Machine Learning Challenge Track: Predict the quality of freshwater

Problem:

Freshwater is one of our most vital and scarce natural resources, making up just 3% of the earth's total water volume. It touches nearly every aspect of our daily lives, from drinking, swimming, and bathing to generating food, electricity, and the products we use every day. Access to a safe and sanitary water supply is essential not only to human life, but also to the survival of surrounding ecosystems that are experiencing the effects of droughts, pollution, and rising temperatures.

Expected Solution:

In this track of the hackathon, you will have the opportunity to apply the oneAPI skills to help global water security and environmental sustainability efforts by predicting whether freshwater is safe to drink and use for the ecosystems that rely on it.

We leveraged the following Intel® AI Analytics Toolkit (AI Kit) - OneAPI Libraries for this model development

1. **Intel® Distribution for Python***
2. **Intel® Extension for Scikit-learn***
3. **Intel optimizations for XGBoost**
4. **Intel® Distribution of Modin***

This has greatly reduced the time of our overall processing compared to standard libraries

In [1]:
```
from sklearnex import patch_sklearn
#running this intel patch so all the sklearn libraries imported will have intel extension for faster
patch_sklearn()
import xgboost
```

```
Intel(R) Extension for Scikit-learn* enabled (https://github.com/intel/scikit-learn-intelex)
```

```
<hr style = "border-top: 3px solid black" >
<h3><font color='blue'> Importing all the required Python libraries (Intel API and others)</font>
</h3>
```

In [2]:

```python
#Leveraging the Modin Distribution for Pandas Loading
import pandas as pd

import numpy as np
import time
from numpy import mean
from numpy import std
import matplotlib.pyplot as plt
import seaborn as sns
import pandas_profiling as pp

#Leveraging the Intel API SKLearn Extension
from sklearn.metrics import f1_score
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error, r2_score

from sklearn import ensemble
from sklearn.linear_model import LogisticRegression
from sklearn.preprocessing import StandardScaler

from xgboost import XGBClassifier
from lightgbm import LGBMClassifier
from catboost import CatBoostClassifier
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import RepeatedStratifiedKFold
```

```
C:\Users\ashutoshvmadmin\AppData\Local\Temp\2\ipykernel_6880\315676513.py:10: DeprecationWarning: `impor
t pandas_profiling` is going to be deprecated by April 1st. Please use `import ydata_profiling` instead.
  import pandas_profiling as pp
```

In [3]:

```python
from sklearn.metrics import accuracy_score, log_loss
from sklearn.neighbors import KNeighborsClassifier
from sklearn.svm import SVC, LinearSVC, NuSVC
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier, AdaBoostClassifier
from sklearn.naive_bayes import GaussianNB
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis
```

Loading the Dataset

In [4]:

```python
#Reading the Provided Dataset
data = pd.read_csv('dataset.csv', index_col = 0)
```

In [5]:
```python
#Having a Preview
data.head(5)

```

Out[5]:

Index	pH	Iron	Nitrate	Chloride	Lead	Zinc	Color	Turbidity	Fluoride	Copper	...	Chlorine	Manga
0	8.332988	0.000083	8.605777	122.799772	3.713298e-52	3.434827	Colorless	0.022683	0.607283	0.144599	...	3.708178	2.269
1	6.917863	0.000081	3.734167	227.029851	7.849262e-94	1.245317	Faint Yellow	0.019007	0.622874	0.437835	...	3.292038	8.024
2	5.443762	0.020106	3.816994	230.995630	5.286616e-76	0.528280	Light Yellow	0.319956	0.423423	0.431588	...	3.560224	7.007
3	7.955339	0.143988	8.224944	178.129940	3.997118e-176	4.027879	Near Colorless	0.166319	0.208454	0.239451	...	3.516907	2.468
4	8.091909	0.002167	9.925788	186.540872	4.171069e-132	3.807511	Light Yellow	0.004867	0.222912	0.616574	...	3.177849	3.296

5 rows × 23 columns

Data Cleansing

In [6]:
```python
data.describe()
```

Out[6]:

	pH	Iron	Nitrate	Chloride	Lead	Zinc	Turbidity	Fluoride	Co
count	5.840788e+06	5.917089e+06	5.851117e+06	5.781311e+06	5.929933e+06	5.800716e+06	5.907027e+06	5.767686e+06	5.757440
mean	7.445373e+00	1.279027e-01	6.169970e+00	1.842970e+02	1.498336e-03	1.550255e+00	5.215093e-01	9.644315e-01	5.161216
std	8.881665e-01	4.799915e-01	3.256667e+00	6.842828e+01	3.250641e-02	1.546368e+00	9.258807e-01	8.247870e-01	5.965534
min	1.057113e+00	2.047587e-53	2.861727e-01	2.363919e+01	0.000000e+00	1.482707e-08	1.029712e-16	4.550148e-06	2.982735
25%	6.894328e+00	9.992949e-06	3.973078e+00	1.381341e+02	1.500283e-122	4.148202e-01	3.872368e-02	3.749503e-01	1.288629
50%	7.449564e+00	2.249640e-03	5.604051e+00	1.760178e+02	2.213625e-62	1.081818e+00	2.097680e-01	7.751792e-01	3.479592
75%	8.014424e+00	5.455290e-02	7.672402e+00	2.179811e+02	3.592165e-27	2.230841e+00	6.249132e-01	1.341508e+00	7.010104
max	1.291072e+01	1.935315e+01	9.639078e+01	1.507310e+03	5.844281e+00	2.836867e+01	2.371527e+01	1.464625e+01	1.207482

In [7]:
```
data.isna().sum()
```

Out[7]:
```
pH                        116054
Iron                       39753
Nitrate                   105725
Chloride                  175531
Lead                       26909
Zinc                      156126
Color                       5739
Turbidity                  49815
Fluoride                  189156
Copper                    199402
Odor                      178891
Sulfate                   197418
Conductivity              163861
Chlorine                   57825
Manganese                 109583
Total Dissolved Solids      1670
Source                     88262
Water Temperature         168233
Air Temperature            29728
Month                      95668
Day                        99603
Time of Day               114519
Target                         0
dtype: int64
```

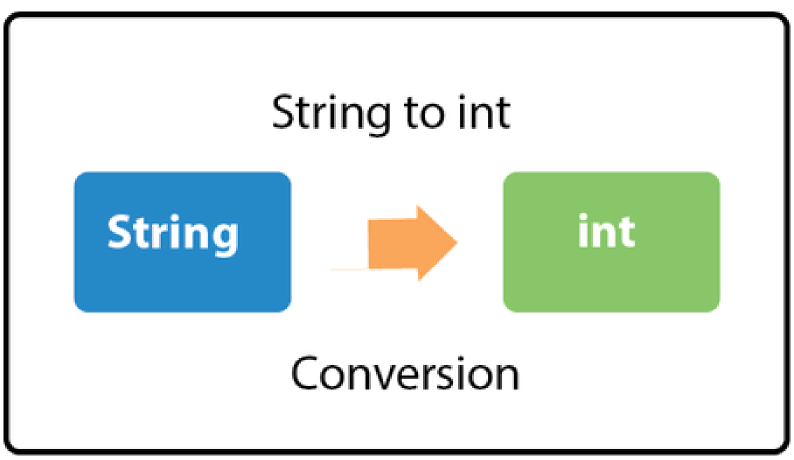
Filling all the Null Values Using Backward Fill Method

In [8]:
```
data.fillna(method='bfill', inplace=True)

```

Converting all the Columns of String Data Type to Integer Type Using Factorization Method

- We are converting all the categorical columns into numerical data type so we can use it for training our model. Since machine learning model only accepts numerical values.



In [9]:

```

#Exclude Object Columns and Factorize all the Number Columns

df_numeric = data.select_dtypes(exclude=['object'])
df_obj = data.select_dtypes(include=['object']).copy()

for c in df_obj:
    df_obj[c] = pd.factorize(df_obj[c])[0]

data = pd.concat([df_obj,df_numeric], axis=1)
```

Correlation Matrix

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

Where,

r = Pearson Correlation Coefficient

x_i = x variable samples $\quad$ y_i = y variable sample

$\bar{x}$ = mean of values in x variable $\quad$ $\bar{y}$ =mean of values in y variable

In [10]:

```python
data.corr(method='pearson').style.format("{:.3}").background_gradient(cmap=plt.get_cmap('coolwarm'),
```

Out[10]:

	Color	Source	Month	pH	Iron	Nitrate	Chloride	Lead	Zinc	Turbidity	Fluoride
Color	1.0	0.000352	-0.000439	-0.00793	0.0423	0.0418	0.0514	0.00997	0.0205	0.0564	0.0422
Source	0.000352	1.0	-7.11e-05	0.000667	0.000206	0.000431	0.000445	0.000496	4.11e-05	-0.000204	0.000251
Month	-0.000439	-7.11e-05	1.0	-0.000294	-0.000135	0.000239	4.57e-05	0.00026	-6.28e-05	-0.000205	-4.39e-05
pH	-0.00793	0.000667	-0.000294	1.0	-0.00975	-0.0095	-0.0124	-0.00233	-0.00509	-0.0134	-0.00988
Iron	0.0423	0.000206	-0.000135	-0.00975	1.0	0.0516	0.0637	0.011	0.0253	0.0693	0.0521
Nitrate	0.0418	0.000431	0.000239	-0.0095	0.0516	1.0	0.0636	0.0116	0.0249	0.0702	0.0519
Chloride	0.0514	0.000445	4.57e-05	-0.0124	0.0637	0.0636	1.0	0.014	0.0303	0.0857	0.0637
Lead	0.00997	0.000496	0.00026	-0.00233	0.011	0.0116	0.014	1.0	0.00588	0.0164	0.013
Zinc	0.0205	4.11e-05	-6.28e-05	-0.00509	0.0253	0.0249	0.0303	0.00588	1.0	0.0338	0.0243
Turbidity	0.0564	-0.000204	-0.000205	-0.0134	0.0693	0.0702	0.0857	0.0164	0.0338	1.0	0.0693
Fluoride	0.0422	0.000251	-4.39e-05	-0.00988	0.0521	0.0519	0.0637	0.013	0.0243	0.0693	1.0
Copper	0.0535	0.000323	0.000334	-0.0132	0.0672	0.0663	0.081	0.0155	0.0321	0.0886	0.067
Odor	0.0406	-2.73e-05	0.000344	-0.00951	0.0497	0.0495	0.0612	0.0113	0.0243	0.0663	0.0497
Sulfate	0.0316	-0.000287	-0.00017	-0.00729	0.0403	0.0392	0.0478	0.00905	0.0191	0.0525	0.0398
Conductivity	-0.000123	0.000156	0.00049	0.000344	0.000163	0.000122	-0.000525	-0.000193	-0.000137	-7.58e-05	-5.34e-05
Chlorine	0.0369	0.000691	0.000867	-0.00777	0.0451	0.045	0.0549	0.0108	0.0217	0.0619	0.0464
Manganese	0.0466	-2.79e-05	-0.000431	-0.0113	0.0588	0.0582	0.0701	0.0133	0.0273	0.0764	0.0567
Total Dissolved Solids	0.0233	0.000445	-0.000121	-0.00521	0.0284	0.0291	0.0361	0.00588	0.0137	0.039	0.0296
Water Temperature	-0.000989	-0.000194	0.000414	-0.000412	0.00107	-6.02e-05	-0.000323	-6.53e-06	-0.00018	0.000297	-0.000461
Air Temperature	-0.000545	0.000354	0.000415	0.000514	-0.000331	0.000169	-0.000315	-0.000547	8.14e-05	-0.000861	1.91e-05
Day	0.000661	0.000204	-0.00589	0.000757	-0.000184	-0.000256	1.08e-05	0.000128	6.58e-05	-0.000331	0.000823
Time of Day	3.48e-05	0.000296	0.000414	-0.000168	0.000559	1.21e-06	-0.000218	0.000697	0.000753	-0.00102	-0.000742
Target	0.147	-7.86e-05	-4.13e-05	-0.0349	0.181	0.183	0.223	0.0421	0.0886	0.244	0.184

In [11]:

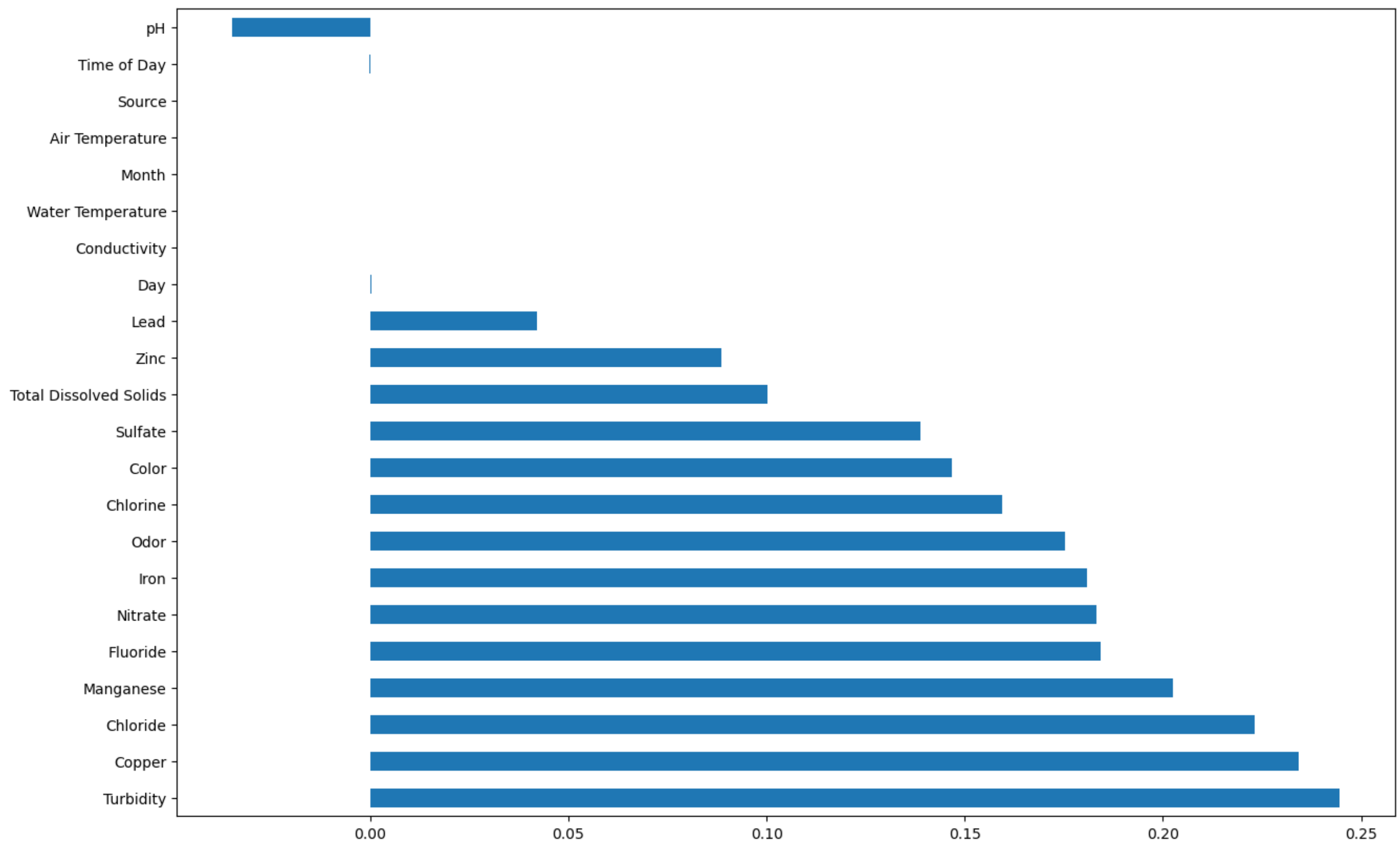
```python
#run the correlation on the data
df_correlation = data.corr()
```

In [12]:

```python
#visualize the highly and least correlated columns..

plt.rcParams['figure.figsize'] = [15, 10]
(df_correlation
     .Target
     .drop('Target')
     .sort_values(ascending=False)
     .plot
     .barh())
```

Out[12]: <AxesSubplot:>



In [13]:

```
#check on the correlated columns
data.corr()['Target'].sort_values()
```

Out[13]:

```
pH                       -0.034884
Time of Day              -0.000116
Source                   -0.000079
Air Temperature          -0.000059
Month                    -0.000041
Water Temperature        -0.000004
Conductivity              0.000004
Day                       0.000253
Lead                      0.042072
Zinc                      0.088646
Total Dissolved Solids    0.100203
Sulfate                   0.138885
Color                     0.146784
Chlorine                  0.159396
Odor                      0.175274
Iron                      0.180904
Nitrate                   0.183262
Fluoride                  0.184222
Manganese                 0.202650
Chloride                  0.223143
Copper                    0.234330
Turbidity                 0.244500
Target                    1.000000
Name: Target, dtype: float64
```

In [14]:

```
cor = data.corr()['Target'].sort_values()
```

In [15]:

```
df = data.copy()
```

Removing all the Columns from the Dataset whose Correlation Value is Less than 0.01 with the Target Column

- Since columns with such low correlation with not be useful for predicting the target column. So we will be dropping through column while training the predictive model

In [16]:

```
#Excluding Columns for Faster Processing and improving Accuracy
arr = []
for k, v in cor.items():
    if abs(v) < 0.01:
        arr.append(k)

df = df.drop(arr, axis=1)

#preview after dripping the non-correlated columns
```

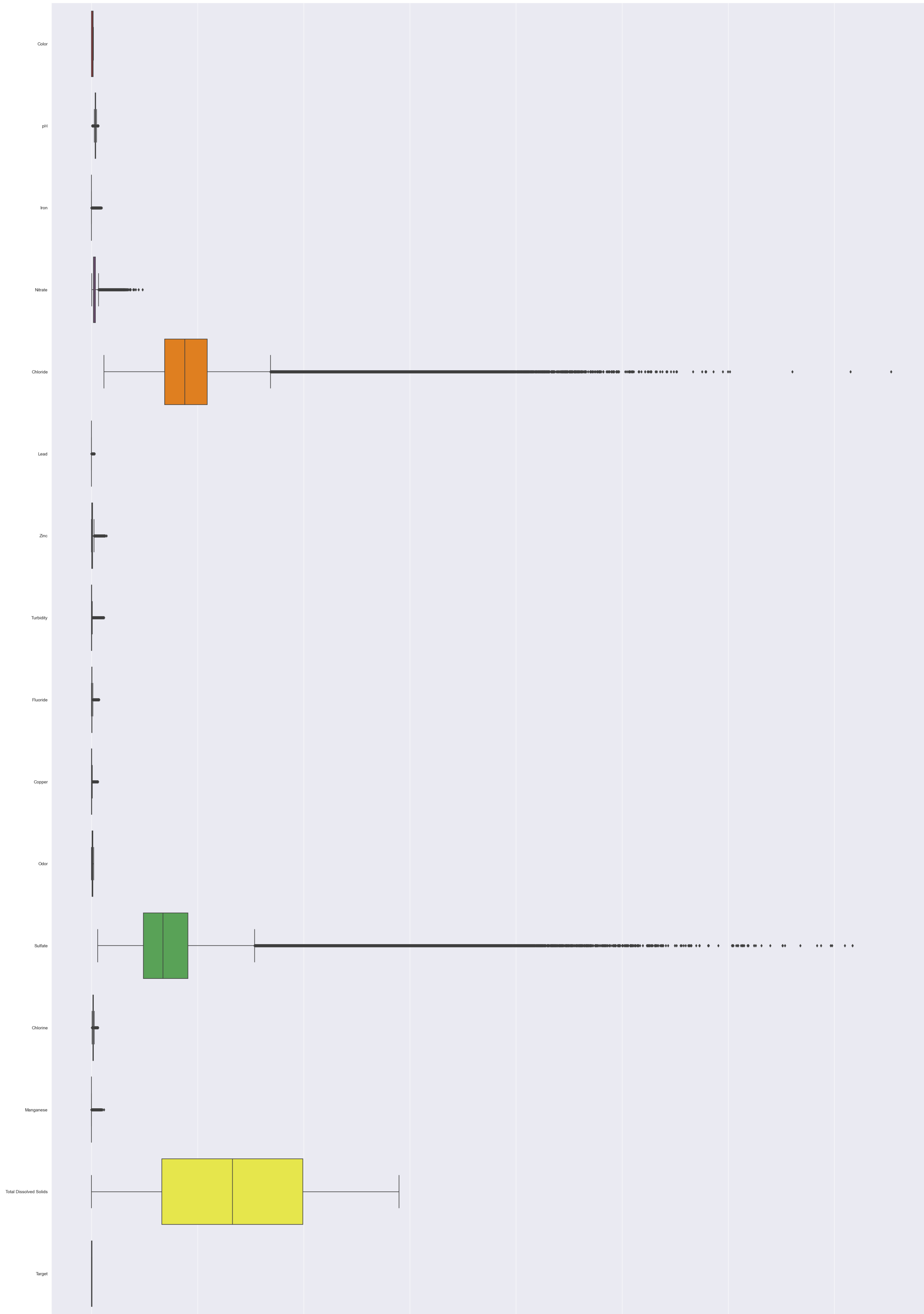
BoxPlot (Pictorial View of all the Outliers in the Data)

In [17]:

```
#visualize the Outliers of which columns are impacting the quality of data..
sns.set(rc={'figure.figsize':(40,60)})
sns.boxplot(data=df, orient="h", palette="Set1")
```

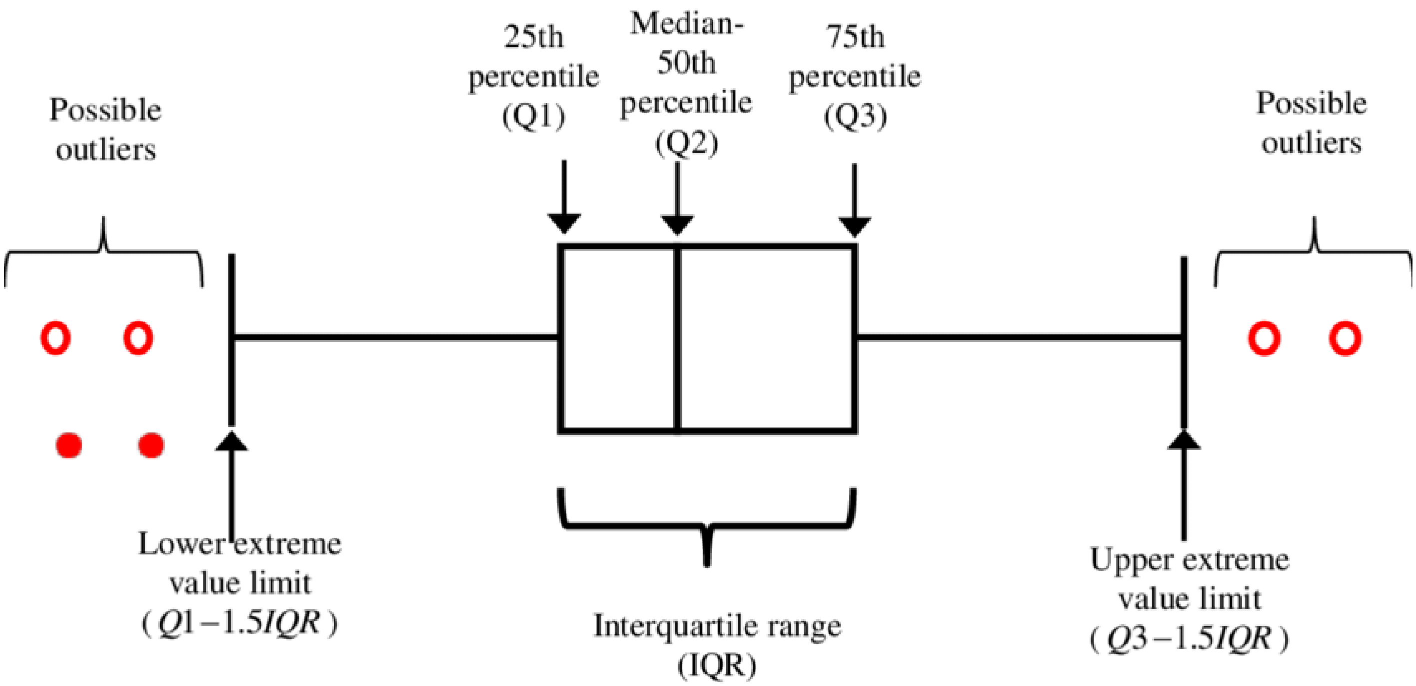
Out[17]:

```
<AxesSubplot:>
```


Color
pH
Iron
Nitrate
Chloride
Lead
Zinc
Turbidity
Fluoride
Copper
Odor
Sulfate
Chlorine
Manganese
Total Dissolved Solids
Target
0
200
400
600
800
1000
1200
1400

Removing all the Outliers from the Dataset

- Since outliers can skew the results of the predictive model. It is better to remove those from the dataset. - Since there is such high standard deviation in the dataset i.e. the values are spread over wider range. So instead of filling null values by mean of a column we are using forward fill method.



In [18]:
```python
#Create the Data Set within the required Quartile..
Q1 = df.quantile(0.25)
Q3 = df.quantile(0.75)
IQR = Q3 - Q1
```

In [19]:
```python
#Check if the datasize is sufficient after removing the quartiles
((df < (Q1 - 1.5 * IQR)) | (df > (Q3 + 1.5 * IQR))).sum()
```

Out[19]:
```
Color                         0
pH                       157747
Iron                     955720
Nitrate                  196843
Chloride                 194005
Lead                    1468586
Zinc                     184192
Turbidity                464318
Fluoride                 207305
Copper                   318595
Odor                          0
Sulfate                  151367
Chlorine                 101531
Manganese                954480
Total Dissolved Solids        0
Target                        0
dtype: int64
```

In [20]:
```python

#refine the dataset by removing outliers..
df = df[~((df < (Q1 - 1.5 * IQR)) |(df > (Q3 + 1.5 * IQR))).any(axis=1)]
df.shape
```

Out[20]: (2698438, 16)

In [21]:

```
#have a look at the refined data
df.head(5)
```

Out[21]:

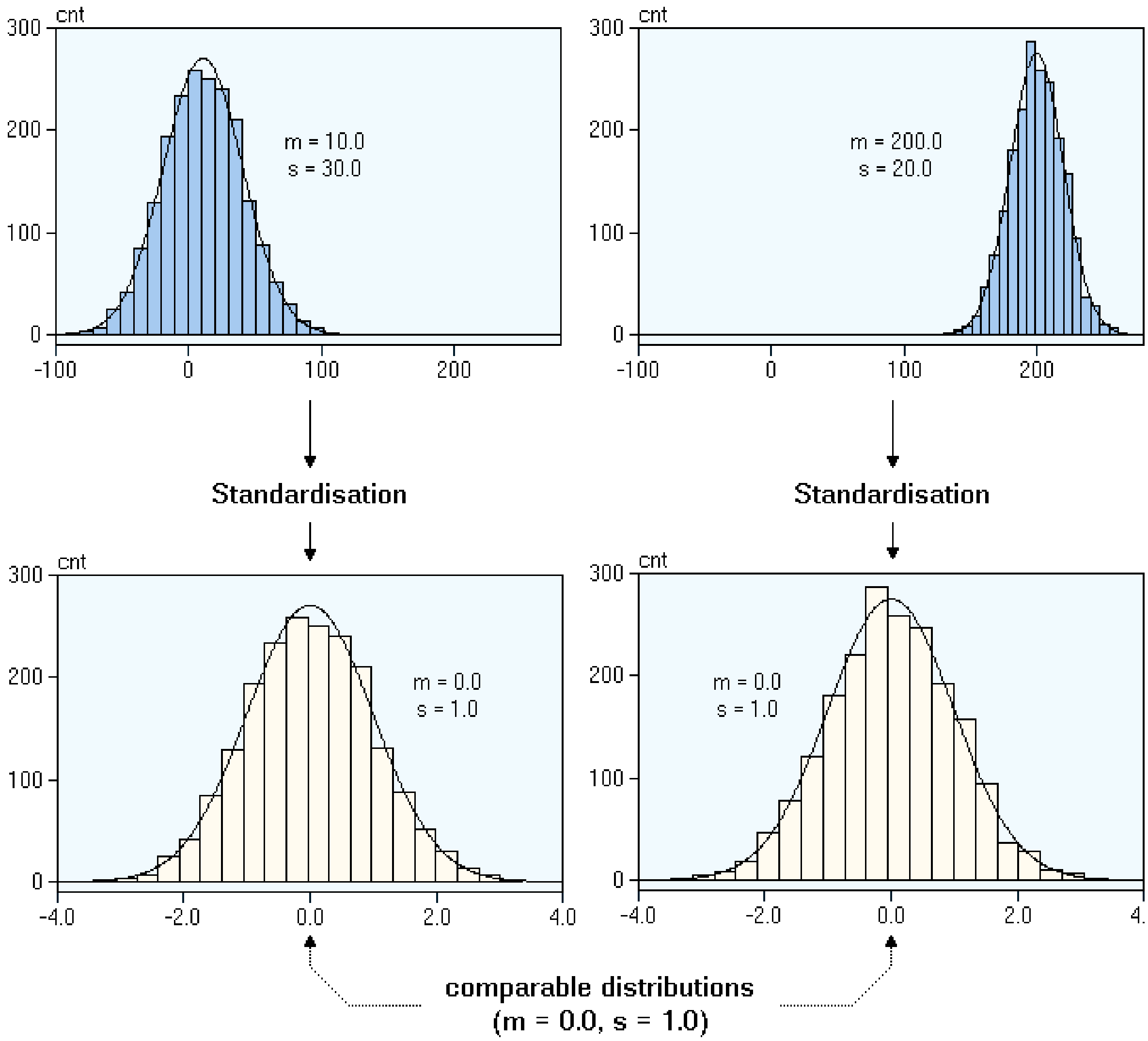
	Color	pH	Iron	Nitrate	Chloride	Lead	Zinc	Turbidity	Fluoride	Copper	Odor	Sulfate
Index												
0	0	8.332988	8.347252e-05	8.605777	122.799772	3.713298e-52	3.434827	0.022683	0.607283	0.144599	1.626212	87.266538
1	1	6.917863	8.053827e-05	3.734167	227.029851	7.849262e-94	1.245317	0.019007	0.622874	0.437835	1.686049	144.010981
4	2	8.091909	2.167128e-03	9.925788	186.540872	4.171069e-132	3.807511	0.004867	0.222912	0.616574	0.795310	175.275175
6	2	8.132455	5.526229e-02	4.288010	94.993978	2.919909e-52	1.770221	0.021703	1.111893	0.247116	0.426404	114.551427
7	0	7.258203	6.107130e-09	9.261676	182.242341	4.399852e-224	0.416478	0.047803	1.016196	0.298093	3.144199	114.551427

In [22]:

```
# Now make the X and Y axis of the data ..
x = df.iloc[:, :-1].values
y = df.iloc[:, -1].values
```

Standardizing all The Columns which will be used for Training the Model

- Strandardizing the columns so some of the machine learning model which assign weights to each column while training should not provide higher weight to a column just based on the magnitude of their value.



In [23]:

```
#use a standard scaler and fit the transformed data
sc_X = StandardScaler()
x = sc_X.fit_transform(x)
```

In [24]:

```
#Taking a 20% for testing and rest for training the data..
x_train, x_test, y_train, y_test = train_test_split(x, y, test_size = 0.2, random_state = 42)
```

Running the Training on FIVE models

1. **Logistic Regression**
2. **XGBoost (Powered by Intel API)**
3. **Light GBM**
4. **CatBoost**
5. **Random Forest**

---

1. Training and Predicting with Logistic Regression

In [25]:
```
regressor = LogisticRegression()
regressor.fit(x_train, y_train)
```

Out[25]:
```
LogisticRegression()
```

In [26]:
```
pred = regressor.predict(x_test)
```

In [27]:
```
accuracy = regressor.score(x_test, y_test)
print(f'Accuracy of Logistic Regression Model is {round(accuracy * 100, 2)} %')
```

```
Accuracy of Logistic Regression Model is 90.5 %
```

---

2. Training and Predicting with XG Boost

In [28]:
```
model = XGBClassifier()
```

In [29]:
```
model.fit(x_train, y_train)
```

Out[29]:
```
XGBClassifier(base_score=None, booster=None, callbacks=None,
              colsample_bylevel=None, colsample_bynode=None,
              colsample_bytree=None, early_stopping_rounds=None,
              enable_categorical=False, eval_metric=None, feature_types=None,
              gamma=None, gpu_id=None, grow_policy=None, importance_type=None,
              interaction_constraints=None, learning_rate=None, max_bin=None,
              max_cat_threshold=None, max_cat_to_onehot=None,
              max_delta_step=None, max_depth=None, max_leaves=None,
              min_child_weight=None, missing=nan, monotone_constraints=None,
              n_estimators=100, n_jobs=None, num_parallel_tree=None,
              predictor=None, random_state=None, ...)
```

In [30]:
```
pred = model.predict(x_test)
```

In [31]:
```
accuracy_xgb = model.score(x_test, y_test)
print(f'Accuracy of XG Boost Model is {round(accuracy_xgb * 100, 4)} %')
```

```
Accuracy of XG Boost Model is 94.7723 %
```

3. Training and Predicting with Light GBM

In [32]:

```
model_lgbm = LGBMClassifier()
```

In [33]:

```
model_lgbm.fit(x_train, y_train)
```

Out[33]:

```
LGBMClassifier()
```

In [34]:

```
pred_new = model_lgbm.predict(x_test)
```

In [35]:

```
accuracy_lgbm = model_lgbm.score(x_test, y_test)
print(f'Accuracy of Light Gradient Boost Model is {round(accuracy_lgbm * 100, 4)} %')
```

```
Accuracy of Light Gradient Boost Model is 95.0297 %
```

---

4. Training and Predicting with CAT Boost

In [36]:

```
model_cat = CatBoostClassifier(verbose=0, n_estimators=100)
```

In [37]:

```
model_cat.fit(x_train, y_train)
```

Out[37]:

```
<catboost.core.CatBoostClassifier at 0x29f4c9540d0>
```

In [38]:

```
predictions = model_cat.predict(x_test)
```

In [39]:

```
accuracy_cbm = model_cat.score(x_test, y_test)
print(f'Accuracy of Light Gradient Boost Model is {round(accuracy_cbm * 100, 4)} %')
```

```
Accuracy of Light Gradient Boost Model is 94.8533 %
```

---

5. Training and Predicting with Random Forest

In [40]:

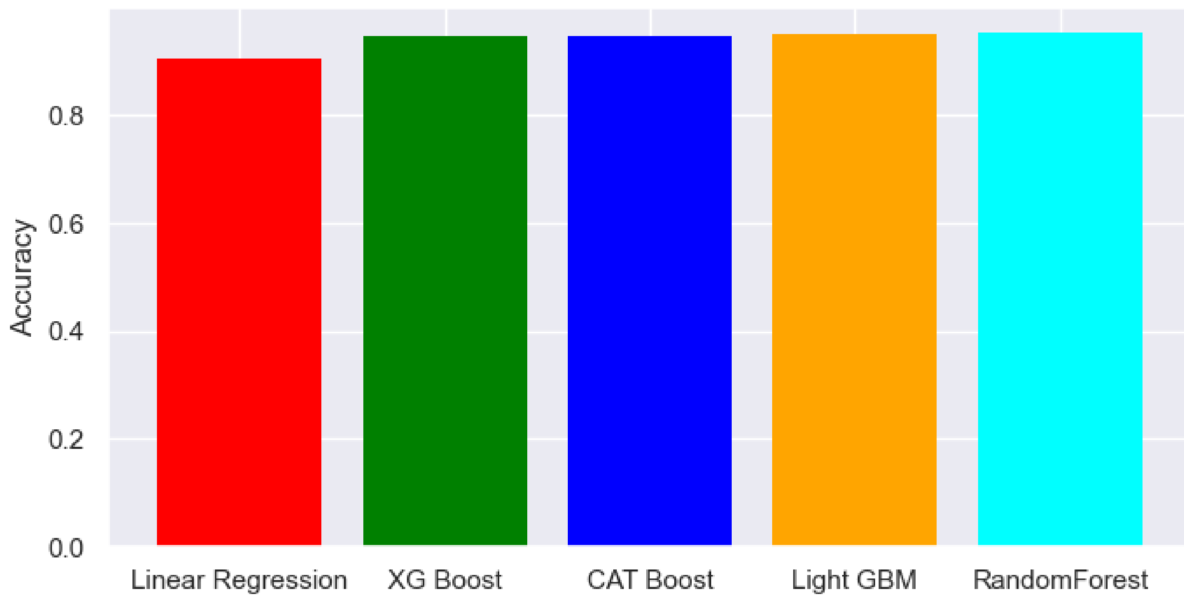
```
model_rfc = RandomForestClassifier()
start_time = time.time()
model_rfc.fit(x_train, y_train)
predictions = model_rfc.predict(x_test)
accuracy_rfc = model_rfc.score(x_test, y_test)
print(f'Accuracy of RandomForest Classifier Model is {round(accuracy_rfc * 100, 2)} %')
end_time = time.time()
training_time = end_time - start_time
```

```
Accuracy of RandomForest Classifier Model is 95.23 %
```

We noticed Random Forest Classifier is giving the best accuracy amongst all the models

In [41]:

```
x = ['Linear Regression', 'XG Boost', 'CAT Boost', 'Light GBM', 'RandomForest']
y = [accuracy, accuracy_xgb, accuracy_cbm, accuracy_lgbm, accuracy_rfc]
colors = ['red', 'green', 'blue', 'orange', 'cyan']
plt.rcParams['figure.figsize'] = [8,4]
plt.bar(x, y, color=colors, edgecolor='none')
plt.ylabel('Accuracy')
plt.show()
```



We are able to achieve 95.23 % Accuracy in this problem statement

- Using sklearn intel api we were able to train our Random Forest Classifier faster than usual

In [42]:

```
print(f'Accuracy of the Model is {round(accuracy_rfc * 100, 2)} %')
print(f"Training time: {training_time:.3f} seconds")
```

```
Accuracy of the Model is 95.23 %
Training time: 62.123 seconds
```