

Machine learning based Unique Perfume Flavour Creation Using Quantitative Structure-Activity Relationship (QSAR)

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Abstract—Artificial intelligence played a vital role in bringing revolutionary changes in the field of perfumery. It is much evident with events including the success of Philyra, exhibitions showcasing the ideas of this concept. Machine learning made it user friendly and more comfortable for the users by means of suggestive interaction. Machine learning also benefited the perfumers in helping them to choose the best combinations and likely successful outcomes. With growing concern about a healthy lifestyle, the thoughts about having an artificial intelligence to predict the user friendliness could be a huge success. This definitely would require a huge database comprising a large detail about diseases and the causes and combinational results of the various chemicals used in perfumery. This system may not be a completely successful one but would be reliable to a better extent. It would gain a positive response from various governmental health departments and would be encouraged by the consumers. Also, another possible development would be Artificial intelligence that is able to predict how long a perfume can last. This would let the consumer choose the one that suits the need. Through this idea we could now get a clear idea about the progress that we have made till this day. Further we can also be driven into vague ideas about how the future of Artificial intelligence would likely grow into. Machine learning and deep learning is a major pillar of artificial intelligence with larger application. Coming to our domain of discussion, artificial intelligence changed the way that things were in the past centuries about fragrance. This article proposed Quantitative structure–activity relationship (QSAR) method is used to predict the best perfume flavour. The proposed system also reduces mean absolute error (MAE). The proposed QSAR is also reducing the chemical composition and increase the perfume quality.

Keywords— Artificial Intelligence; Data Analytics; Machine Learning; Human Intelligence; Natural Language Processing; Perfume industry

I. INTRODUCTION

In the realistic situation artificial intelligence is mirror of human intelligence; it is computed in computer machine. The modern economy produces larger employability in this machine learning field. Apart from this natural language processing is also incorporate this human machine system [1]. The Traditional idea that is passed on to our minds about AI is that it is something that could function on its own to some

extent without actually needing any external assistance. The following contents are designed to explain the concepts and ideas about AI in a broader perspective. The intervention of technology into the field of perfumes has brought up immense change. Perfume industry in leading countries like France, Spain, Germany and many more has slowly inclined towards AI since the 1980s. Symrise's Philyra marked the beginning of this era [2]. Technology has upgraded our lifestyles with its various features that we use in our day to day life, one such example is the Global Positioning System commonly known as GPS, the Android technology are few of it [3]. AI is the contemporary coexisting technology that possibly would outsmart humans in the near future. Technology has influenced almost all the fields that exist. Be it contaminant existent or a non-contaminant existent technology exists everywhere. The evolution of technology in a nutshell would be the one that was created for the ease of humans to the present scenario where it poses as a threat to human existence. The recent developments of technology are immense that it has been successful in even observing the human activities and learning from it that evolved into a dimension that is termed as machine learning. As a result of machine learning, human interaction with computers has grown more interesting in the recent past [4]. One such field that AI entered and is successful over the years is the fragrance industry. Technology impacted from the way fragrant products are created till the way humans interacted with it. The Aromatic product usage by humans can be traced back to the Indus valley civilization. In the recent past Artificial Intelligence happened to be the preferable essence to create a variety of essences [5]. The major setback to perfumery was the time it took to bring out a new fragrance. This posed a huge problem to the fragrance industry. The Cologne water was a combination of various chemicals like methanol and ethanol which required a lot of precautions to be handled. The olfactory property of a substance is determined by how carefully the chemicals in it are managed and mixed. A fragrant product can't be either too pungent or too mild. Technology was assigned to solve all these problems. A remarkable note about the perfume industry is that it is a huge industry that generates revenue of more than 50 billion US dollars. TechSci Research deliberated the market size for India perfumes market using a data-driven processing, wherein perfume manufacturers' value share data for type was

documented and predicted for the following years. Research sourced these values from industry specialist and company representatives. They externally proved through examining historical sales data of respective perfume manufacturers to arrive at the overall market size [6].

II. STATE OF ART

Focusing on Machine learning, it is an incredible development in this field. The artificial intelligence is the pillar of building, there is many floors in that building. Machine learning is one of the floors in that building. The main focus on machine learning is used to develop the intelligence programme. This particular programme is used to split the data in the form of pattern. The main objective of this programme is to work without human intervention to meet the particular goal [7]. The normal data analysis is work on without this kind of machine learning program, but at the same time larger data set is need this technology. This machine learning program is providing higher accuracy. The combination technology of AI and ML is used to handle numerous amounts of data alternate name is big data [8]. It is an inevitable fact that ever since AI came into existence the major field of its application was Machine learning. The technologies mentioned in this article uses machine learning in one way or the other. The primary use of machine learning to suggest the best for the consumers based on the previous interaction interests [9]. The AI learns every day from the interaction it makes with the users. The result of this is satisfied customers and perfumers whose work is made simple. The machine learns to be best suggestive in flavours and fragrant when it comes to perfumery. The other application of Artificial intelligence that is not very uncommon here is deep learning. Deep learning is a method based on artificial neural networks and representation-based learning systems [10]. The whole idea of neural networks was inspired from the biological neural networks found in the brains of animals. It is usually learned by the already defined data and processing the raw data [11]. For example, the system is fed with examples of images having cats and a labeled cat. The system processes the images and further can differentiate and identify the raw data that has cat in them. This is widely applied throughout the different existing technologies in one form or the other to ensure the increased ease of using them. The topic of discussion gets wider and more interesting when we start learning more about it. Let us extend this discussion to different branches of technology in perfumery by analyzing the progress and its disadvantages and drawing conclusions.

III. PROBLEM STATEMENT

The existing technology, it would find a variety of interesting dimensions that AI has grown into the field of perfumery. The first one on the row would be Symrise's Philyra. The IBM research is designing pattern identification particularly larger data set. The algorithm that is used by the system works by speeding up the creation of fragrance by creating formulas which are new-fangled. This comprises algorithms that acquire knowledge and forecast the original formulas. This machine learning algorithm to generate the alternate formula and test patterns generated. These test patterns are used to analysis different composition. Philyra's data-driven approach also leverages data on fragrance families,

historical data, and industry trends. Philyra uses machine learning to come across empty-spaces in the global fragrance market and create new formulas. Symrise's perfumers are used to generate the end stage preparation [12]. This can be used on fragrance of different combination preparation. Apart from this many Brazilian company try these kind of technology to innovate new product [13]. The Quantitative structure–activity relationship (QSAR) is mainly used for the purpose of drug designing. It is also designing different kind of molecules [14]. This technique includes the toxicity and biochemical methodology. This is majorly two categories that is one dimensional and two-dimensional models; it is alternate name of classical QSAR model. This QSAR model is cost effective at the same time medium throughput. Philyra and David Apel (perfumer), created three different versions for O Boticário's Valentine's Day launch. In the machine world, this kind of AI suggestion is taken in secondary part. The final decision is taken for technical expert in that field. All three were tested, and the "overwhelming majority opted for the 100% AI-generated perfume". What about the future of humans if the usage of AI is Augmented? In general, this perfume manufacturing field is one kind of art. The reason is they can think and produce different kind of flavours. This process will take more time minimum of one year and maximum of three to four years. To avoid this kind long duration researchers, use AI technology, the first company use this AI in perfume industry is IBM with Symrise. These IBM research centers develop different kind of flavour by using AI technology. This year, flavour and fragrance company Givaudan unveiled CARTO, a system designed to use the Odours Value Map to maximize olfactory performance in final formulas of flavours and fragrances. Turns out creating fragrances are an art and a science. Master perfumers still have the emotional advantage over AI, so until that changes, AI will augment human expertise in fragrance development.

The next one on the list is Scent Bird's Confessions of a Rebel [15]. The famous direct-to - consumer based company Scent bird launched a new gender -fluid sub-brand confessions of a Rebel. It also used AI in this project. The working of AI that was used is based on the consumer data and consumer reviews that are collected [16]. The AI used these data to create four initial mother fragrances of its own [17]. This feat of new application of AI was successful with the help of over million data points from as many as 3 lakhs users that it utilized [18]. Adding to their new development the company introduced another innovative move to let the customers select their own descriptors that included fresh, clean and sexy rather than the old ones like citrus, floral or woody. The edge that has over the others is that this AI software is capable of giving access to the patterns within the large subscriber database. This consequently resulted in letting the company produce new fragrances by considering the user reviews and their preference in accordance to the fragrance notes. It finds its application in confessions of a Rebel's four gender fluid fragrances. The next one is, Sommelier Du Parfum, the AI used in this was very handy and could be said as one of the best user-friendly software in the field. This is an AI powered phone application that helps the user in identifying the fragrance of one's choice. The application uses a set of questionnaires to analyses the user's lifestyle and their preferences. It processes the data and

gives out a suggestion from its database of over 30,000 fragrances. This allows the user to choose the product of their choice. It then shows the user the nearby supermarket where one could try them. The suggestion includes any shop from smaller boutiques to the largest retailers. The fragrance information includes olfactory notes, perfumer and fragrance history and toxicity assessment along with ingredients. The major edge it has got over the rest of all technologies is that it is a mobile friendly application. And it also makes the consumers aware of the various other fragrance products available in the marketplace. This application is currently used in the US where it helps customers to buy in over 8000 stores. The next one is Algorithmic Perfumery. In Layman's terms it can be simply said as the best interactive personalized perfumery method. The AI allows the user to create their own personalized fragrance. It uses a variety of software for this process. This algorithmic perfumery is refined all the time as new users keep letting the AI learn new things every time. So, it adapts and learns from every exchange. The Dutch based founder Frederik Duerinck who started a company in Netherlands has presented this Algorithmic perfumery at many major festivals and exhibitions throughout the last year. This was aimed to make a difference in the way everyone interacts with the fragrance, to leave them with a unique experience since everyone one has their own ideas. This includes the Fragrances with under explored locative categories. Where it is used today, it was exhibited in almost all the major exhibitions and festivals throughout Europe, and North America.

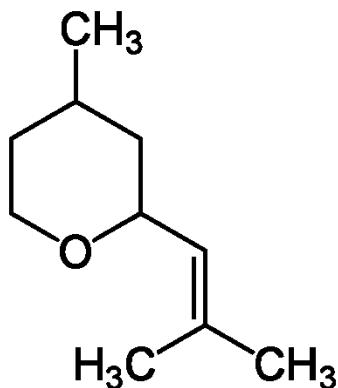


Figure 1: Rose Oxide Molecular Sample

The figure 1 is to sample molecular diagram of rose oxide. The next one on the list is Coty's VR Experience, this is a multi-sensorial VR experience launched in Argentina. It was launched in collaboration with a retailer Julie Rague and powered by AI again. It uses the senses of touch, smell, sound and sight to match the consumers with the right fragrance without making an error on the fragrance of being more intense on unexpected accounts. So, it works basically when a user wears a VR headset and picks up a fragrant stone that is associated with a broad variety of scents like citrus watery, and at the end of the video the consumer is offered with many suggestions related to that. This gives the consumer a better experience with the fragrance and thus making the interaction

more live. This can be made to adapt at any market situation and is most useful to guide the consumer into the World of fragrance. Coty is planning to bring this experience to the additional markets and tailoring the experience into a broader way. The last and a perfumer-based AI is Givaudan's Carto, this one enhances the Perfumers imagination to create a fragrance. The advantage is it accelerates the rate at which the new flavour of perfume is developed. The interactive touch screen enabled AI could refer to anything from the historical fragrance notes to the now available stock of the company and the ones that are in R&D and from consumer's data. The system also involves a sampling robot that could immediately produce a fragrance trail. It allows the perfumer to play and experiment with the fragrance in the same time taking reference from all the sources. It is also being able to give out fast samples. This is used in Givaudan's fragrance creative centers in all regions.

IV. PROPOSED METHODOLOGY

Bringing in development over a period of time alone enhances the survival of any industry. In an industry like perfumery bringing in consumer-centred developments would result in multiplying the profits. One drawback that the industry would face is the side effects due to the usage of the products. To overcome this best solution was needed. Fragrant products mostly have a direct contact to the skin. The common products like roll on, deo sticks and body spray interact directly with the skin. The effects caused by these products should be minimal so that it is more user-friendly also the production cost involved must be economical in order to ensure the product's success. The QSAR processing is three major steps. First one is preparation; this step is to prepare the data set and sent to further process. Second step is data analysis, after preparing the data that data should analysis and sent to further and final process of validation.

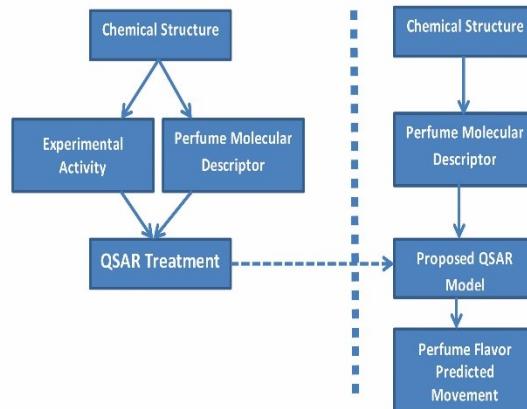


Figure 1: Proposed flow model using QSAR

The Fig. 1 is the proposed flow analysis model in the QSAR treatment. This flow model will help to demonstrate the perfume flavour prediction. The initial level of this proposed model is chemical structure that should be connected with experimental activity with perfume molecular descriptor. This

experimental activity is used to analysis the different composition; this process is automatically design different types of perfume flavour by using different chemical. That same block another subcomponent is molecular descriptor; this will help to analysis molecular calculation. The calculation process is done and sent the quality and unique perfume composition will send to QSAR module. This QSAR block is working with the principle of quantitative structure that will be predict the activity relationship. The proposed block diagram finally predicts the unique perfume flavour. Proposed QSAR model is to find the quality and unique perfume composition. The improvement of quality is to minimize the mean absolute error (MAE). The main role of experimental activity is to find the chemical reaction; this is pre-process step of QSAR.

This interaction with perfume products is often associated with high level risks of skin diseases like cancer. One of the important scenarios in this perfume industry is smell. This smell plays a vital role different manufacturing industry. This smell is varying in the basis of chemical composition, at the same time possibilities of opposite reaction in human body is more because of wrong chemical composition. Whilst we can't point to single compounds as being the cause of perfumes scents, we can identify those that have a major impact on the aroma that our noses detect; in many cases, there will be molecules that make a large contribution, and it's those we'll speak off here. The table 1 gives us an idea about how different chemicals are involved in the process of perfume making. Not all chemicals are harmful, but a few are quite dangerous and are found to be responsible for a variety of diseases. The reports from the research work carried out by the National Academy of Sciences concluded that styrene, a basic building chemical used in perfume, could cause cancer in the long run. Adding on to this it was found that 35% of Americans suffered from respiratory migraine caused due to fragrance products. The study made by Silent spring Institute in 2018 found that a fragrant marker called Diethyl phthalate was responsible for causing endocrine-disruption and asthma.

Table 1: Different Chemicals Composition in Perfume Making

Flavours	Component 1	Component 2	Component 3
Roses	(-)-cis-rose oxide	(-)-stereoisomer	beta-ionone
Carnations	eugenol	beta-caryophyllene	methyl salicylate
Violets	Alpha-ionone	Beta-ionone	Beta-dihydroionone
Lilies	Linalool	(E)-beta-ocimene	Myrcene
Hyacinth	Ocimenol	cinnamyl alcohol	ethyl 2-methoxybenzoate
Chrysanthemums	eucalyptol	chrysanthenone	alpha-pinene
Lilacs	(E)-beta-ocimene	Lilac aldehyde	Lilac alcohol

The reports are never ending with another one that is Benzyl Chloride that is associated with Vanilla scent that was found to be responsible for breast cancer. We would end up in a plethora of cases and reports filed at different times which are related to the hazards caused by the chemicals associated with fragrance products. We could conclude that the need of the

hour is to reduce the growing rates of developing diseases. Taking in consideration the recent developments in the AI based Cancer prediction system, it is more based on data and trend-based analysis than actual cell testing and test-results based methods. So, the best possible AI development that can be brought up is one that takes in details about all the inputs added to the perfume and pre fed data about its impacts. The data must include the possible combination of chemicals and how they could cause harm to humans when they come in contact whenever they are in any given propositions. The huge data might need a lot of experimentations but it's a one-time effort that could be of huge result. This can be added with possible alternative chemicals that could substitute the harmful ones. The developments in this aspect of perfumery could be beneficial to both the sellers and consumers. This can be installed in the next stage after bringing out the formulas. The perfumer can feed in his ideas and the possible chemicals it would require to the AI and the AI would in turn give a result about how the chemicals can be harmful. And the already existing AI Givaudan's Carto which is capable of using all the data as we know already and that could be linked with this get the alternative suggestions. This AI may also be associated with the algorithm to predict how efficient and how much lasting can a perfume be based on the chemicals and consumer feedbacks. How successful will this be? With growing concern about health and healthy lifestyle, we can be assured that this would be encouraged and in fact would be funded easily since it has a lot to do with the consumers. In the most competitive era earning the trust of the consumers is the major need and these improvements are a step towards it.

V. RESULT AND DISCUSSION

The proposed methodology provides different flavour of perfume. That flavour will design with the help of AI. There are several parameters will help to analyze the performance of proposed solution. The analysis will made quality check, that quality check will compare the chemical level with smell. The initial level comparison is chemical level analysis that is minimal level of chemical and provides higher quality. So, this analyze will compare chemical level with AI and without AI usage. The table 2 and figure 2 is to elaborate chemical level comparison. That indicates different flavour of perfume is having chemical composition levels. For example, rose flavour of perfume using AI selection chemical level is 72%, at the same time without using AI chemical level is 80%. Without AI process totally 8% higher chemical levels. Similar to those other flavours also providing lesser chemical level by using AI. This proposed method provides better result compare to existing methodology.

The table 2 and Fig. 2 are to elaborate chemical level comparison. That indicates different flavour of perfume is having chemical composition levels. For example, rose flavour of perfume using AI selection chemical level is 72%, at the same time without using AI chemical level is 80%. Without AI process totally 8% higher chemical levels. Similar to those other flavours also providing lesser chemical level by using AI. This proposed method provides better result compare to existing methodology. There are several parameters to check QoS, one of the major constraint in the marketing is cost. The proposed AI based perfume composition analysis is also

providing cost effectiveness. The manufacturing cost is compared with the chemical usage cost and flavour base material cost.

Table 2 - Chemical Molecule Level Comparison

Flavours	Chemical Level With AI (%)	Chemical Level Without AI (%)
Roses	72%	80%
Carnations	81%	84%
Violets	69%	69%
Lilies	56%	59%
Hyacinth	62%	63%
Chrysanthemums	85%	81%
Lilacs	74%	75%

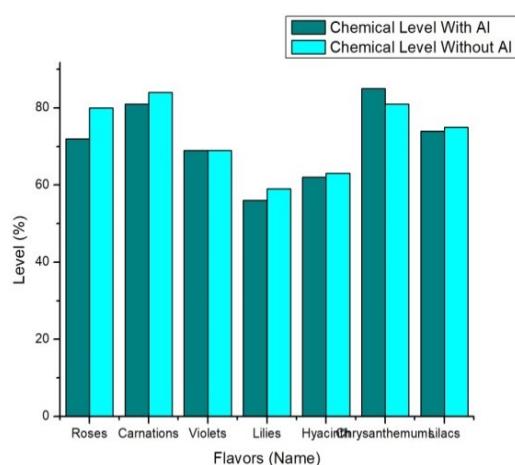


Figure 2: Different Molecule Chemical Level Analysis

Table 3 - Cost Analysis Comparison

Flavours	Manufacturing Cost Using With AI	Manufacturing Cost Using Without AI
Roses	Rs. 280	Rs. 300
Carnations	Rs. 320	Rs. 350
Violets	Rs. 510	Rs. 500
Lilies	Rs. 240	Rs. 210
Hyacinth	Rs. 170	Rs. 160
Chrysanthemums	Rs. 230	Rs. 220
Lilacs	Rs. 410	Rs. 400

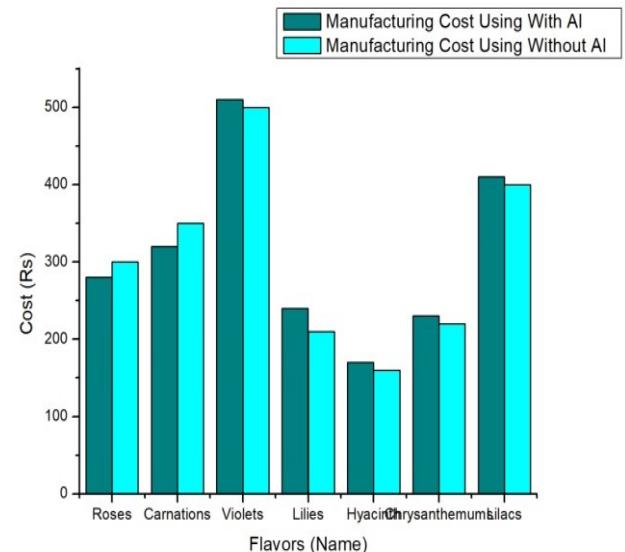


Figure 3: Manufacturing Cost Analysis

The table 3 and Fig. 3 is to compare manufacturing cost of different perfume flavour. Based on the result, by using AI provide the better result. That indicates manufacturing cost is reduced compare to without AI involvement. Reason for this is using AI chemical is reduced so automatically manufacturing cost also reduced. The equation 1 α is measuring the mean absolute error. X_i is the without QSAR and Y_i is the with QSAR.

$$\alpha = \sum_i \cup_{n=1}^m (X_i \cap Y_i) \quad \dots \quad (1)$$

The table 4 and Fig. 4 are to compare Mean Absolute Error (MAE) of different perfume flavour. Based on the result, by using QSAR is reduce the error rate. That indicates manufacturing quality is increased compare to without QSAR model. The error rate indicates direct and indirect level of quality. The mean absolute error rate is highly important because based on that value the proposed chemical flavour quality is measured.

Table 4 - Mean Absolute Error (MAE) Comparison

Flavours	Mean Absolute Error Value Without QSAR (eV)	Mean Absolute Error Value Without QSAR (eV)
Roses	0.42	0.36
Carnations	0.51	0.42
Violets	0.34	0.22
Lilies	0.39	0.26
Hyacinth	0.42	0.37
Chrysanthemums	0.65	0.58
Lilacs	0.37	0.25

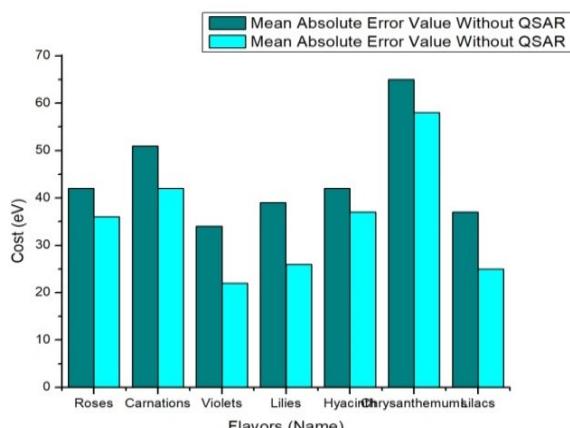


Figure 4: Mean Absolute Error (MAE) Analysis Using QSAR

VI. CONCLUSION

This article is help that the need of the hour is to realize that the time left before artificial intelligence challenges human existence is less since AI has already outdistanced its early stages. When it comes to Perfumery, AI inflicted an immense change in the way that humans interacted with fragrance and made the life of Perfumers more comfortable over the years. The near future would witness Symrise's Philyra taking over the complete process from designing to producing or Sommelier Du parfum completely assisting the consumers from choosing a fragrant product of their choice to getting it to their home step or anything much more that won't be a surprise. The proposed method prefers artificial intelligence as the best solution of this hour since it is better when it comes to performance since it is reliable and specified. But the entire process will result in a disaster if it fails in bringing out new and much deserved inventions in the field like the above discussed ideas. Stephen Hawking predicted that Artificial intelligence is taking away our jobs. This leaves us with options to grow with the flow or be prepared to be left out. Elon Musk on multiple occasions quoted that Artificial intelligence would not result in something really positive. At this part of the history the things that we need to be really worried about are, one is the prediction about artificial intelligence being equally smart as humans in the 2060s and the second is the net economic contribution of around \$15.7 trillion by 2030. The proposed QSAR method is providing less error rate, it is providing 0.0914eV less error rate compare to existing method.

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