ODOR PREDICTION
Using Machine Learning

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Abstract

ML and data science are rapidly employed in the chemical realm for quantitative structure-property relation applications. One such application is the perception of odorant stimuli, as olfaction is the least worked among all other senses in the prediction domain. The usefulness of employing a data-based strategy to predict the characteristics of perception of an odorant, precisely the attributes of an odorant, is investigated using ML-based algorithms and data science. We first analyze an Odor dataset [1], a repository of odor names, smiles, and primary and secondary odors. We next utilize the data to train multiple ML algorithms [2] for olfactory character prediction, including random forest, decision tree, XGBoost, and K-nearest-neighbors and provide the structural elements that correlate with the smell based on the optimum model.

Furthermore, we try to find the impact of data quality on model execution by contrasting the semantic descriptors often related to a specific aroma to how the bulk of the contributors recognize it. The research gives a structure for constructing odor perceptive models and intuition into odor perception and the effect of intrinsic bias in perception data on model performance. The programs and approaches described here might be utilized to anticipate novel odorant odor characteristics. In this article, we narrate a model that merges data preprocessing and scaling methods to clean the dataset. Different classifiers are applied to the dataset, and we obtained the highest accuracy of 97.01% using a random forest classifier on the test data.

Introduction

One or more volatilized chemical components, generally found in low quantities and may be detected by humans and animals using their sense of smell, cause an odor or scent. An odor is sometimes known as a "smell" or "scent," and it can be either pleasant or unpleasant [3]. Aromas are also often added to a diversity of chemical goods or Mixtures (moisturizer, soaps, lotion, cleansers, and so on) to increase their sensory qualities by impersonating the items' otherwise "chemical" smell.

Olfaction is the least known of all the senses regarding why an odorant smells the way it does. According to research, there may be discrepancies in how specialists and unskilled participants perceive odors [4,5,6]. In the business, there is limited consensus on how to quantify odorant qualities, including quality, intensity, and resemblance. Researchers use various methods to

obtain odor perception data, including verbal profiling, similarity scores, and sorting [7,8]. Over the years, scientists have sought to figure out how physical stimulation affects olfactory perception. The stimulus-percept issue, on the other hand, is fraught with difficulties. In addition to the unpredictable nature of the Composition-odor relationship, the expanse and largeness of the perceptive olfactory space are ambigious[9,10,11].

It has been proposed that, rather than only the chemical properties of the stimuli, experience variables such as memory are crucial for odor discrimination [12]. Nonetheless, as machine learning has progressed, there has been an increasing interest in adopting a data-driven method to forecast structure-odor connections in recent years. Many people have attempted to show that the structural properties of odorant molecules may be used to predict olfactory perception [13]. However, the methodologies employed for the predictions range substantially regarding the data utilized. Some use intuitive data from ignorant persons, and others use comparative data from skillful experts, making differentiation impossible.

This work aims to take untrained individuals' perceptual data and apply a machine learning-based classification strategy to predict the 68 distinct odor characteristics (OC) of odorant molecules using 11 descriptors as input features.

The study has been divided into 3 sub parts

1. Literature review
2. Proposed Methodology
3. Results and Analysis

Literature Review

This study paper covers four distinct aspects of olfaction; however, our focus was on Machine-learned odor detection based on Physico-chemical characteristics of volatile molecules. In this section, the author outlines how the dataset was gathered and the various accuracy measurements. A classifier based on RF correctly predicted eight out of nineteen evaluated connotative descriptors ("garlic," "fish," "sweet," "fruit," "burnt," "spices," "flower," "sour"). SVM, RF, and extreme learning machines were among the machine-learning methods employed. An extensive psychophysical data collection was compiled from 49 people who profiled 476 constitutionally and subjectively distinct compounds. ELM has the highest

identification accuracy (97.53%), followed by SVM (97.19%) and RF (97.19%). (92.79 percent) [13].

The study's goal is to anticipate the olfactory features, which are mostly sweet and musky. They use some ML methods such as RF, gradient boosting, and SVM for olfactory character prediction. The work proposes a technique for constructing odor perception models and insights into how untrained human participants perceive odorants and the impact of innate bias in the perception data on model execution. The odorant property data for 480 structurally varied chemicals are included in the dataset [14].

This article uses the "Flavors and Fragrances" library to create an olfactory character predicting model. In the Sigma-Aldrich catalog, the descriptor's application is supplied in binary form, but in Dravnieks' sensory evaluation, it is offered on a scale of 0 to 5. For data with a binary representation. The article and its supporting information files include half of the necessary data (odor character data). The NIST database [16] has the other half (mass spectrum) of the data [15].

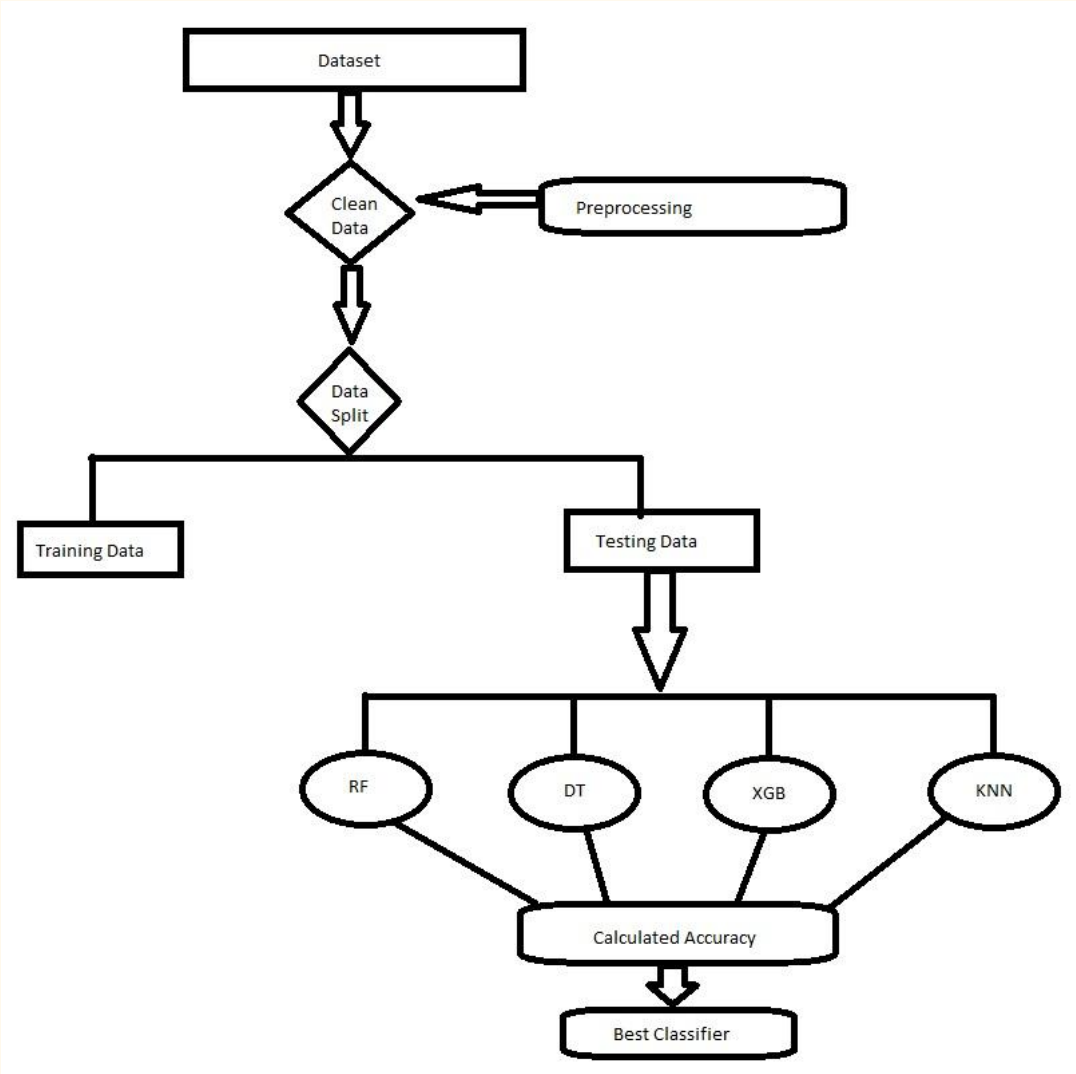
This study proposes a proof-of-concept approach for obtaining olfactory information from odorant molecules' molecular properties (MPs) using machine learning-based prediction. Molecular computation software was used to get the physicochemical properties of the odorant molecules (DRAGON). The Dragon chemo information program was used to import SMILES strings. The MPs' characteristics were retrieved using either non-autonomous(principal component analysis) or autonomous(Boruta, BR) methods and then utilized as input to ML models to fine-tune them. The findings revealed that SVM-calibrated models had higher accuracies than others [17].

By accumulating OMs from rat odor bulbs and drawing out attribute profiles of the related odorant molecules, this study investigated the connection between order maps (OMs) and molar parameters (MPs) of odorants. The OdorMapDB provided 178 pictures of glomerular (network of tiny blood veins) activity in the olfactory bulb corresponding to odorants. In 2D space, all odorants were depicted, and similar odorants were collected in the t-SNE area. The models were measured using olfactory particulars or molecular data to see how well they could identify functional groupings. The OM-PCA19 ELM (extreme learning machine) offers a lot of potential for identifying available categories [18].

Proposed Methodology

The proposed approach worked on an odor dataset [1] and predicted the odor of the given molecule. First, we have to analyze the dataset; then, we apply preprocessing on the dataset; after that, we create dummy variables (One Hot Encoding) for absolute values; then, In an 80:20 ratio, we split the data into training and testing. After breaking the dataset, we apply various machine learning classifiers.

The proposed approach's framework is depicted in Figure 1.



Fig(1): Proposed Methodology

1. Dataset Description

We have worked on the Odor Dataset [1], which we have obtained from the Olfaction base section of IIIT Allahabad. The dataset consists of 3686 unique molecule information, and this dataset contains five attributes, namely Primary Odor, Sub-Odor, CAS-id, chemical name, and smiles.

2. Dataset Preprocessing

We used the padelpy library of python and generated 1875 descriptors. Then we used Pearson correlation with Primary Odor as a target variable and generated 13 descriptors that were highly correlated with the target variable. After that, we used correlation among the 13 descriptors and the 0.99 thresholds to generate 11 descriptors used for the final prediction.

```
Index(['nS', 'AATS8i', 'AATSC1i', 'MATS1i', 'SM1_Dzs', 'SpMin6_Bhm',
       'SpMin7_Bhm', 'minHBa', 'gmin', 'MAXDN', 'ETA_Psi_1', 'Primary Odor'],
      dtype='object')
12
```

Fig(2): Dataset with 11 descriptors and 1 target variable

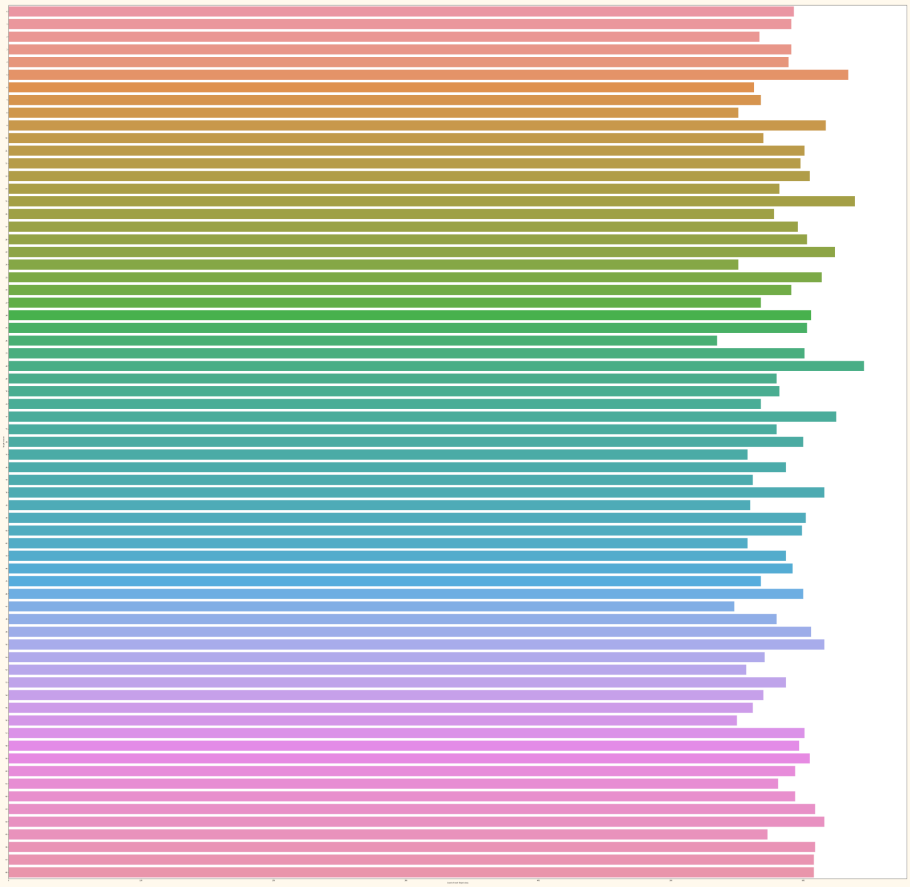
```
Score:  [1.76127945e+04 4.86215913e+05 2.08792612e+03 1.59196886e+03
 1.96011348e+04 2.65091540e+03 3.63092270e+03 1.51829871e+04
 5.45063048e+04 5.37428012e+03 1.49251532e+02]
Columns:  Index(['nS', 'AATS8i', 'AATSC1i', 'MATS1i', 'SM1_Dzs', 'SpMin6_Bhm',
       'SpMin7_Bhm', 'minHBa', 'gmin', 'MAXDN', 'ETA_Psi_1'],
      dtype='object')
```

Fig(3): Chi2 Feature Selection with Scores

```
Score:  [334.98792417 268.66128205 306.4886707  260.35426046 326.39462235
 340.64812168 290.05154283 214.11588818 419.89170005 242.54792843
 347.71306518]
Columns:  Index(['nS', 'AATS8i', 'AATSC1i', 'MATS1i', 'SM1_Dzs', 'SpMin6_Bhm',
       'SpMin7_Bhm', 'minHBa', 'gmin', 'MAXDN', 'ETA_Psi_1'],
      dtype='object')
```

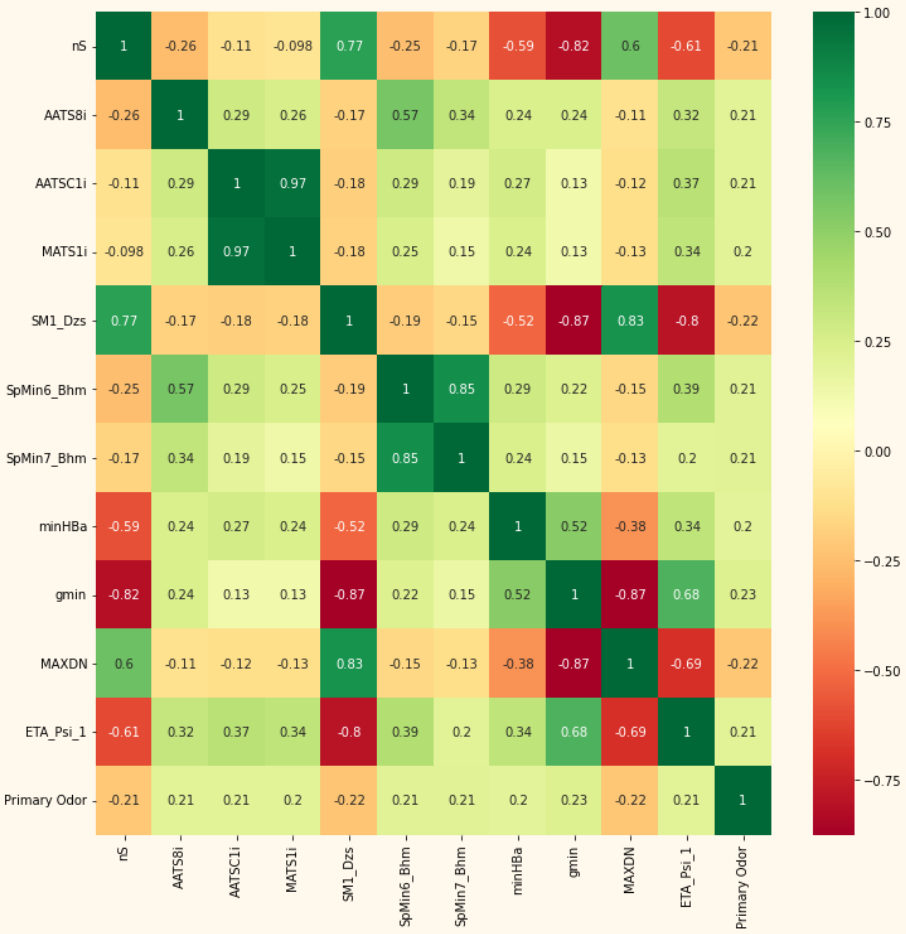
Fig(4): F_classif Feature Selection with Scores

After this, we used resampling of classes/weights such that the 68 unique odor characteristics (OC) had an equal distribution of count. Which made the size of the dataset 40641 rows.

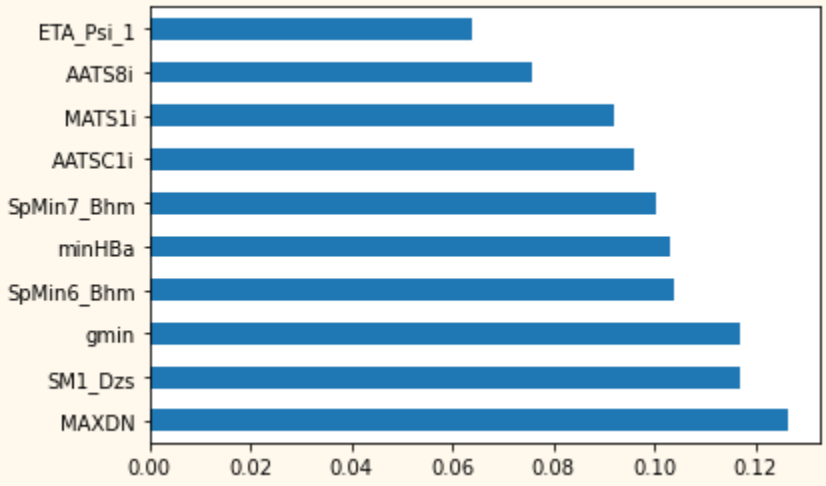


Fig(5): Dataset Primary Odor count of each Target class

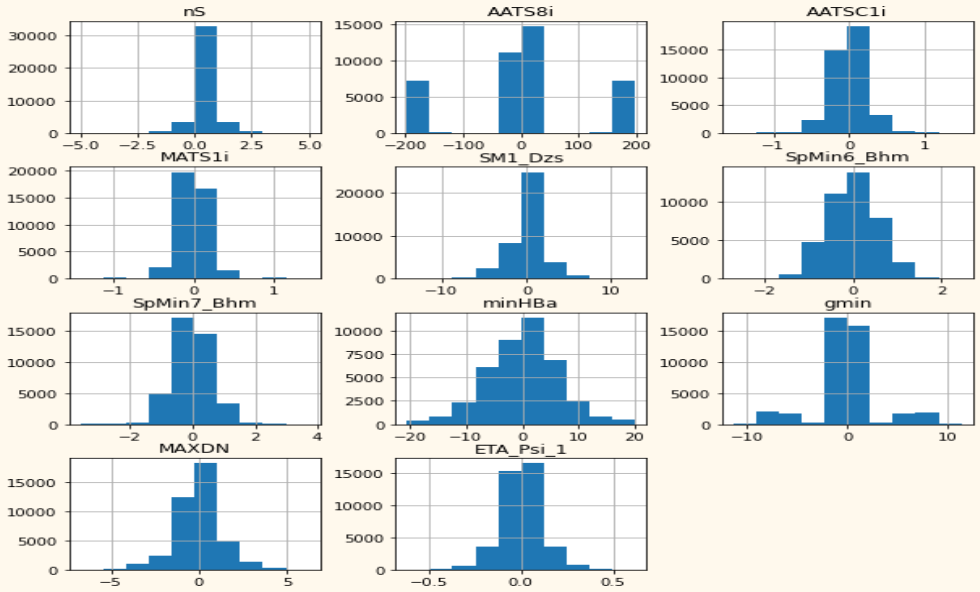
In the preprocessing part of the dataset, we worked on the **Robust scaler** (Use statistics that are resistant to outliers to scale features. The mean is separated, and the data is mounted according to the bivariate range (defaults: IQR). The IQR is the interval linking the first and third quartiles (twenty-fifth and third quantiles) (seventy-fifth quantile).) and **Quantile Transformer** (Quantile data is used to change attributes. The characteristics are transformed into a constant or standard dispensation utilizing this plan).



Fig(6): Distribution of correlation between all the 11 features and target feature



Fig(7): Most important features according to the Target



Fig(8): Features Distribution According to count and scale

3. Machine Learning Classifiers

As we get the 11 features and one target variable, we divide the dataset into X and Y, with X.Shape=(27852,11) and Y.Shape=(27852,). X contains 11 features, and Y has only the target variable.

Then we work on the Train_Test_Split method to cut the dataset into Train and Test with 80:20, such that the training dataset comprises 80% of the data, whereas the testing dataset only contains 20% of the data.

Then We apply different machine learning classifiers to the dataset, such as Random Forest, Decision Tree, K-Nearest Neighbor, and XGBoost [2]. The accuracy of the classifiers was calculated using the confusion matrix. A classifier that the highest accuracy bags can identify as the best classifier.

Random Forest -The RF is created via supervised machine learning. Random forest is a user-friendly and adaptable algorithm. Random forest is a method that, in most cases, produces good results without the use of hyper-parameter tweaking. It creates a forest out of a collection of DTs.

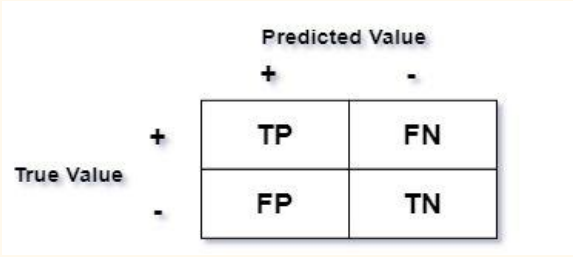
Decision tree - The DT is a supervised machine learning approach for segmenting data based on specific features. It splits the dataset into smaller and smaller subgroups as it develops the tree. There are two sorts of nodes in the tree: decision nodes and leaf nodes. In a DT, decision nodes indicate outcomes, whereas leaf nodes are where the data is split.

K-Nearest Neighbor(KNN) - K-NN is a supervised ML technique that may be used for regression and classification. However, classification is the most prevalent use. The K-NN technique implies that the latest and elderly data are similar, and it assigns the latest data to the category nearest to the standard types. During the training phase, the K-NN approach saves the data, and when new data is received, it is classified into a class that is close to the most recent data.

XGBoost(XGB)- XGBoost is a toolkit for scattered inclined boosting optimized for efficiency, versatility, and compactness. It creates ML algorithms using the Inclined Boosting framework. XGBoost is an aligned tree extending (GBDT, GBM) technique that addresses a wide range of data science problems rapidly and reliably.

Evaluation Parameters - For the assessment, we utilized the confusion matrix, accuracy, sensitivity, specificity, f1-score, Matthews correlation coefficient (MCC) score, and Cohen kappa score. The confusion matrix is a table-like structure with actual and projected values. The below we describe the confusion matrix and evaluation parameters formulas:-

Confusion Matrix -



$$\text{Accuracy} = \frac{True\ Positive + True\ Negative}{True\ Positive + True\ Negative + False\ Positive + False\ Negative}$$

$$\text{Specificity} = \frac{True\ Negative}{True\ Negative + False\ Positive}$$

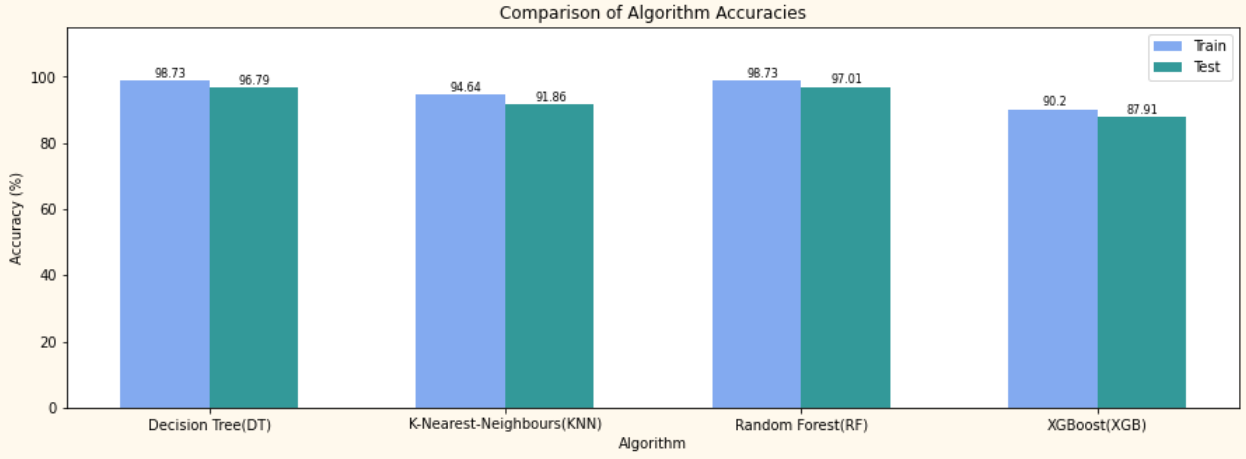
$$\text{Sensitivity} = \frac{True\ Positive}{True\ Positive + False\ Negative}$$

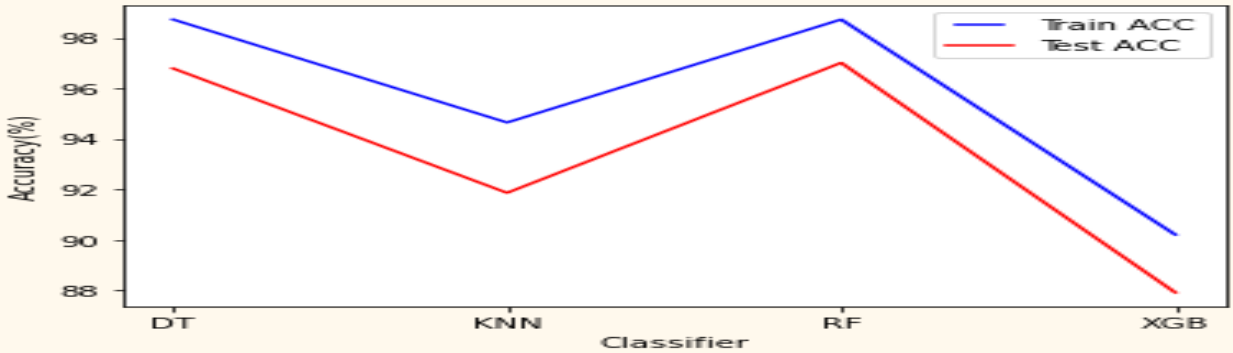
$$\text{F1-Score} = \frac{True\ Positive}{True\ Positive + 1/2(False\ Positive + False\ Negative)}$$

Results and Analysis

For our research, we divided our dataset 80:20 for training and testing. Our work achieves the best accuracy of 97.01% by using the random forest algorithm. We have used different ML classifiers for our work, and the algorithms used are RF,k-NN, DT, and XGB[2]. By using the Decision Tree, we got an accuracy of 96.79%. When we used the K- Nearest neighbor algorithm, we got an accuracy of 91.86%. The accuracy of the XGB classifier is 87.91%.

Classifier	Accuracy	Specificity	Sensitivity	F1-Score	MCC	Kappa
DT	96.79	96.79	96.79	96.79	0.97	0.97
KNN	91.86	91.86	91.86	91.86	0.92	0.92
RF	97.01	97.01	97.01	97.01	0.97	0.97
XGB	87.91	87.91	87.91	87.91	0.88	0.88





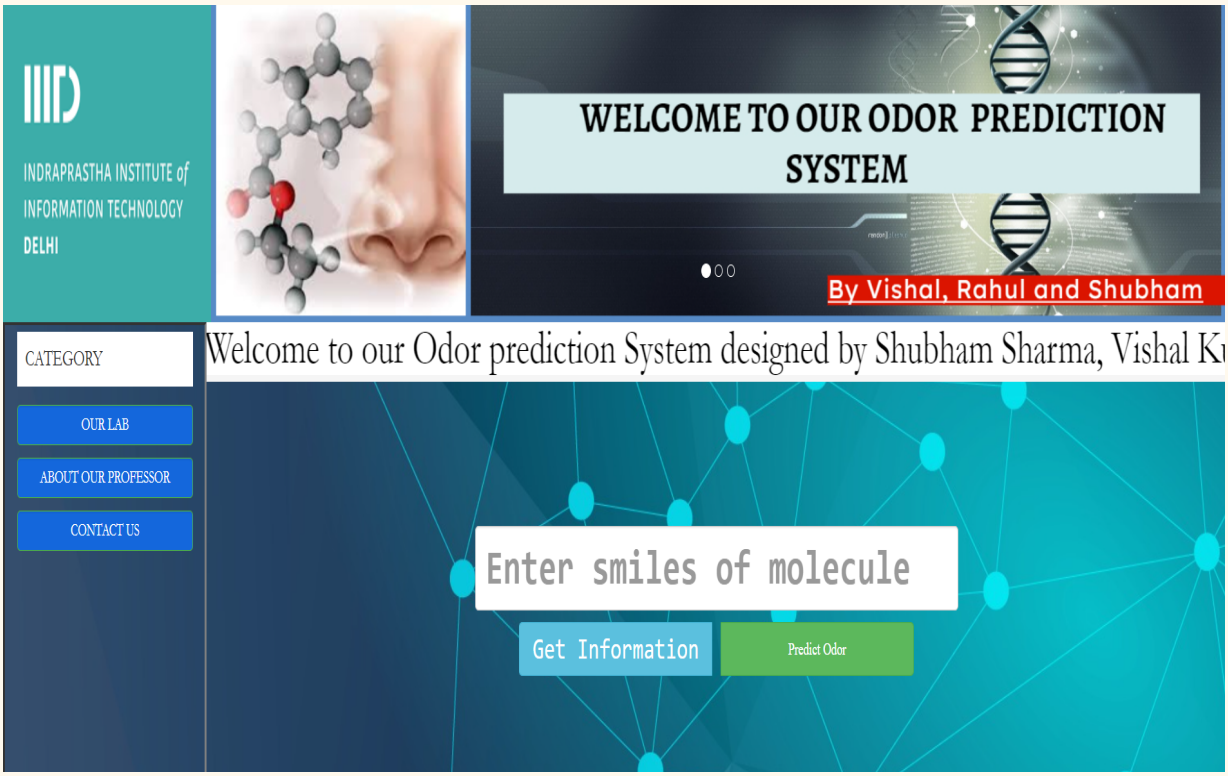
About Odor Prediction WebPage

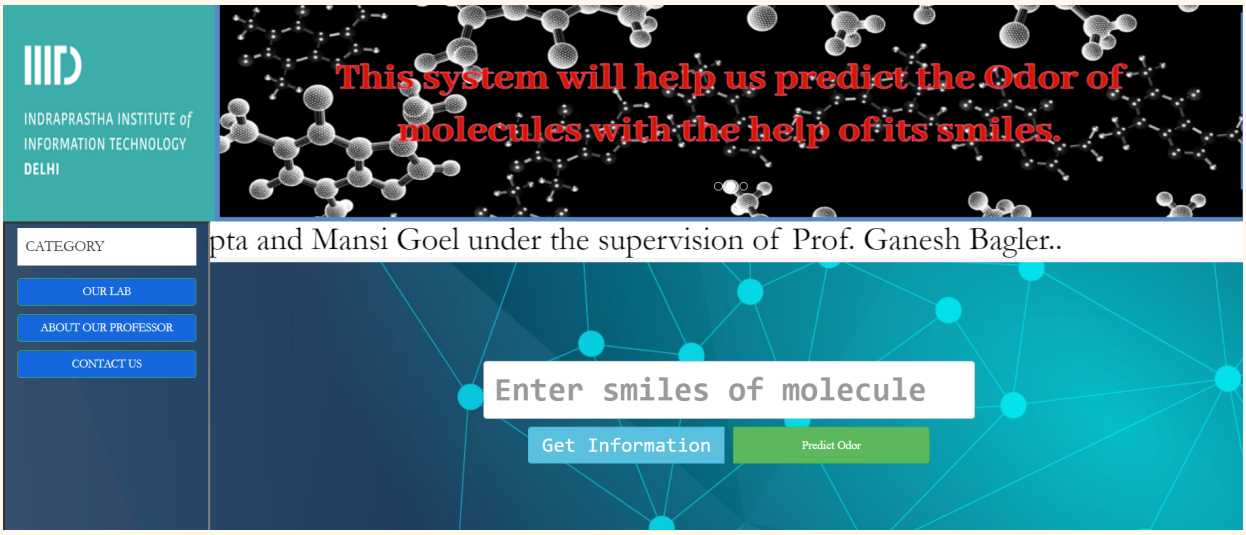
We have used different tool/technologies for building the webpage :

- HTML for displaying our web page on a web browser.
- CSS used for presentation of our webpage and managing styles etc.
- JavaScript used for creating dynamic and interactive web page.
- Bootstrap for developing responsive websites..

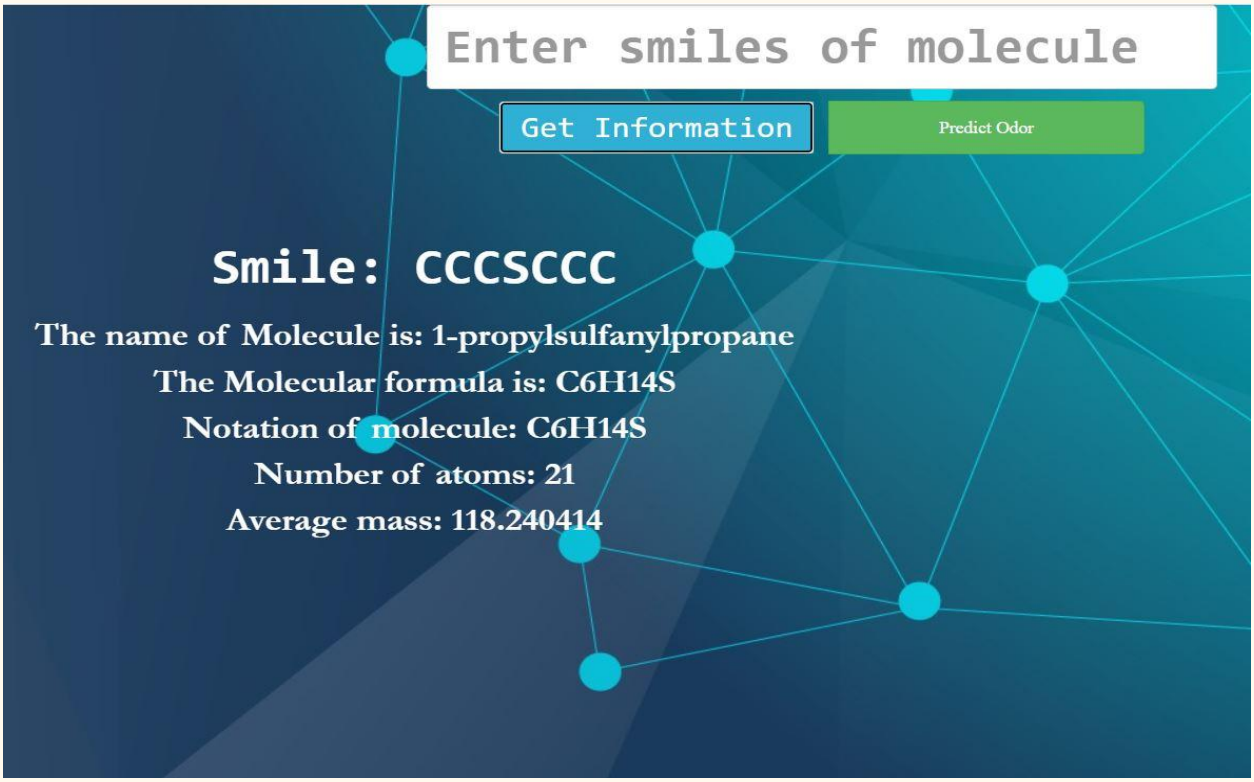
Odor Prediction WebPage

a. Our Front view of webpage

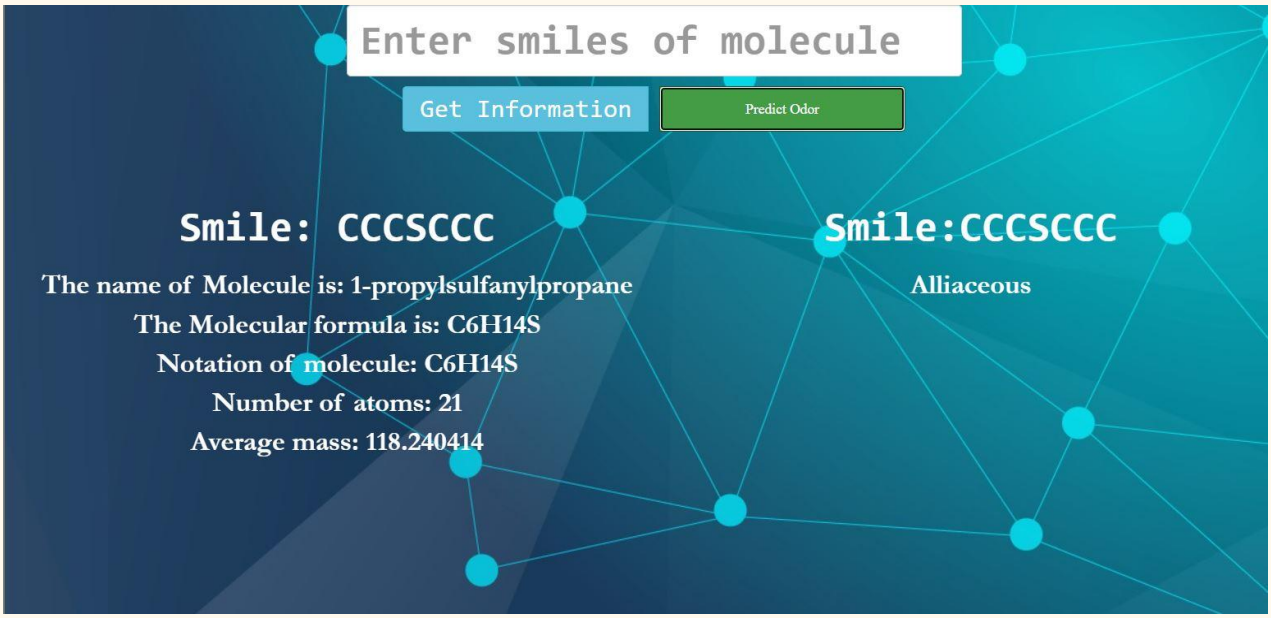




b. Enter the smile of the molecule in the text box to get molecular information of that particular smile by clicking on Get Information Button.



c. To Predict the Odor of a molecule through smile as input, click on the Predict odor button.



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