plt.xlabel('Month')
plt.ylabel('Total Nitogen Oxides (NO2) in ppb')   # Parts per billion (ppb)
plt.title("Mean Total Nitrogen Oxides(NO2) Level by Month")
```

[35]: Text(0.5, 1.0, 'Mean Total Nitrogen Oxides(NO2) Level by Month')



[36]:
```python
airq['PT08.S5(O3)'].resample('M').mean().plot(kind='bar', figsize=(18,6))
plt.xlabel('Month')
plt.ylabel('Total Ozone (O3) in ppb')    # Parts per billion (ppb)
plt.title("Mean Total Ozone(O3) Level by Month")
```

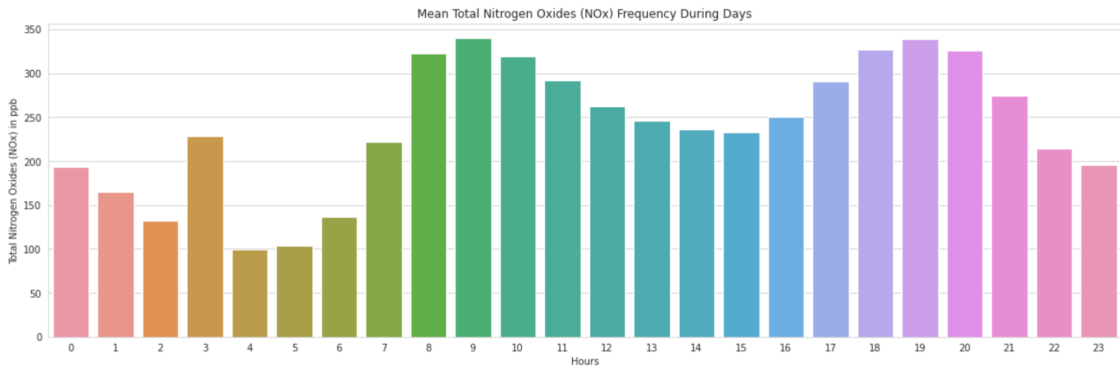
[36]: Text(0.5, 1.0, 'Mean Total Ozone(O3) Level by Month')



[37]:
```python
plt.figure(figsize=(20,6))
sns.barplot(x='Time',y='NOx(GT)',data=airq, ci=False)
plt.xlabel('Hours')
```

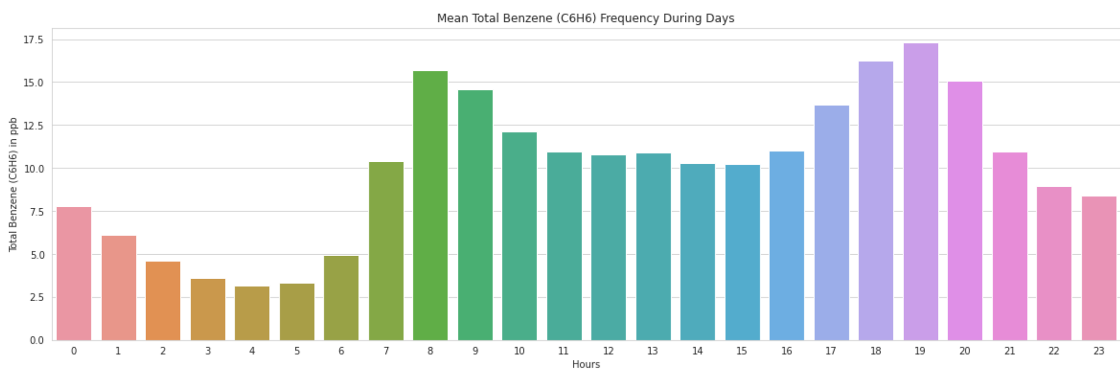
```
plt.ylabel('Total Nitrogen Oxides (NOx) in ppb') # Parts per billion (ppb)
plt.title("Mean Total Nitrogen Oxides (NOx) Frequency During Days")
```

[37]: Text(0.5, 1.0, 'Mean Total Nitrogen Oxides (NOx) Frequency During Days')



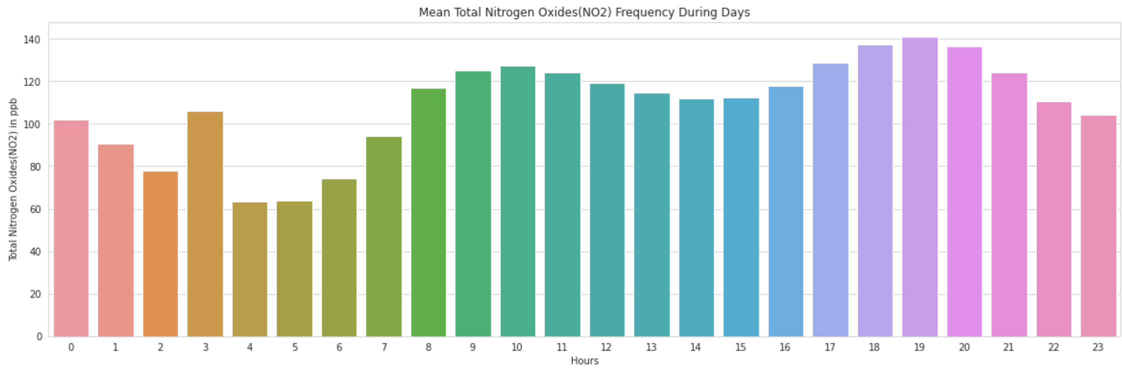
[38]:
```
plt.figure(figsize=(20,6))
sns.barplot(x='Time',y='C6H6(GT)',data=airq, ci=False)
plt.xlabel('Hours')
plt.ylabel('Total Benzene (C6H6) in ppb') # Parts per billion (ppb)
plt.title("Mean Total Benzene (C6H6) Frequency During Days")
```

[38]: Text(0.5, 1.0, 'Mean Total Benzene (C6H6) Frequency During Days')



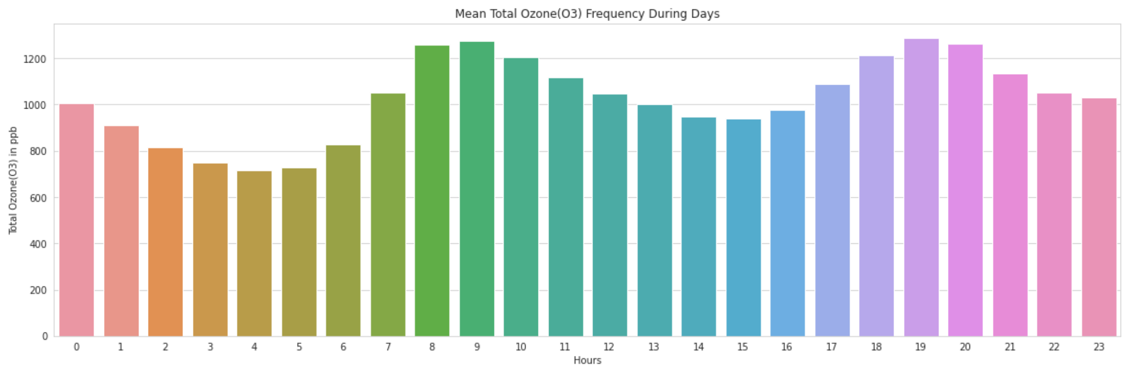
[39]:
```
plt.figure(figsize=(20,6))
sns.barplot(x='Time',y='NO2(GT)',data=airq, ci=False)
plt.xlabel('Hours')
plt.ylabel('Total Nitrogen Oxides(NO2) in ppb') # Parts per billion (ppb)
plt.title("Mean Total Nitrogen Oxides(NO2) Frequency During Days")
```

[39]: Text(0.5, 1.0, 'Mean Total Nitrogen Oxides(NO2) Frequency During Days')

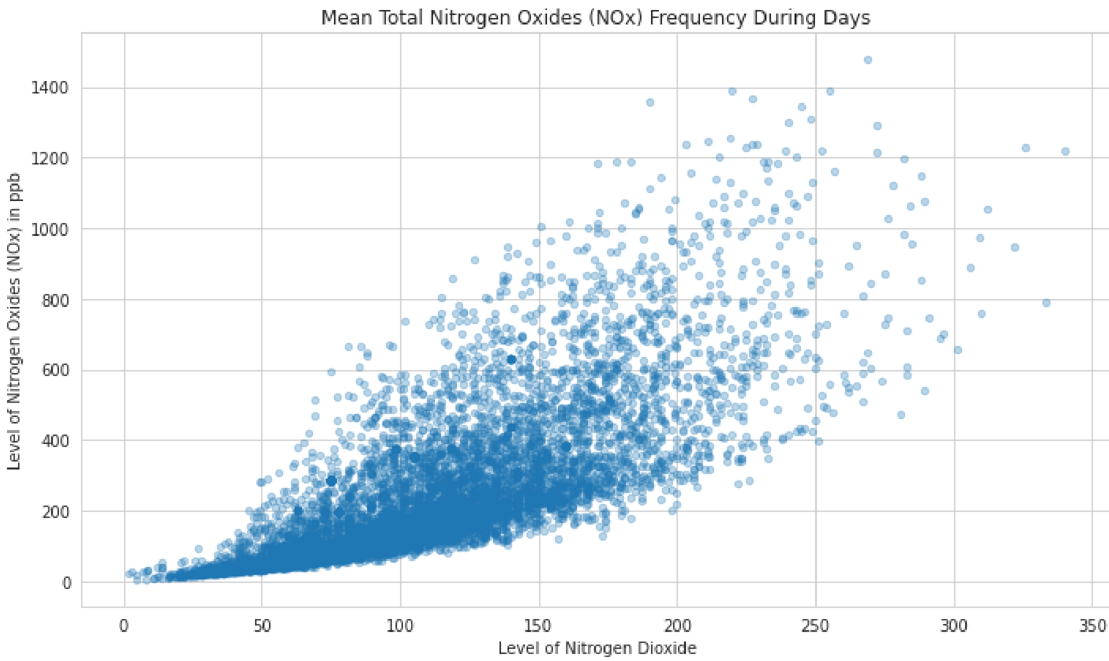


[40]:
```
plt.figure(figsize=(20,6))
sns.barplot(x='Time',y='PT08.S5(O3)',data=airq, ci=False)
plt.xlabel('Hours')
plt.ylabel('Total Ozone(O3) in ppb') # Parts per billion (ppb)
plt.title("Mean Total Ozone(O3) Frequency During Days")
```

[40]: Text(0.5, 1.0, 'Mean Total Ozone(O3) Frequency During Days')

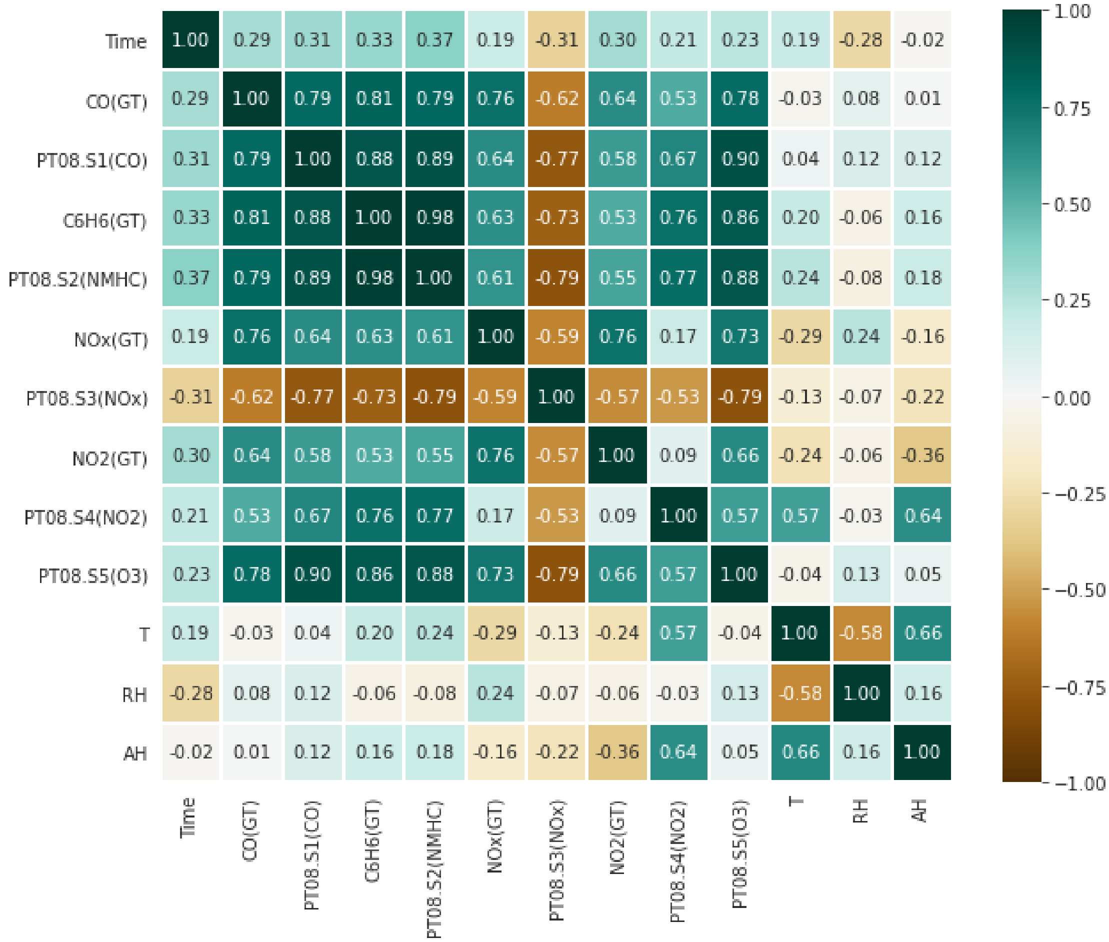


[41]:
```
airq.plot(x='NO2(GT)',y='NOx(GT)', kind='scatter', figsize = (10,6), alpha=0.3)
plt.xlabel('Level of Nitrogen Dioxide')
plt.ylabel('Level of Nitrogen Oxides (NOx) in ppb') # Parts per billion (ppb)
plt.title("Mean Total Nitrogen Oxides (NOx) Frequency During Days")
plt.tight_layout();
```



[42]:
```
corrPearson = airq.corr(method="pearson")


plt.figure(figsize=(10,8))
sns.heatmap(corrPearson,
            annot=True,
            fmt=".2f",
            linewidth=.20,
            cmap='BrBG',
            vmin=-1,
            vmax=+1
           )
```

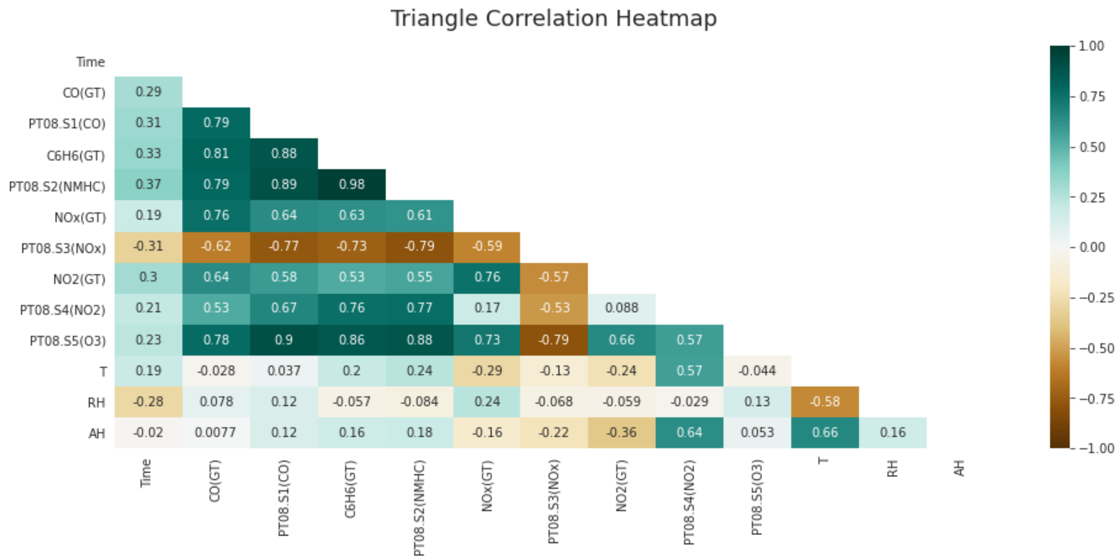
[42]: <AxesSubplot:>



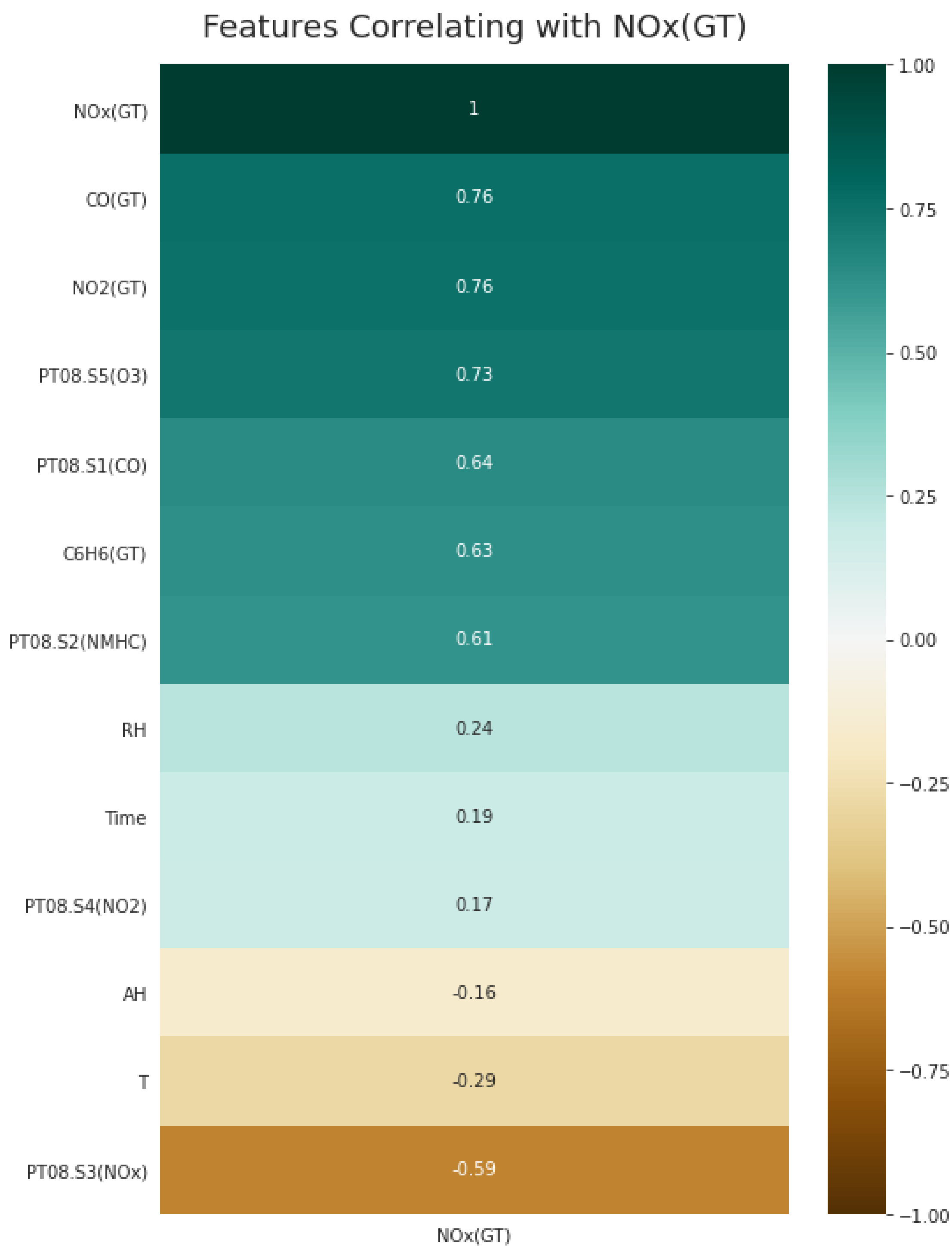
[43]:

```
plt.figure(figsize=(16,6))

mask = np.triu(np.ones_like(corrPearson, dtype=np.bool))

heatmap = sns.heatmap(corrPearson, mask=mask, vmin=-1, vmax=1, annot=True,␣
↪cmap='BrBG')

heatmap.set_title('Triangle Correlation Heatmap', fontdict={'fontsize':18},␣
↪pad=16);
```

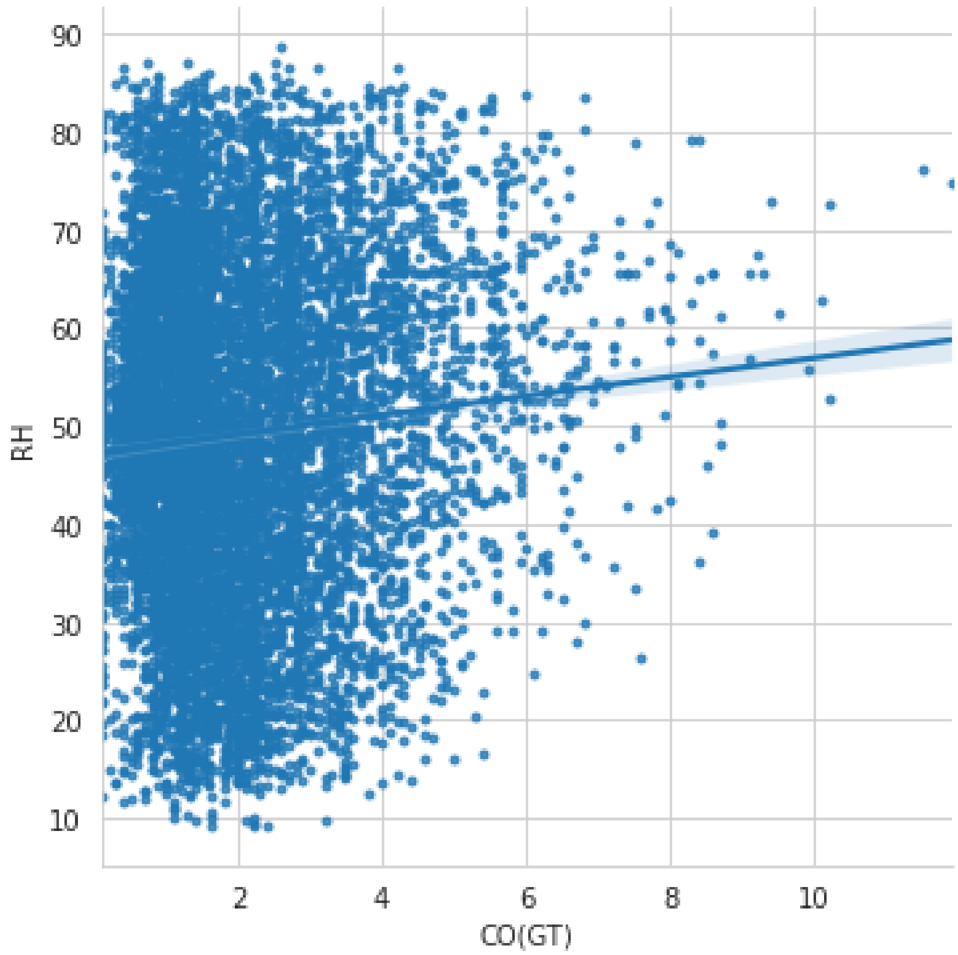
```
<ipython-input-43-b13df2c2b04c>:3: DeprecationWarning: `np.bool` is a deprecated
alias for the builtin `bool`. To silence this warning, use `bool` by itself.
Doing this will not modify any behavior and is safe. If you specifically wanted
the numpy scalar type, use `np.bool_` here.
Deprecated in NumPy 1.20; for more details and guidance:
https://numpy.org/devdocs/release/1.20.0-notes.html#deprecations
  mask = np.triu(np.ones_like(corrPearson, dtype=np.bool))
```



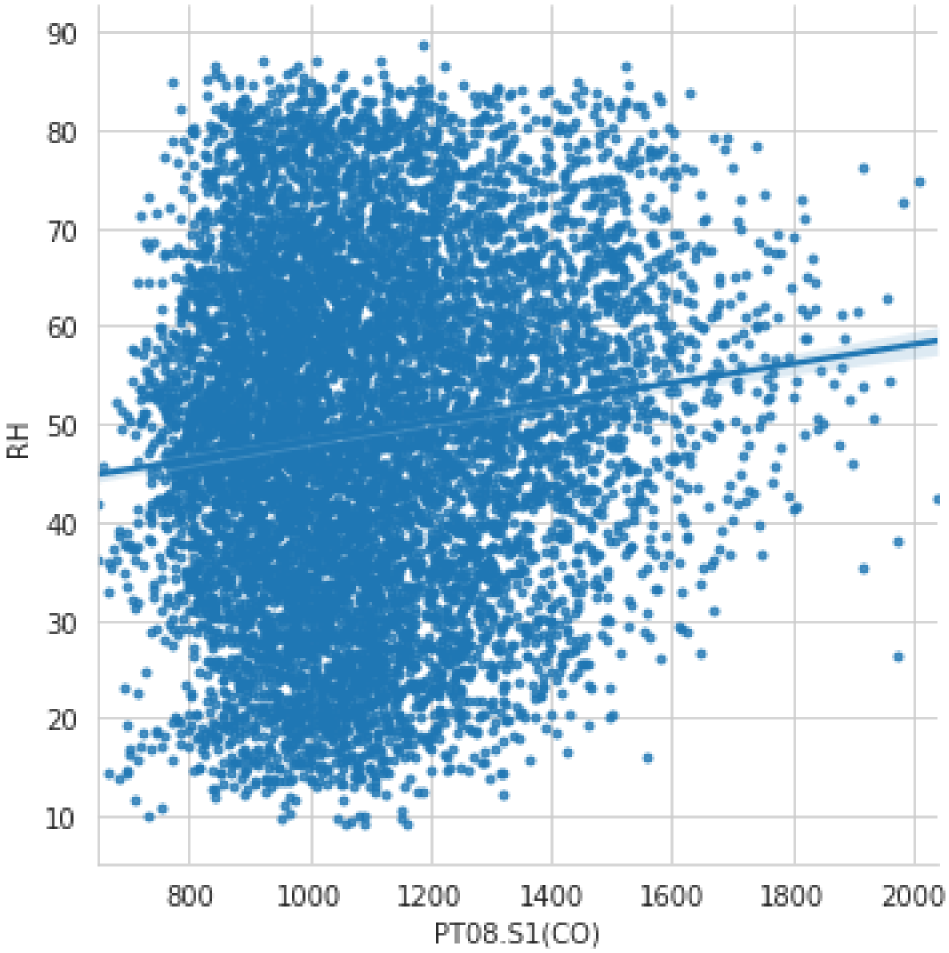
[44]:
```
plt.figure(figsize=(8, 12))
heatmap = sns.heatmap(corrPearson[['NOx(GT)']].sort_values(by='NOx(GT)',␣
↪ascending=False), vmin=-1, vmax=1, annot=True, cmap='BrBG')
heatmap.set_title('Features Correlating with NOx(GT)', fontdict={'fontsize':
↪18}, pad=16);
```

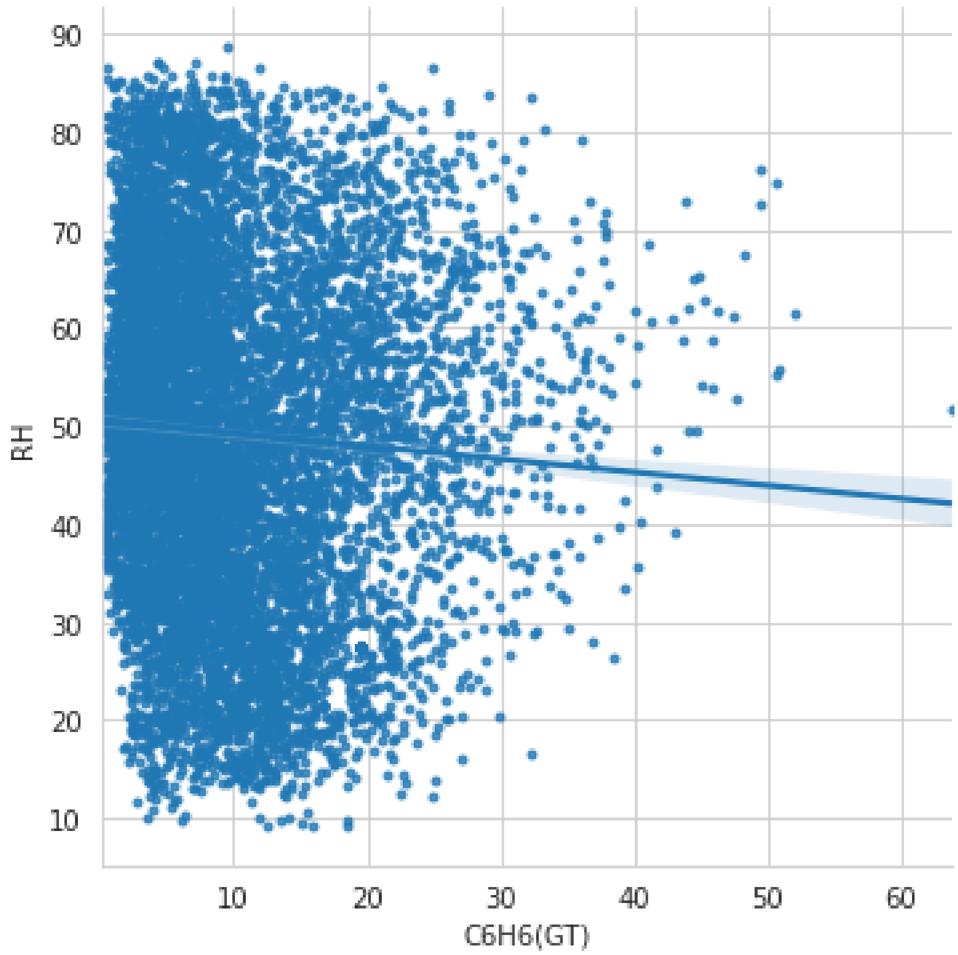


[45]:
```python
column_=airq.columns.tolist()[1:]
for i in airq.columns.tolist()[1:]:
    sns.lmplot(x=i,y='RH',data=airq,markers='.')
```

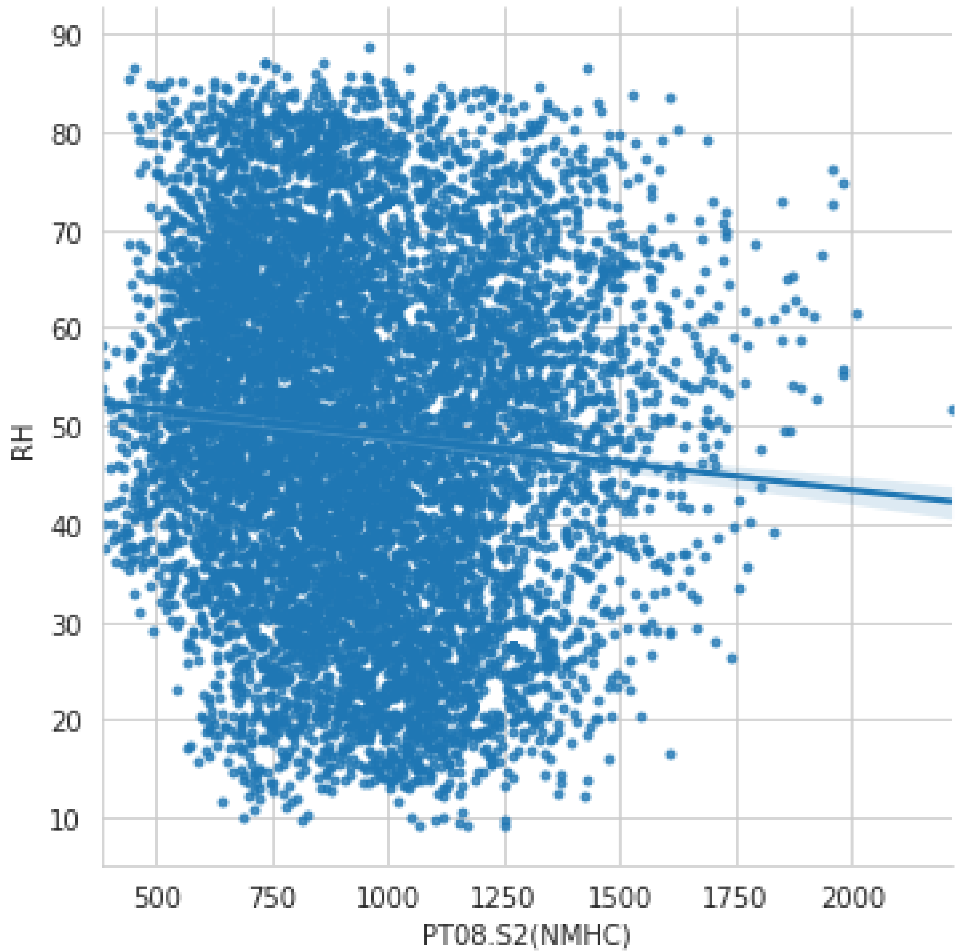


90
80
70
60
50
40
30
20
10
RH
2
4
6
8
10
CO(GT)

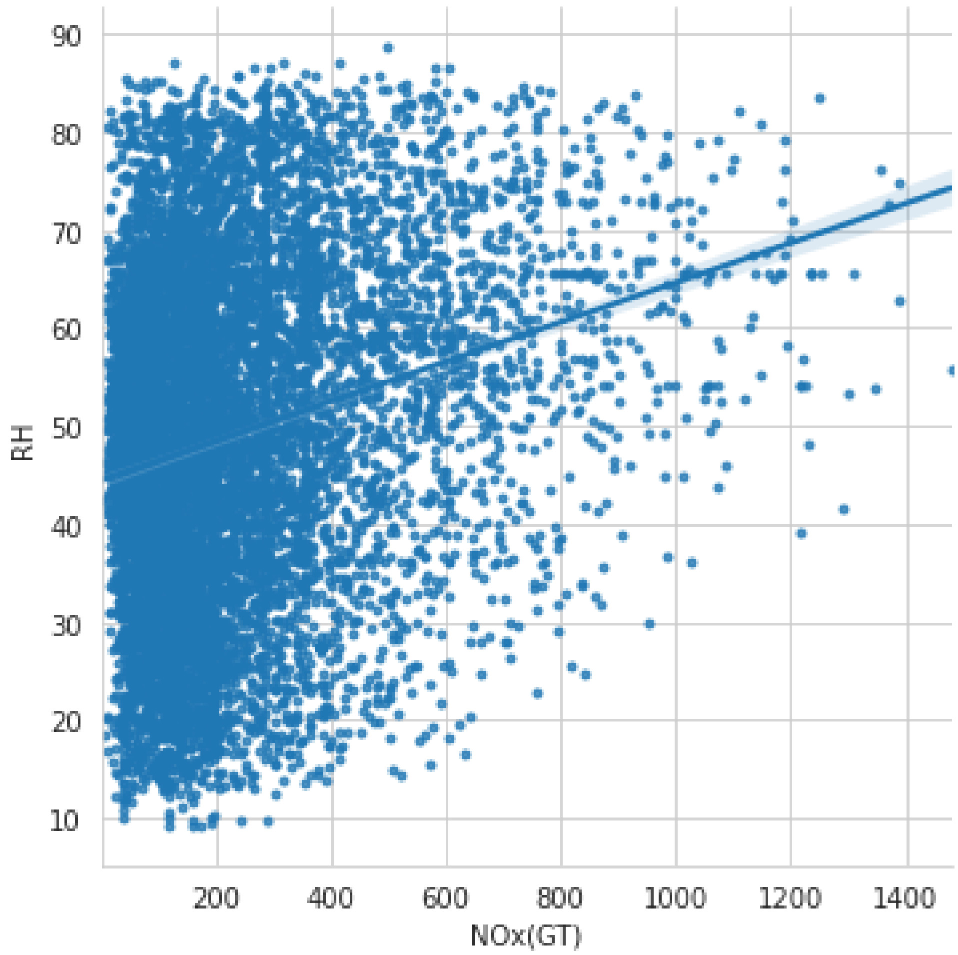

90
80
70
60
50
40
30
20
10
RH
800
1000
1200
1400
1600
1800
2000
PT08.S1(CO)

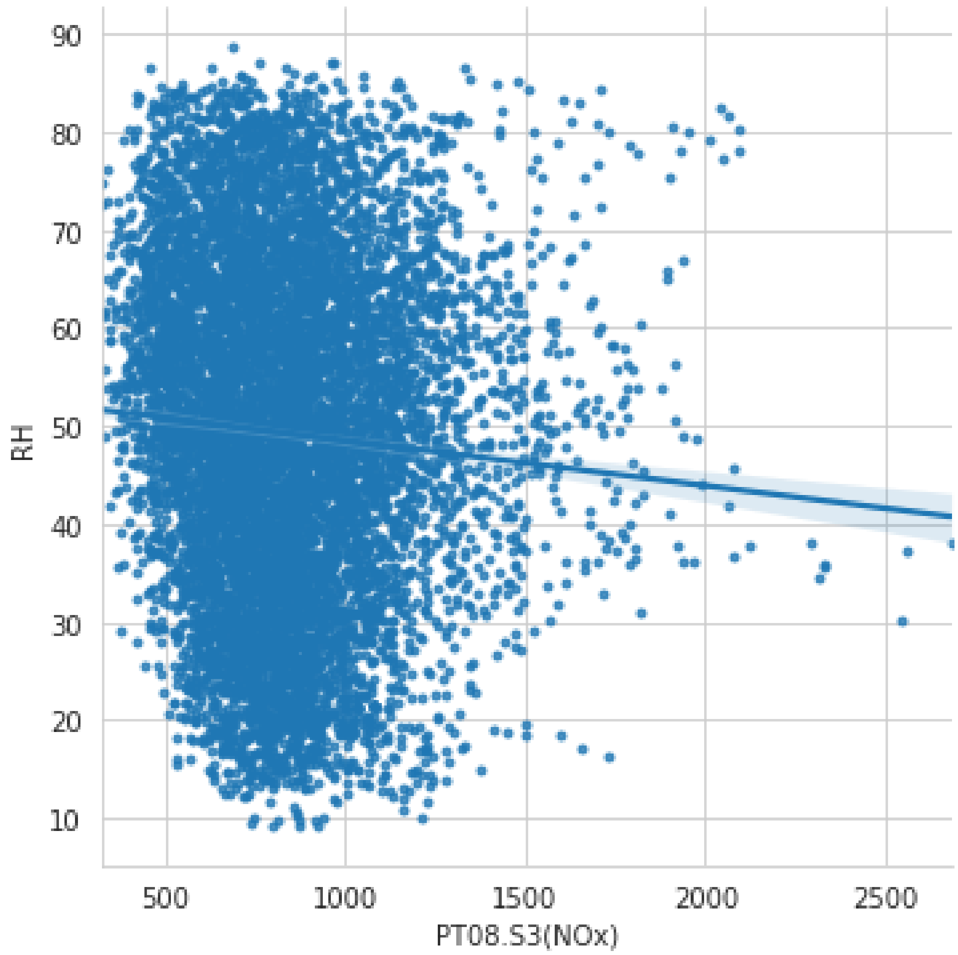


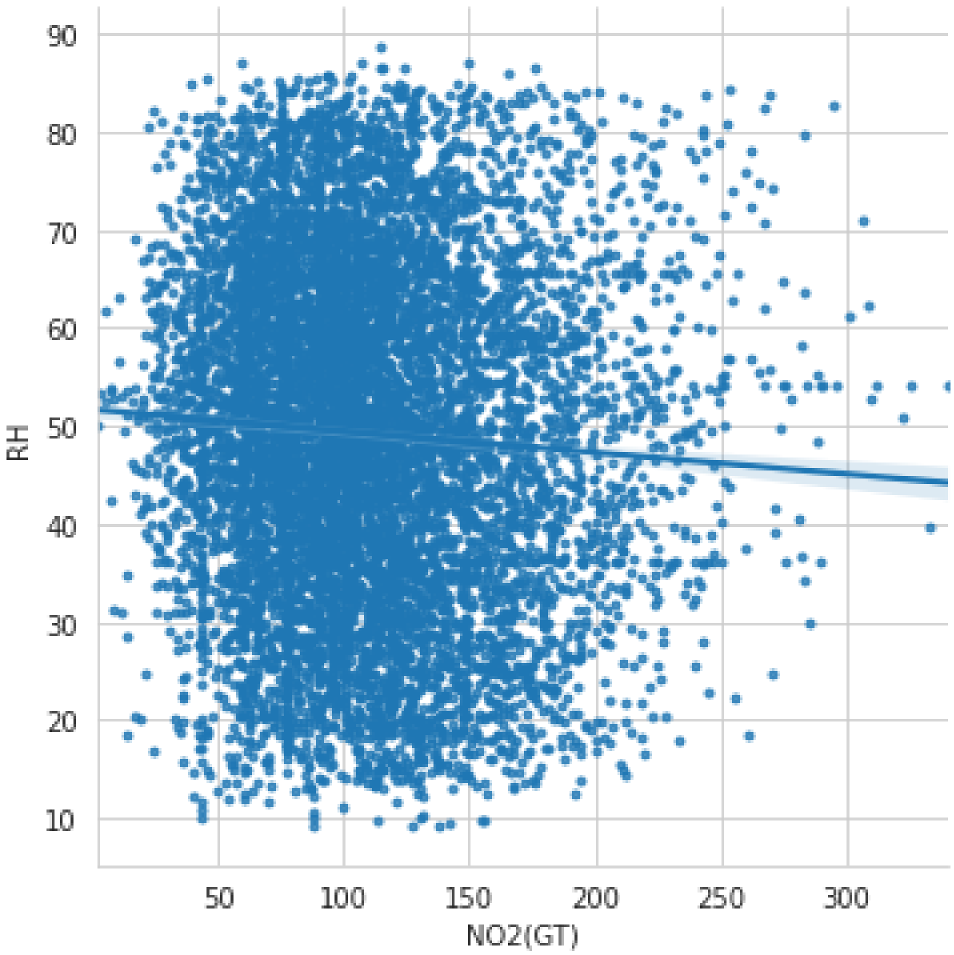
90
80
70
60
50
40
30
20
10
RH
10
20
30
40
50
60
C6H6(GT)



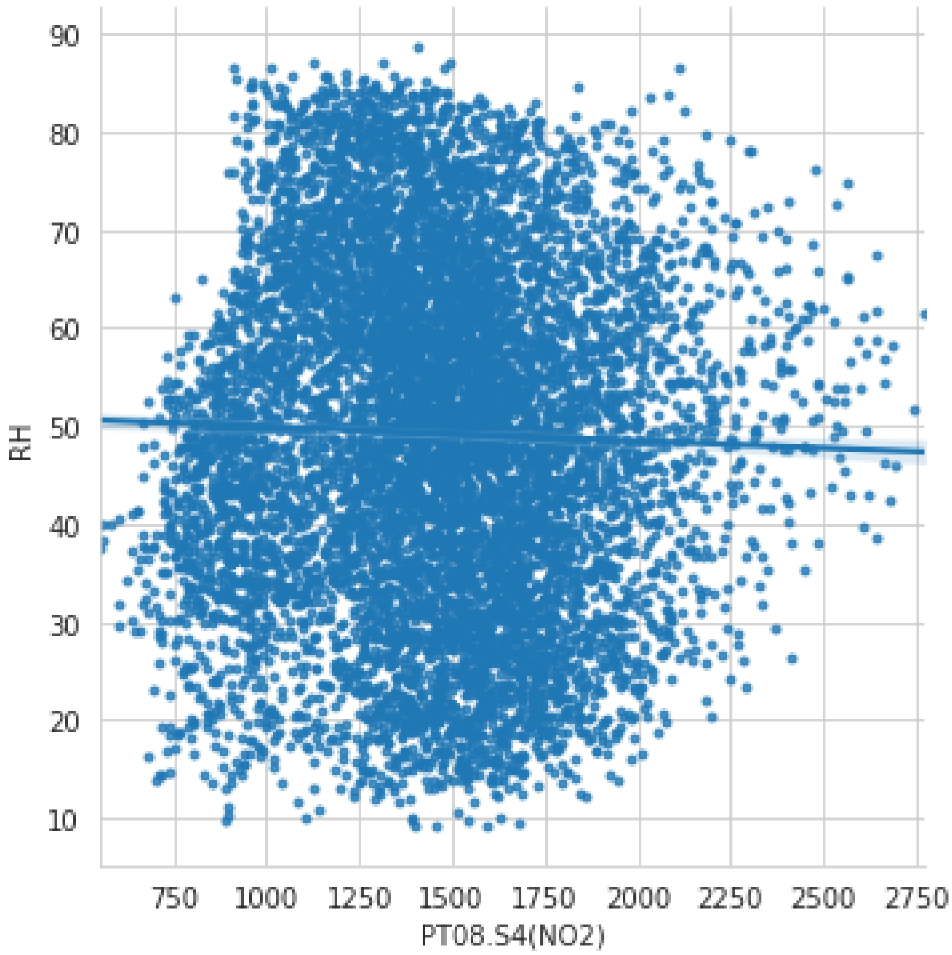
90
80
70
60
50
40
30
20
10
RH
500
750
1000
1250
1500
1750
2000
PT08.S2(NMHC)

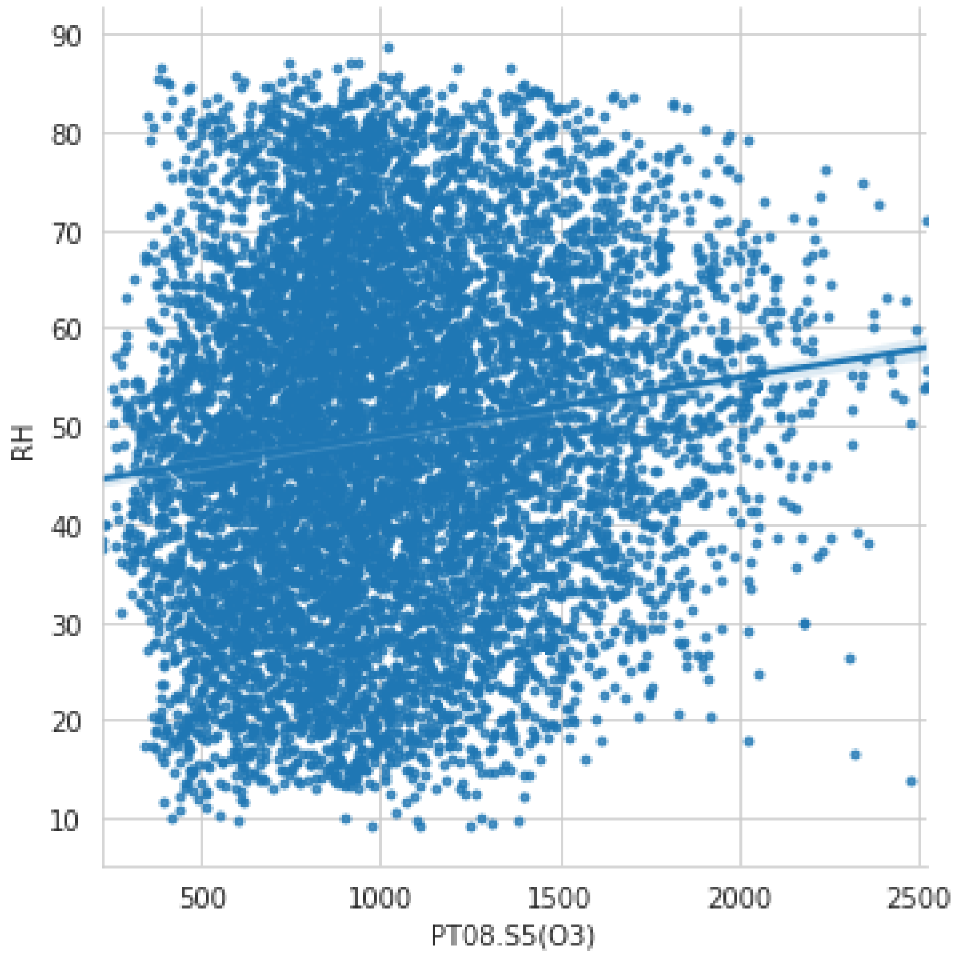

90
80
70
60
50
40
30
20
10
RH
200
400
600
800
1000
1200
1400
NOx(GT)

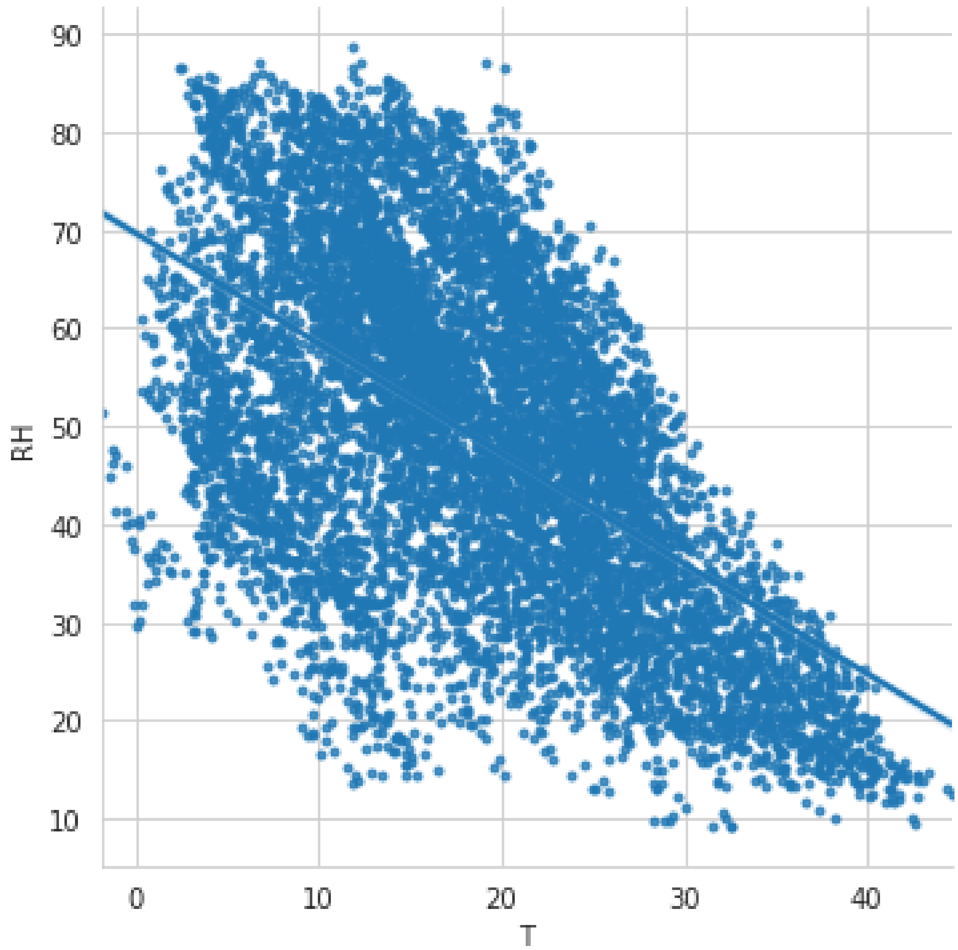

90
80
70
60
50
40
30
20
10
RH
500
1000
1500
2000
2500
PT08.S3(NOx)



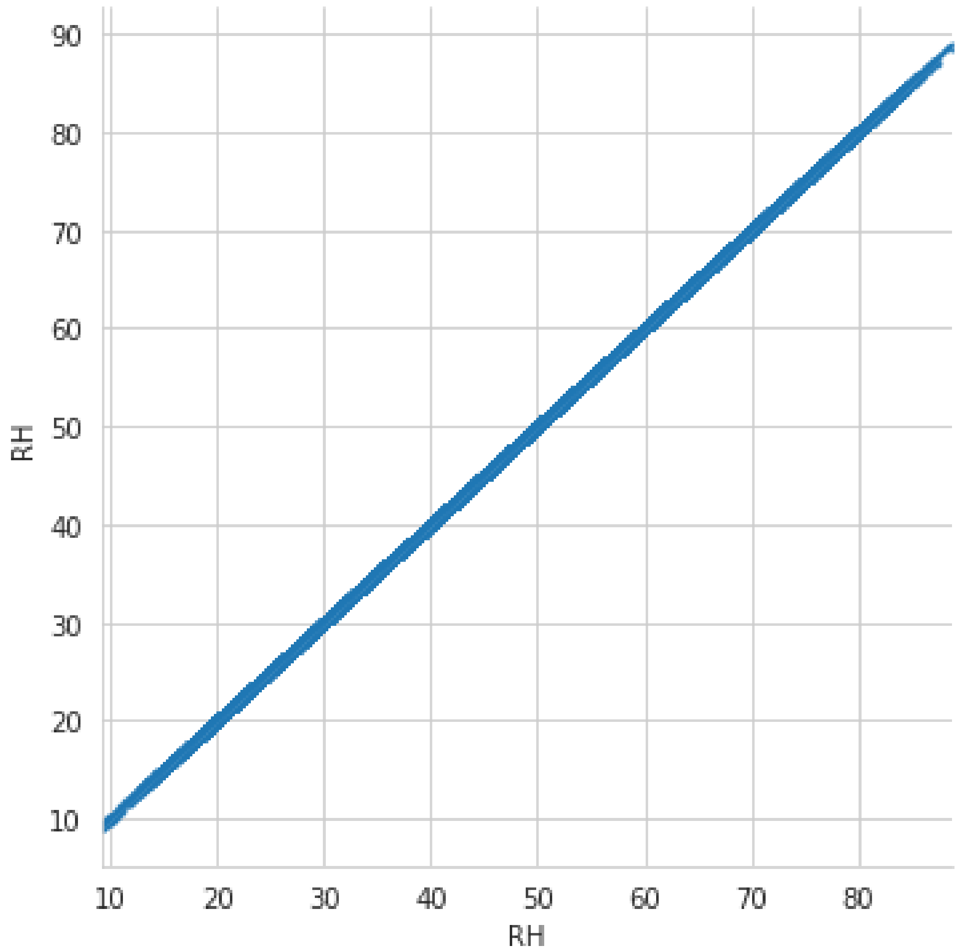
90
80
70
60
50
40
30
20
10
RH
50
100
150
200
250
300
NO2(GT)

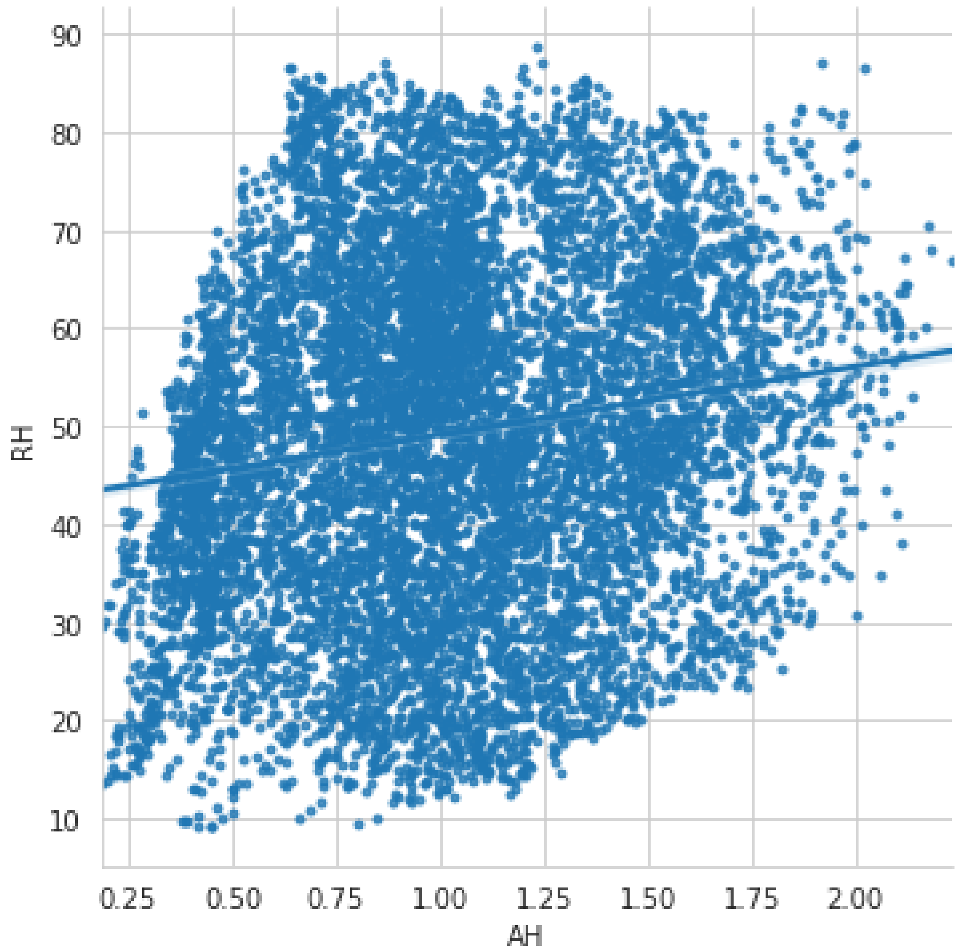

90
80
70
60
50
40
30
20
10
RH
750
1000
1250
1500
1750
2000
2250
2500
2750
PT08.S4(NO2)


RH
PT08.S5(O3)



90
80
70
60
50
40
30
20
10
RH
0
10
20
30
40
T


90
80
70
60
50
40
30
20
10
RH
10
20
30
40
50
60
70
80
RH



1.5 ML Linear, Lasso, Ridge, Elastic Net models

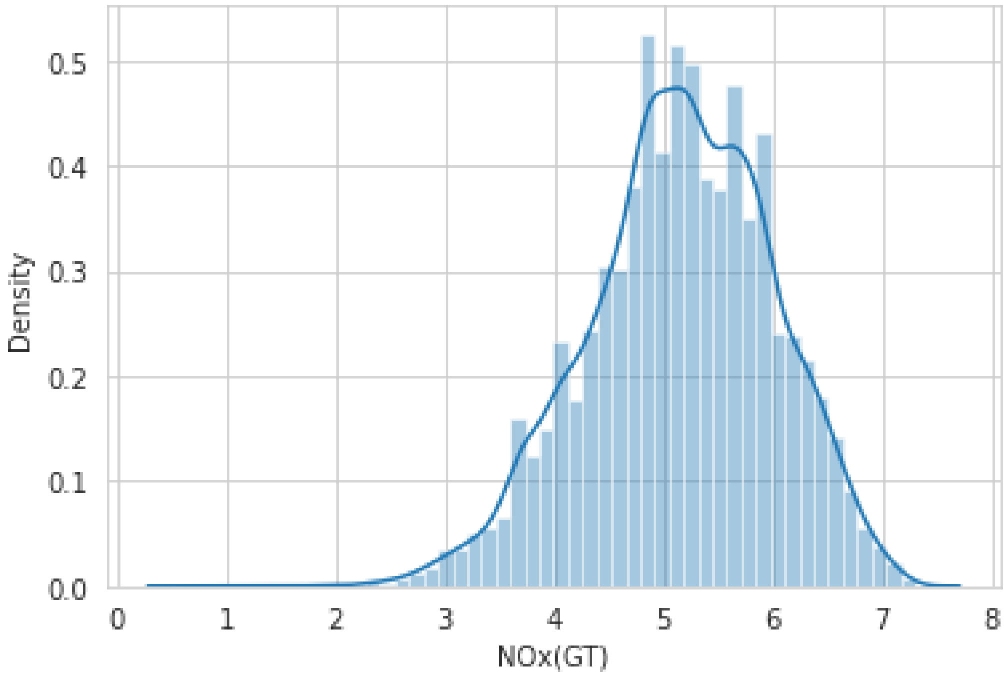
[46]:
```
X = airq.drop(['NOx(GT)','T','Time'], axis=1)

y= airq['NOx(GT)']
```

[47]:
```
X = np.log(X)
y = np.log(y)
```

[48]:
```
sns.distplot(y)
```

```
/home/tselest/.local/lib/python3.9/site-packages/seaborn/distributions.py:2557:
FutureWarning: `distplot` is a deprecated function and will be removed in a
future version. Please adapt your code to use either `displot` (a figure-level
function with similar flexibility) or `histplot` (an axes-level function for
histograms).
  warnings.warn(msg, FutureWarning)
```

[48]: <AxesSubplot:xlabel='NOx(GT)', ylabel='Density'>



[49]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
                                                    random_state=101)
```

[50]:
```
# Show the results of the split
print("Training set has {} samples.".format(X_train.shape[0]))
print("Testing set has {} samples.".format(X_test.shape[0]))
```

```
Training set has 6549 samples.
Testing set has 2808 samples.
```

[62]:
```
kf = KFold(shuffle=True, random_state=72018, n_splits=3)

s = StandardScaler()
lr = LinearRegression()

X_train = s.fit_transform(X_train)
X_test = s.transform(X_test)
lr.fit(X_train, y_train)

y_pred = lr.predict(X_test)
score = r2_score(y_test, y_pred)

# with pipeline
```

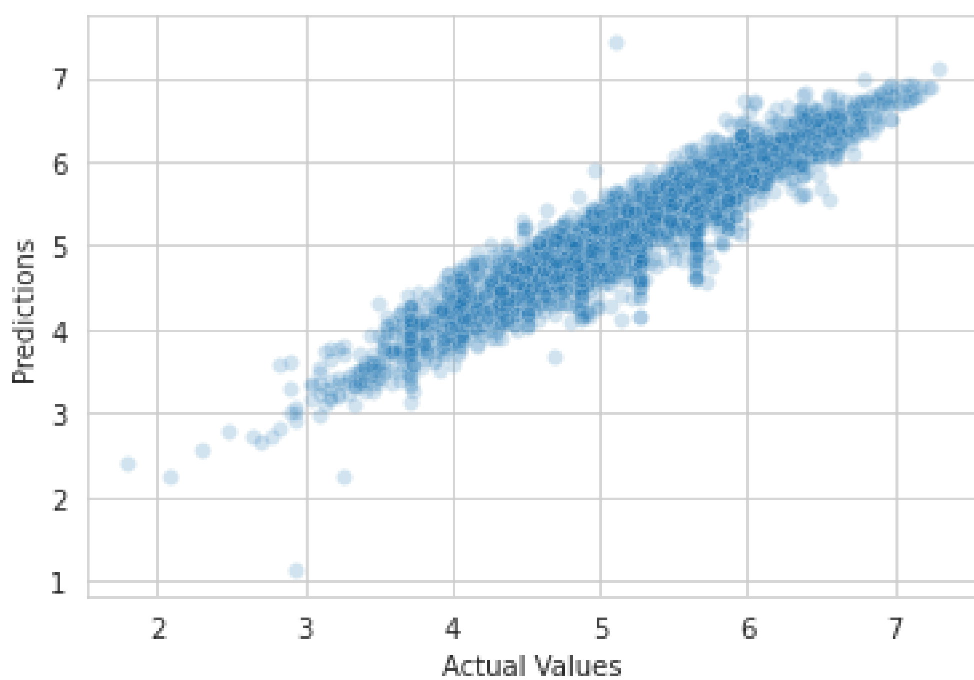
```
estimator = Pipeline([("scaler", s),("regression", lr)])
predictions_lr = cross_val_predict(estimator, X_train, y_train, cv=kf)
linear_score = r2_score(y_train, predictions_lr)

linear_score, score #almost identical
```

[62]: (0.8773345173587086, 0.8765640967999826)

[63]:
```
sns.scatterplot(y_test, y_pred, alpha = 0.2)
plt.xlabel('Actual Values')
plt.ylabel('Predictions')
```

```
/home/tselest/.local/lib/python3.9/site-packages/seaborn/_decorators.py:36:
FutureWarning: Pass the following variables as keyword args: x, y. From version
0.12, the only valid positional argument will be `data`, and passing other
arguments without an explicit keyword will result in an error or
misinterpretation.
  warnings.warn(
```

[63]: Text(0, 0.5, 'Predictions')

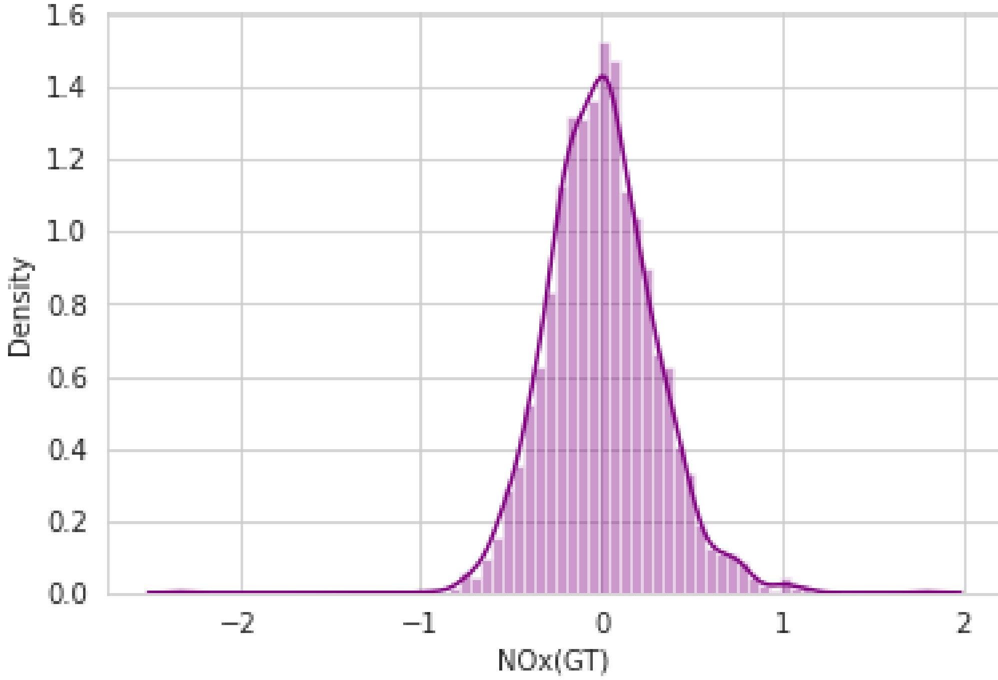


[72]:
```
sns.distplot((y_test-y_pred), bins=70, color="purple")
```

```
/home/tselest/.local/lib/python3.9/site-packages/seaborn/distributions.py:2557:
FutureWarning: `distplot` is a deprecated function and will be removed in a
future version. Please adapt your code to use either `displot` (a figure-level
```

```
function with similar flexibility) or `histplot` (an axes-level function for
histograms).
  warnings.warn(msg, FutureWarning)
```

[72]: <AxesSubplot:xlabel='NOx(GT)', ylabel='Density'>

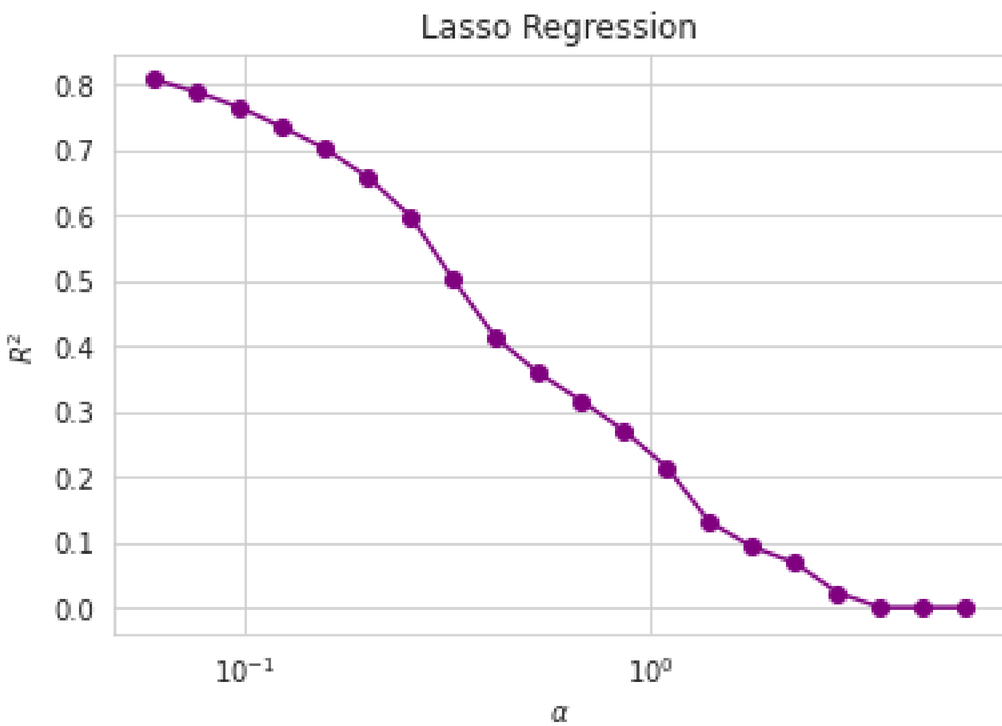


[64]:
```
print('MAE:',metrics.mean_absolute_error(y_test, y_pred))
print('MSE:',metrics.mean_squared_error(y_test, y_pred))
print('RMSE:',np.sqrt(metrics.mean_squared_error(y_test, y_pred)))
```

```
MAE: 0.2290190551198133
MSE: 0.08797015944419892
RMSE: 0.2965976389727317
```

[65]:
```
# lasso regression and K-fold cross validation
pf = PolynomialFeatures(degree=3)
kf = KFold(shuffle=True, random_state=72018, n_splits=3)
scores = []
alphas = np.geomspace(0.06, 6.0, 20)
predictions_lsr = []
for alpha in alphas:
    las = Lasso(alpha=alpha, max_iter=100000)

    estimator = Pipeline([
        ("scaler", s),
```

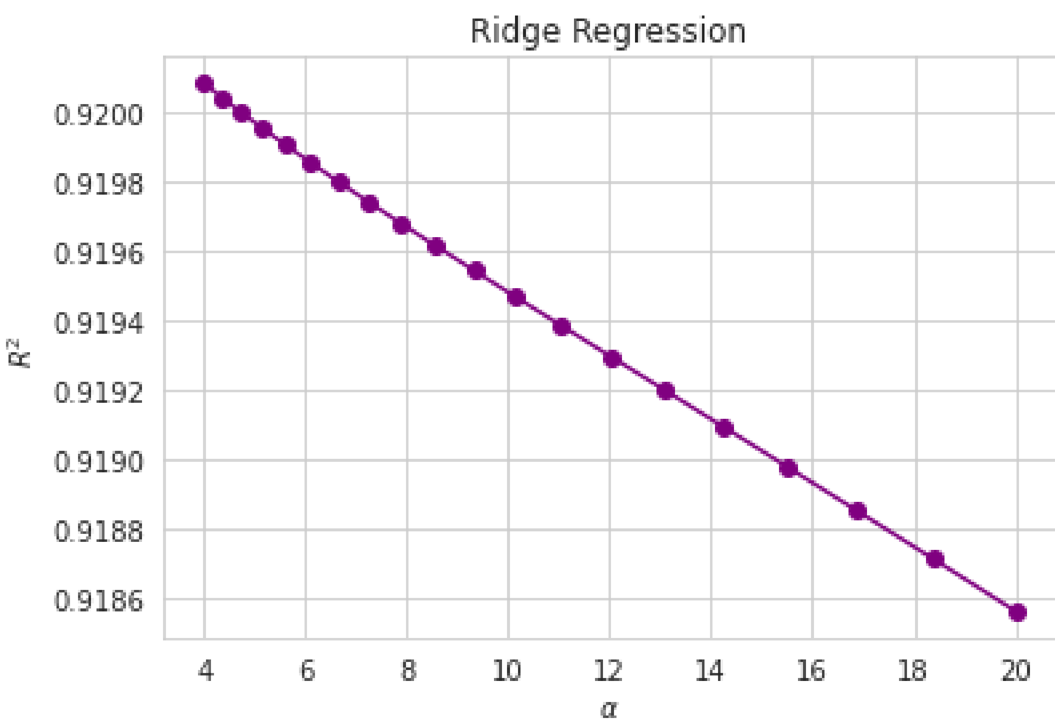
```
        ("make_higher_degree", pf),
        ("lasso_regression", las)])

    predictions_lsr = cross_val_predict(estimator, X_train, y_train, cv = kf)

    score = r2_score(y_train, predictions_lsr)

    scores.append(score)
plt.semilogx(alphas, scores, '-o', color='purple')
plt.title('Lasso Regression')
plt.xlabel('$\\alpha$')
plt.ylabel('$R^2$');
```



[66]:
```
best_estimator = Pipeline([
                    ("scaler", s),
                    ("make_higher_degree", PolynomialFeatures(degree=2)),
                    ("lasso_regression", Lasso(alpha=0.03))])

best_estimator.fit(X_train, y_train)
lasso_score = best_estimator.score(X_train, y_train)
```

[67]:
```
# ridge regression and K-fold cross validation
pf = PolynomialFeatures(degree=2)
```

```
alphas = np.geomspace(4, 20, 20)
scores=[]
predictions_rr = []
for alpha in alphas:
    ridge = Ridge(alpha=alpha, max_iter=100000)

    estimator = Pipeline([
        ("scaler", s),
        ("polynomial_features", pf),
        ("ridge_regression", ridge)])

    predictions_rr = cross_val_predict(estimator, X_train, y_train, cv = kf)
    score = r2_score(y_train, predictions_rr)
    scores.append(score)

plt.plot(alphas, scores, '-o', color='purple')
plt.title('Ridge Regression')
plt.xlabel('$\\alpha$')
plt.ylabel('$R^2$');
```



[68]:
```
best_estimator = Pipeline([
                    ("scaler", s),
                    ("make_higher_degree", PolynomialFeatures(degree=2)),
```

```
                    ("ridge_regression", Ridge(alpha=0.03))])

best_estimator.fit(X_train, y_train)
ridge_score = best_estimator.score(X_train, y_train)
```

[69]:
```
# comparing accuracy scores
pd.DataFrame([[linear_score, lasso_score, ridge_score]],columns=['linear',␣
↪'lasso', 'ridge'], index=['score'])
```

[69]:

	linear	lasso	ridge
score	0.877335	0.847026	0.924211

[70]:
```
def rmse(ytrue, ypredicted):
    return np.sqrt(mean_squared_error(ytrue, ypredicted))

# Fit a basic linear regression model
linearRegression = LinearRegression().fit(X_train, y_train)
linearRegression_rmse = rmse(y_test, linearRegression.predict(X_test))

# Fit a regular (non-cross validated) Ridge model
alphas = [0.005, 0.05, 0.1, 0.3, 1, 3, 5, 10, 15, 30, 80]
ridgeCV = RidgeCV(alphas=alphas, cv=4).fit(X_train, y_train)
ridgeCV_rmse = rmse(y_test, ridgeCV.predict(X_test))

# Fit a Lasso model using cross validation and determine the optimum value for
alphas2 = np.array([1e-5, 5e-5, 0.0001, 0.0005])
lassoCV = LassoCV(alphas=alphas2,
                  max_iter=5e4,
                  cv=3).fit(X_train, y_train)
lassoCV_rmse = rmse(y_test, lassoCV.predict(X_test))

# Fit elastic net with the same set of alphas as lasso
l1_ratios = np.linspace(0.1, 0.9, 9)
elasticNetCV = ElasticNetCV(alphas=alphas2,
                            l1_ratio=l1_ratios,
                            max_iter=1e4).fit(X_train, y_train)
elasticNetCV_rmse = rmse(y_test, elasticNetCV.predict(X_test))


rmse_vals = [linearRegression_rmse, ridgeCV_rmse, lassoCV_rmse,␣
↪elasticNetCV_rmse]

labels = ['Linear', 'Lasso', 'Ridge' 'ElasticNet']

# creating a pandas dataframe for comparing root-mean square errors
```

```
rmse_df = pd.DataFrame([[linearRegression_rmse, ridgeCV_rmse, lassoCV_rmse,␣
↪elasticNetCV_rmse]],columns=['Linear', 'Lasso', 'Ridge', 'ElasticNet'],␣
↪index=['rmse'])
rmse_df
```

[70]:

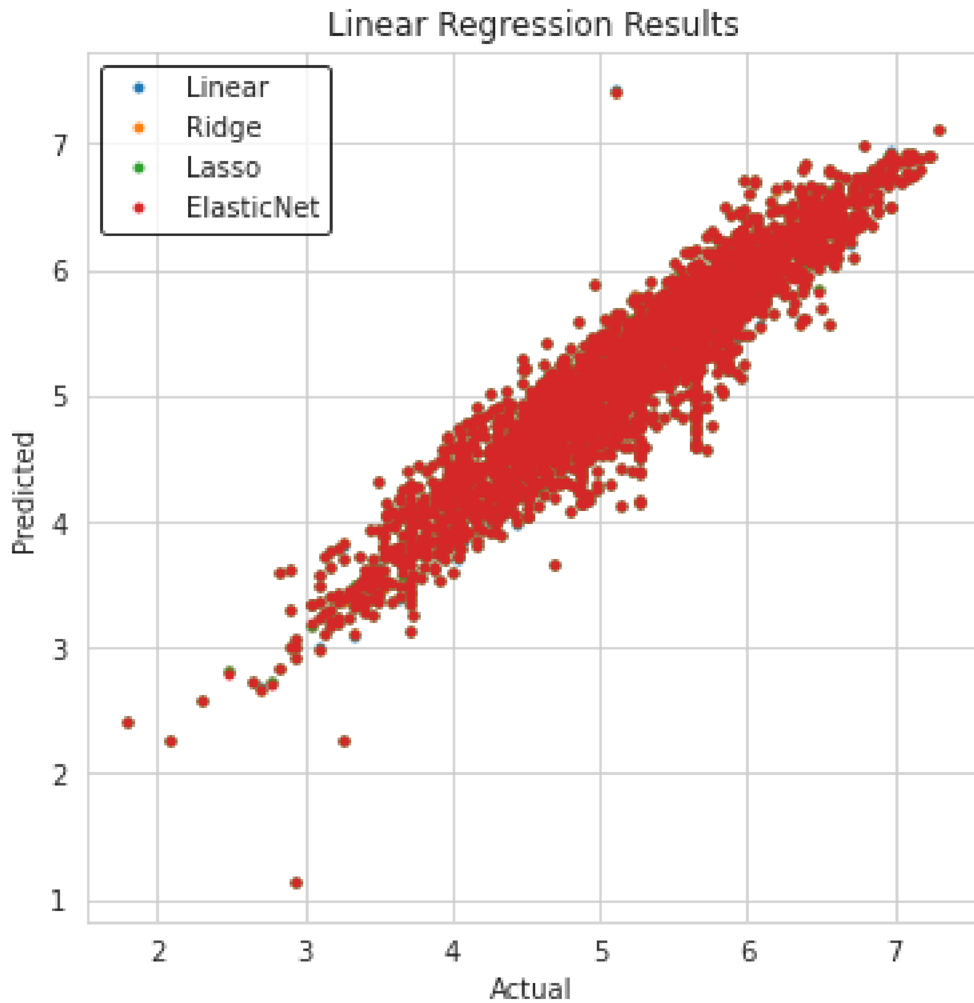
	Linear	Lasso	Ridge	ElasticNet
rmse	0.296598	0.296621	0.296621	0.29665

[71]:

```
# plotting the results: prediction vs actual values

f = plt.figure(figsize=(6,6))
ax = plt.axes()

labels, models = ['Linear', 'Ridge', 'Lasso', 'ElasticNet'], [linearRegression,␣
↪ridgeCV, lassoCV, elasticNetCV]

for mod, label in zip(models, labels):
    ax.plot(y_test, mod.predict(X_test), marker='o', ls='', ms=3.0,␣
↪label=label, alpha=1)

leg = plt.legend(frameon=True)
leg.get_frame().set_edgecolor('black')
leg.get_frame().set_linewidth(1.0)

ax.set(xlabel='Actual', ylabel='Predicted', title='Linear Regression Results')
```

[71]:

```
[Text(0.5, 0, 'Actual'),
 Text(0, 0.5, 'Predicted'),
 Text(0.5, 1.0, 'Linear Regression Results')]
```



1.6 Conclusion

Two of the most toxicologically significant compounds are nitric oxide (NO) and nitrogen dioxide (NO2). Nitrogen Oxides (NOx) are among the most dangerous forms of air pollution. They are produced from the reaction of nitrogen and oxygen gases in the air during combustion, especially at high temperatures. In areas of high motor vehicle traffic, such as in large cities, the amount of nitrogen oxides emitted into the atmosphere as air pollution can be significant. It is mainly due to fossil fuel combustion from both stationary sources, i.e. power generation (21%), and mobile sources, i.e. transport (44%). Other atmospheric contributions come from non-combustion processes, for example nitric acid manufacture, welding processes and the use of explosives.

In addition, these create serious health issues. These mainly impact on respiratory conditions causing inflammation of the airways at high levels. Long term exposure can decrease lung function, increase the risk of respiratory conditions and increases the response to allergens. NOx also contributes to the formation of fine particles (PM) and ground level ozone, both of which are associated with adverse health effects.

In this project, the AirQuality dataset from UCI was used, for exploratory data analysis and the prediction of NOx. linear regression models (Linear baseline, ridge, lasso and elasticnet) were created and trained, using the same training and test splits, and then compared to find the best model among them.

Based on the models findings, the simple linear model gives the smallest Root-mean-square error. However, the difference in scores and errors are not significant and almost identical. Therefore it is recommended as a final model as it best fits the data in terms of accuracy.

The above models could give even better results if we used GridSearchCV or RandomizedSearchCV to optimize the models' hyperparameters. Alternatively, different techniques like Random Forest Regression or SUpport Vector Machine could be used.

Here, NOx levels were predicted, using the Air Quality dataset. However, there are many others ways to measure air pollution, including PM10 (particulate matter around between 2.5 and 10 microns in diameter), carbon monoxide, sulfur dioxide, nitrogen dioxide, ozone (O3), etc.