

Qualitative Analysis of Chemical Components of Jasminum Sambac and Rosa Damascena by Gas Chromatography-Mass Spectrometry and Its Influences on E-nose to Classify Odour

Sasedharen Chinnathambi*, Gopinath Ganapathy*

School of Computer Science and Engineering, Bharathidasan University, Tiruchirappalli, TamilNadu, India

*Corresponding author: sasedharentc@gmail.com, gganapathy@gmail.com

Received November 14, 2022; Revised December 23, 2022; Accepted January 05, 2023

Abstract The significance of insight of smell, the equivalent olfactory communication and the perspective of culture towards olfaction vary through the ages. The E-nose research discipline has experienced a tremendous growth in recent times, creating a new need for tools and algorithms to quickly analyse olfactory representation in digital format, i) detects substance smell, ii) implements pattern matching theorem for acknowledging those substances (Chemical Compounds), iii) the accuracy and reliability of reproducing predicted data, over internet. The current research aims to identify the Chemical Compounds of Indian Jasminum Sambac and Rosa Damascena, calculating the Molecular Mass, and Parts Per Million by Solid Phase Extraction and Natural Drying method using Gas Chromatography-Mass Spectrometry. For each chemical compound, Peak Area is converted into Parts Per Million and this is the key factor for the classification of Future E-nose technology. The two floral plants Jasmine and Rose chemical composition were taken for the study of E-nose since these flowers have attained commercial significance in India. In the current study, Jasminum Sambac and Rosa Damascena concrete extraction was carried out by solvent extraction with Hexane. A procedure for Solid Phase Extraction and Natural Drying of Gas Chromatography-Mass Spectrometry analysis of Rose and Jasmine Flower is presented. This paper describes the state of Gas Chromatography-Mass Spectrometry considering the Solid Phase Extraction for Chemical Characterization of Chemical Compounds and its influence on Odour Classification by E-nose. The Odour of this absolute sample was examined as intense and heavy floral-flowery. The main advantages of these two methodologies are an expeditious, selective, and sensitive determination of chemical compounds in floral flowery.

Keywords: gas chromatography, mass spectrometry, Odour, volatiles, natural drying, solid phase extraction

Cite This Article: Sasedharen Chinnathambi, and Gopinath Ganapathy, "Qualitative Analysis of Chemical Components of Jasminum Sambac and Rosa Damascena by Gas Chromatography-Mass Spectrometry and Its Influences on E-nose to Classify Odour." *Applied Ecology and Environmental Sciences*, vol. 10, no. 12 (2022): 766-775. doi: 10.12691/aees-10-12-10.

1. Introduction

Numerous studies have focused on olfactory media content to enhance the perception of an aroma's presence in form of multimedia contexts. Though the human olfaction system is the most essential system and analytic, the effective instrumentation for odour evaluation, there exists a demand! Since their creation, the widely utilised aromatic and medicinal plants have been used to flavour food and medicines as well as for their medical and preservation properties. The physical attributes of a flower-Odour, Shape, Size, Color, and Weight-are traditionally used to assess its quality. There is inadequate research had been done on Jasmine and Rose Flowers of Indian Origin especially based on their chemical profile and the importance of PPM for the classification of odour

by E-nose. It is fascinating to discover that while the E-nose is effective at identifying grade differences brought on by volatile organic concentrations, it falls short when it comes to identifying the key scents that contribute to the distinctive qualities of outstanding grade jasmine samples [1]. GC-MS is an ideal tool for identifying those unknown substances or contaminants which identifies and evaluates untold samples, contaminants, trace elements in specimens, environmental effects on samples and more.

Gas chromatography for the identification of chemical compounds and quantitative analysis of floral extracts are carried out in the current study. The E-nose is now transposed with the exposure of digital olfaction concentrated on the digital detection and examination of various odours (classification). GC-MS segregates each compound into ionized fragments and identifies those fragments according to their mass-to-charge ratio [2]. Many of the organic pollutants that are found in complex

food and environmental samples at detectable amounts may only be measured effectively using GC-MS [3]. The therapeutic properties of *Jasminum* samples are important in perfumery, cosmetics, food flavouring, and medical applications because they act as an antidepressant, expectorant, antiseptic, sedative, and other things [4]. A comparison of GC-MS detected volatiles in flower extracts and distilled rose extracts of different rose genotypes was conducted in order to assess the impact of floral volatile composition and abundances on the rate of recovery of the volatile compounds [5]. It's a vital module that the sensor array of metal oxide semiconductors, can simulate the human nose and generate corresponding signals for floral gases [6].

2. Material and Methods

2.1. Fabrication of Floral Fragrance

An effective investigation of an odour, requires smell measurement techniques by implementing standard scientific methods. In comparison with other analytical approaches, the reason behind Natural Drying [7] is characterized by a better perception of odour, minimal time implemented for sample preparation, the benefits of promptness, and relatively inexpensive analysis. Moreover, the physical property of a dried sample is essentially fundamental w.r.t re-moisten, which is defined in terms of the capacity of dried floral flowers back to their natural flavors. SPE [8] is considered the most appropriate method for the identification of the desired analytes and compounds since it is suitable for detecting Physicochemical properties.

2.2. Sample Preparation and Storage

The sampling process ensures the sample integrity, regulates the odour primitively associated with the sample, and decreases losses and chemical-physical phenomena between odourants and the sampler medium.



Figure 1. Natural dried Fresh flowers in the well-ventilated room, temperature range at 28-32°C (Day 1)

2.2.1. Natural Drying Method (ND)

The Indian *Jasminum Sambac* and *Rosa Damascena* were collected from farmers, air-dried for 8-10 days, and crushed into powder. For extraction of the concrete, the flowers were dried (Figure 1, Figure 2) by spreading the samples on the paper to avoid moisture and drying at ambient air temperature in a well-ventilated room with temperature ranges between 28–32°C. The traditional drying method also includes, Blast or Oven drying at the

temperature range of 50°C; Heat pump or Hot-air drying at the temperature of 50°C and air velocity at 1.5 ms⁻¹; Vacuum Freeze-drying at the temperature of -45°C and vacuum pressure of 10–30 Pa for 24 h.



Figure 2. Moistureless dried J.Sambac and R.Damascena (Day 8)



Figure 3. Samples ready to be treated with Ultrasonication water bath



Figure 4. Ultrasonication removes the dirt and makes the samples solvable by breaking the bonded particles

Note that, the various drying processes had multiple effects on the color, odour index, and volatile compounds [9] of the given sample. The Concrete content of flowers was analyzed by solvent extraction method with Hexane, averaged, and expressed in percent of the concrete recovery. A 5.0 g of Moistureless dried J.Sambac & R.Damascena was grounded into a fine powder and transferred into a polyethylene centrifuge tube (Figure 3) containing 20 ml of Hexane as solvent. The centrifuge tube was kept in an ultrasonic bath (Figure 4) for 10 min. The solution was filtered with membrane filter paper to remove the impurities and was used for SPE extraction of chemical components. Practically, 1-5 gm of sediment is weighted and transferred to the bottle. 20ml (15 mins x 2 times) to break the particles and make them solvable. 90% of the Hexane-containing chemical components were recovered after ultrasonic extraction and the rest were lost during the cleaning process. The upper layer of the extract is transferred into Rotavapor Evaporating Flask (Figure 5) to remove the solvent from the flower sample through evaporation under reduced pressure. It leaves a concentrated compound in the original round bottom flask. The excess solvent is then evaporated to bring the volume to 1 ml. Finally, samples are analyzed in GC-MS.



Figure 5. Rotavapor evaporating, to remove the solvent from the flower sample

2.2.2. Solid Phase Extraction (SPE)

This identifies odour-causing compounds, and analyses long-lived volatile organic compounds given off by a sample during heating or overtime. 1 gm of a typical sample uses a “purge and trap” method where the sample is placed in a heated vessel and the vessel is purged with a carrier gas. Here, Helium is the carrier gas at a flow rate of 4 ml/min with a supply pressure of 300 – 980 kPa. The volatile components escape into the head-space [10] above the sample. The head-space gas is then injected into a gas chromatograph which separates the various components of the sample based on size and polarity.

3. Chemical Analysis (with Speciation)

In general, odour measurement methods are categorized as *sensorial* or *instrumental*; and they can be applied at the *emission level* or *receptor level*. At the emission level, the *sensorial method* includes, i) Dynamic Olfactometry, ii) Gas Chromatography-Olfactometry (GC-O) and the *instrumental method* involves, i) Chemical Analysis, ii) E-Nose. The chemical analysis (with speciation) of odourous emergence belongs to the complete identification and measurement of odourous chemical components in an odour sample. GC-MS has been widely used to examine air quality in order to bring forth a list of substances involved and their concentration, it hardly relies on the complexity of odour [11]. To clarify the components of the J.Sambac and R.Damascena in this present study, at first, a method for identifying the volatile compounds was determined (SPE), and then the major chemical components were investigated, including their absolute configurations. In particular, Hexane is recommended as a solvent surfactant for use in GC-MS, as it can produce good results of even low levels of Semi-Volatiles/VOCs and often gives cleaner extracts. In

addition, alkanes in general are very stable and doesn't react with any other substances, likely to be in a sample for GC-MS analysis. A non-polar solvent such as Hexane is used here to draw out the aromatic compounds from the flowers.

4. Analysis of Chemical Compounds in Injected Samples

To identify the unknown chemical compounds in the 1-2 μ l of the injected sample, we used a SHIMADZU's GCMS-QP2010 SE (Figure 6), installed with a Capillary Column (0.25 mm $\times$ 30.0 m $\times$ 0.25 μ m). We used Helium as the carrier gas at a flow rate of 4 ml/min with a supply pressure of 300 - 980 kPa. The injector temperature was set at 200°C. The oven temperature was initially programmed at 40°C for 2 min, then increased from 40°C to 200 °C at 15°C/min, and held at the temperature for 1 min.

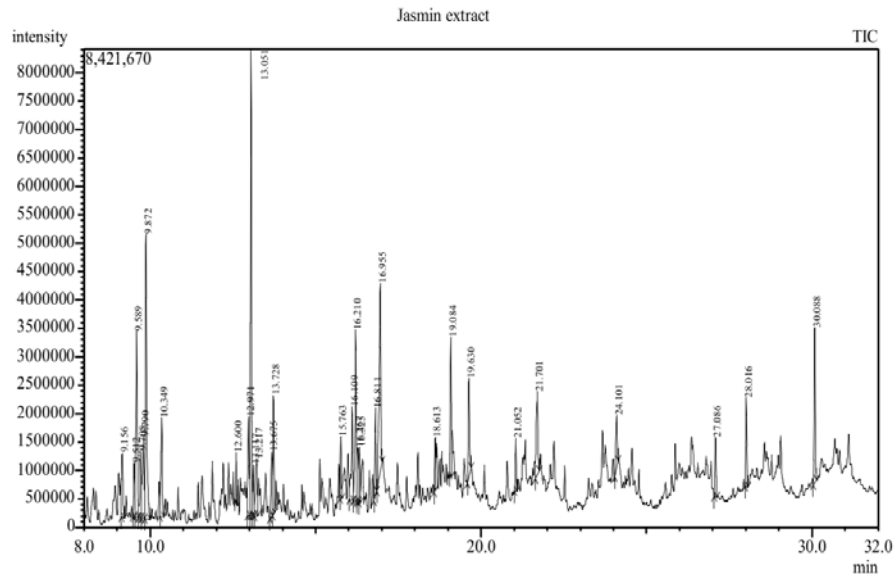
The best outputs in terms of the peak quality and coherence of the extracts were obtained which were examined for further analysis. The mass spectrometer breaks each molecule into ionized fragments and discloses these fragments using their mass-to-charge ratio and identifies every compound individually.

5. GC-MS Data and Statistical Analysis

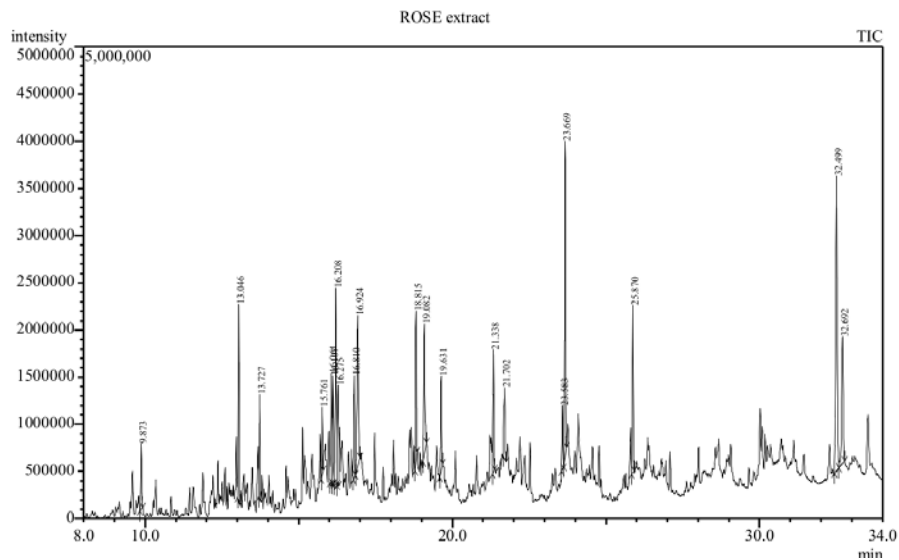
The following graphs shows, Total chromatograms of authentic standards of the identified constituents of Jasminum Sambac and Rosa Damascena; We obtain a chromatogram, a graph where we can discover different peaks, each peak attributable to the different compounds distributed by the GC column in the function of time; Graph 1 & 2 determines Sonication followed by Solid Phase Extraction (SPE) and Graph 3 & 4 outcomes, Sonication followed by Natural Drying (ND) Method.



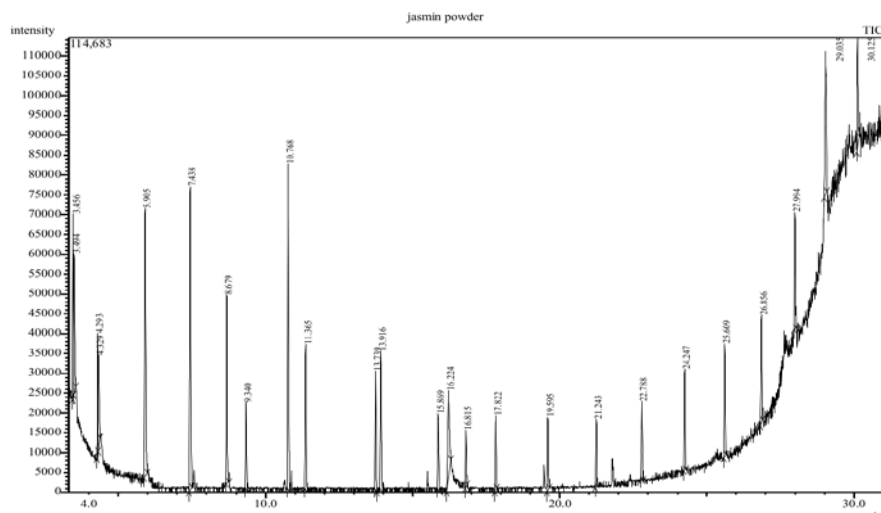
Figure 6. SHIMADZU's GCMS-QP2010 SE with a Capillary Column (0.25 mm $\times$ 30.0 m $\times$ 0.25 μ m)



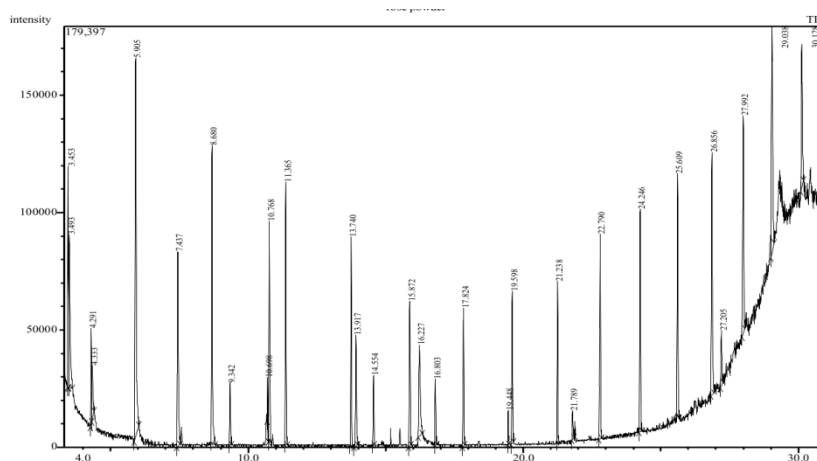
Graph 1. Total chromatograms of authentic standards of the identified constituents of *Jasminum Sambac*; peaks shows retention factors corresponding to identical compounds found in Solid Phase Extraction in chromatograms



Graph 2. Total chromatograms of authentic standards of the identified constituents of *Rosa Damascena*; peaks shows retention factors corresponding to identical compounds found Solid Phase Extraction in chromatograms



Graph 3. Total chromatograms of authentic standards of the identified constituents of *Jasminum Sambac*; peaks shows retention factors corresponding to identical compounds found Natural Drying Method in chromatograms



Graph 4. Total chromatograms of authentic standards of the identified constituents of Rosa Damascena; peaks shows retention factors corresponding to identical compounds found Natural Drying Method in chromatograms

We have identified the set of chemical compounds for a given odour and investigated major aroma characteristics with jasmine and rose samples through distinct techniques. More than 25 components have been found in indian jasmine and rose samples, with the main chemical compounds being 2,4-Di-tert-butylphenol, Eicosane, Heptadecane, Pentadecane, Heneicosane, Octadecane, Tetracosane, Tetracontane. Some volatile compounds have also been found either in low concentrations or as trace elements. Here we present a mechanism SPE for solvent extraction of native jasmine flowers and comparative GC-MS analysis of rose flowers and related volatiles.

6. Calculating Molecular Weight (g/mol), % Composition of a Mixture, and PPM

To calculate the **Molecular Weight** of an identified chemical compound, we need to find the Atomic Mass of individual elements.

Step 1: Identify the Atomic Mass of individual elements (Ex: Carbon, Oxygen, Hydrogen, Nitrogen, Phosphorous)

Step 2: Calculate the Total No. of Individual Elements among identified Chemical Compounds

Step 3: Multiply the Total No. of Individual Elements by their Atomic Mass

Step 4: Finally Add those Values together gives the Total Molecular Weight in g/mol.

Example,

Atomic Mass of Carbon, 12.011; Atomic Mass of Hydrogen, 1.0078;

Atomic Mass of Oxygen, 15.999; Atomic Mass of Silicon, 28.0855;

Atomic Mass of Silicon, 28.0855; Atomic Mass of Phosphorus, 30.973762

For **Undecane, 2,4-dimethyl, $C_{13}H_{28}$** (One of Chemical Compound of Jasminum Sambac, identified by GC-MS, See [Table 1](#) below)

Total No. of Elements C, H, among identified compounds => C - 13, H - 28

Calculating the Molecular Weight

$$= C * 12.011 + H * 1.0078$$

$$= 13 * 12.011 + 28 * 1.0078 = 184.36 \text{ g/mol}$$

The % Composition of a Mixture

Here we determine the amount of each compounds, the percent composition of a mixture of volatile liquids. In general, the percent composition is directly related to the area of each peak in the chromatogram. The percent composition of a compound can be found by using one of the following methods:

Method 1: Calculating the area of each peak

Step 1: Calculate the area under the peaks using the equation:

$$\text{Area} = \text{Height of Peak} * \text{Width at half the height}$$

Step 2: To obtain a percent composition for the mixture, we first add all the peak areas from Gas Chromatogram.

Step 3: Then, to calculate the percentage of any compound in the mixture, we divide its individual area by the total area.

Step 4: Finally, multiply the result by 100.

Example,

% Composition of 1-Undecanol (One of Chemical Compound of Jasminum Sambac, identified by GC-MS, See [Table 3](#) below)

$$= \frac{\text{Area of Undecane, 2,4-dimethyl}}{\text{Total Area of Identified Compounds}} * 100$$

$$= \frac{47577}{1151148} * 100$$

$$= 4.13\%$$

Method 2: Calculating the molar mass of the elements

Step 1: Calculate the molar mass of all the elements in the compound in grams per mole.

Step 2: Calculate the molecular mass of the entire compound.

Step 3: Divide the component's molar mass by the total molecular mass.

Step 4: Finally, multiply it by 100% to get percent composition

% Composition of Eicosane

(One of Chemical Compound of Jasminum Sambac, identified by GC-MS, See [Table 2](#) below)

$$= \frac{\text{Molar Mass of Eicosane}}{\text{Total Molecular Mass / Weight}} * 100$$

$$= \frac{282.6}{4618.7} * 100 = 6.12\%$$

Calculating Parts Per Million (PPM)

- To perform the conversion, from Percent of Composition of a Mixture(a chemical compound) to PPM, multiply the value in percent by 10,000 or 10^4

$$PPM = \% \text{ Composition of a Mixture} * 10^4$$

For **Heptadecane**, One of Chemical Compound of Jasminum Sambac, See [Table 1](#) below

$$\% \text{ Composition of a Mixture} * 10^4 = 20800 PPM$$

The following tables ([Table 1](#) – [Table 4](#)) shows the chemical composition and odour description of some major constituents of Jasminum Sambac and Rosa Damascena absolute samples from India (Tamilnadu)

Table 1. The Chemical Composition and Odour Description of Some Major Constituents of Jasminum Sambac – SPE Method

Compound	Chemical Formulae	RT	MW	BP °C	MP °C	Area in % (% Composition of a Mixture)	PPM	Odour
Undecane, 2,4-dimethyl	C ₁₃ H ₂₈	9.16	184.3614	218.9 ± 7.0	N/A	1.89	18900	Gasoline-like to Odorless
Eicosane	C ₂₀ H ₄₂	9.51	282.5476	343.1	36 - 38	1.46	14600	Colorless, Odourless, Waxy Crystals
Eicosane	C ₂₀ H ₄₂	9.59	282.5476	343.1	36 - 38	6.68	66800	Colorless, Odourless, Waxy Crystals
Heptadecane	C ₁₇ H ₃₆	9.71	240.4678	301.9	21.1 - 22.9	2.08	20800	Colorless Liquid, Odourless
Pentadecane	C ₁₅ H ₃₂	9.79	212.4146	270	16.8 - 10	3.52	35200	Oil of D. Guineense Fruit, Colourless Liquid
2,4-Di-tert-butylphenol	C ₁₄ H ₂₂ O	9.87	206.3246	253	37	9.57	95700	Characteristic Odour
Eicosane	C ₂₀ H ₄₂	10.35	282.5476	343.1	36 - 38	3.43	34300	Colorless, Odourless, Waxy Crystals
Heneicosane	C ₂₁ H ₄₄	12.60	296.5742	356.10	40.5	1.05	10500	Waxy Solid
Heneicosane	C ₂₁ H ₄₄	12.97	296.5742	356.10	40.5	3.06	30600	Waxy Solid
Heptadecane	C ₁₇ H ₃₆	13.05	240.4678	301.9	21.1 - 22.9	11.62	116200	Colorless Liquid, Odourless
Eicosane	C ₂₀ H ₄₂	13.117	282.5476	343.1	36 - 38	1.20	12000	Colorless, Odourless, Waxy Crystals
Eicosane	C ₂₀ H ₄₂	13.217	282.5476	343.1	36 - 38	2.66	26600	Colorless, Odourless, Waxy Crystals
Eicosane	C ₂₀ H ₄₂	13.68	282.5476	343.1	36 - 38	2.26	22600	Colorless, Odourless, Waxy Crystals
Eicosane	C ₂₀ H ₄₂	13.73	282.5476	343.1	36 - 38	3.02	30200	Colorless, Odourless, Waxy Crystals
Eicosane	C ₂₀ H ₄₂	15.76	282.5476	343.1	36 - 38	1.56	15600	Colorless, Odourless, Waxy Crystals
Octadecane	C ₁₈ H ₃₈	16.11	254.4944	317	28 - 30	3.34	33400	White Crystals or Powder, Odourless
Octadecane	C ₁₈ H ₃₈	16.21	254.4944	317	28 - 30	4.97	49700	White Crystals or Powder, Odourless
Tetracosane, 2,6,10,15,19,23-Hexame	C ₃₄ H ₇₀	16.27	478.92	391	50.3	2.00	20000	Oil of Hamamelis Leaves
Tetrapentacontane	C ₅₄ H ₁₁₀	16.33	759.452	596.4 ± 13.0	94 - 97	1.42	14200	Odourless
Tetracosane	C ₂₄ H ₅₀	16.81	338.654	391	50.3	2.22	22200	Oil of Hamamelis Leaves
n-Hexadecanoic Acid	C ₁₆ H ₃₂ O ₂	16.96	256.4236	351 – 352	62.9	7.99	79900	A Waxy Type Odor
Tetrapentacontane	C ₅₄ H ₁₁₀	18.61	759.452	596.4 ± 13.0	94 - 97	1.46	14600	Odourless
Octadecane	C ₁₈ H ₃₈	19.084	254.4944	317	28 - 30	3.71	37100	White Crystals or Powder, Odourless
Eicosane	C ₂₀ H ₄₂	19.630	282.5476	343.1	36 - 38	3.06	30600	Colorless, Odourless, Waxy Crystals
9-Tricosene, (Z)-	C ₂₃ H ₄₆	21.05	322.6118	110 – 120	32	1.22	12200	The Smell of Apple Cider Vinegar
Octadecane	C ₁₈ H ₃₈	21.701	254.4944	317	28 - 30	3.65	36500	White Crystals or Powder, Odourless
Octadecane	C ₁₈ H ₃₈	24.101	254.4944	317	28 - 30	1.83	18300	White Crystals or Powder, Odourless
Farnesol <cis,cis->	C ₁₅ H ₂₆ O	27.09	222.3668	283.4 ± 0.0	N/A	1.61	16100	Floral , Colorless Liquid
Tetracontane	C ₄₀ H ₈₂	28.02	563.0796	523.9 ± 13.0	80 - 84	2.21	22100	Solid White, Odourless
Tetracontane	C ₄₀ H ₈₂	30.09	563.0796	523.9 ± 13.0	80 - 84	4.27	42700	Solid White, Odourless
Total			9756.62			100	1000200	

RT – Retention Time, MW – Molecular Weight, BP – Boiling Point, MP – Melting Point.

Total No. of Carbon, Hydrogen, Oxygen among above identified compounds => C - 688, H - 1418, O - 4

Total Molecular Weight Jasminum Sambac - SPE Method(g/mol)

$$= C * 12.011 + H * 1.0078 + O * 15.999 = 688 * 12.011 + 1418 * 1.0078 + 4 * 15.999$$

Table 2. The Chemical Composition and Odour Description of Some Major Constituents of Rose Damascena – SPE Method

Compound	Chemical Formulae	RT	MW	BP °C	MP °C	Area in % (% Composition of a Mixture)	PPM	Odour
2,4-Di-tert-butylphenol	C ₁₄ H ₂₂ O	9.873	206.324	253	37	2.13	21300	Pale Yellow Crystalline Solid, with Characteristic Odour
Eicosane	C ₂₀ H ₄₂	13.046	282.547	343.1	36 - 38	6.11	61100	Colorless, Odourless, Waxy Crystals
Eicosane	C ₂₀ H ₄₂	13.727	282.547	343.1	36 - 38	3.03	30300	Colorless, Odourless, Waxy Crystals
Pentacosane	C ₂₅ H ₅₂	15.761	352.680	401.0	53 - 55	1.92	19200	Floral
Nonadecane	C ₁₉ H ₄₀	16.061	268.521	330	32	3.84	38400	White Crystals or Powder
L-Lysine, N(6)- [(1,1-dimethylethoxy) carbonyl]-N(2)- [(9H-fluoren-9 methyloxy)carbonyl]	C ₁₉ H ₂₈ N ₂ O ₆	16.107	380.434	N/A	N/A	3.17	31700	N/A
Octadecane	C ₁₈ H ₃₈	16.208	254.494	317	28 - 30	7.12	71200	White Crystals or Powder , Odourless
Oxalic acid, monoamide, N-(2-phenylethyl)-, isohexyl ester	C ₁₆ H ₂₃ NO ₃	16.275	277.359	N/A	N/A	4.29	42900	N/A
Tetracosane	C ₂₄ H ₅₀	16.810	338.654	391.4	48 - 54	3.16	31600	Oil of Hamamelis Leaves, Colorless Waxy Crystals
Palmitic acid	C ₁₆ H ₃₂ O ₂	16.924	256.423	351 - 352	62.9	7.48	74800	Fruit of Oil Palms
Heneicosane	C ₂₁ H ₄₄	18.815	296.57	356.1	40.5	4.27	42700	Waxy Solid
Octadecane	C ₁₈ H ₃₈	19.082	254.494	317	28 - 30	4.95	49500	White Crystals or Powder , Odourless
Tetracosane	C ₂₄ H ₅₀	19.631	338.65	391.4	48 - 54	3.27	32700	Oil of Hamamelis Leaves, Colorless Waxy Crystals
Heneicosane	C ₂₁ H ₄₄	21.338	296.574	356.1	40.5	3.81	38100	Waxy Solid
Octadecane	C ₁₈ H ₃₈	21.702	254.494	317	28 - 30	3.54	35400	White Crystals or Powder , Odourless
Z-12-Pentacosene	C ₂₅ H ₅₀	23.583	350.665	401.0	53.00	1.81	18100	An Intensive Citrus-like Odor
Pentacosane	C ₂₅ H ₅₂	23.669	352.680	401.0	53 - 55	9.82	98200	Floral
Pentacosane	C ₂₅ H ₅₂	25.870	352.680	401.0	53 - 55	5.21	52100	Floral
.gamma.-Sitosterol	C ₂₉ H ₅₀ O	32.499	414.708	719.6	147 - 148	14.43	144300	Waxy Powder with a Characteristic Odor
Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)	C ₂₉ H ₄₈ O	32.692	412.692	220 - 230	118 - 120	6.63	66300	White Solid Odourless
Total			6224.19			100	999900	

RT – Retention Time, MW – Molecular Weight, BP – Boiling Point, MP – Melting Point.

Total No. of Carbon, Hydrogen, Oxygen, Nitrogen among above identified compounds => C - 426, H - 835, O - 14, N – 3
 Total Molecular Weight Rose Damascena - SPE Method (g/mol) = $C * 12.011 + H * 1.0078 + O * 15.999 + N * 14.0067$
 = $426 * 12.011 + 835 * 1.0078 + 14 * 15.999 + 3 * 14.0067 = 6224.2 \text{ g/mol}$

Table 3. The Chemical Composition and Odour Description of some Major Constituents of Jasminum Sambac – Natural Drying Method

Compound	Chemical Formulae	RT	MW	BP °C	MP °C	Area in % (% Composition of a Mixture)	PPM	Odour
Cyclopentasiloxane, Decamethyl	C ₁₀ H ₃₀ O ₅ Si	3.46	258.424	210	-38	3.92	39200	A Colorless and Odorless Liquid
Cyclopentasiloxane, Decamethyl	C ₁₀ H ₃₀ O ₅ Si	3.49	258.424	210	-38	4.27	42700	A Colorless and Odorless Liquid
1-Undecanol	C ₁₁ H ₂₄ O	4.29	172.307	243	19	2.52	25200	A Waxy Type Odor
1-Undecanol	C ₁₁ H ₂₄ O	4.33	172.307	243	19	2.94	29400	A Waxy Type Odor
Cyclohexasiloxane, Dodecamethyl	C ₁₂ H ₃₆ O ₆ Si	5.91	304.492	245	-3	10.42	104200	Odorless
1-Tetradecanol	C ₁₄ H ₃₀ O	7.44	214.387	>260	38	10.43	104300	Aroma of Cooked and Raw Beef
1,1,1,3,3,5,7,7-Nonamethyl-5-[(Trimethylsilyl)oxy]Tetrasiloxane	C ₁₂ H ₃₆ O ₄ Si ₅	8.68	384.836	N/A	N/A	5.57	55700	N/A
15-Methyltricyclo [6.5.2(13,14).0(7,15)] Pentadeca-1,3,5,7,9,11,13-Heptene	C ₁₃ H ₁₅ N ₃	9.34	213.280	N/A	N/A	2.15	21500	N/A

Compound	Chemical Formulae	RT	MW	BP °C	MP °C	Area in % (% Composition of a Mixture)	PPM	Odour
1-Hexadecene	C ₁₆ H ₃₂	10.77	224.425	285	4	8.6	86000	Odor Mild Hydrocarbon Odor
Benzoic Acid, 2,4-bis(trimethylsiloxy)-, Trimethylsilyl Ester	C ₁₆ H ₃₀ O ₄ Si ₃	11.37	370.662	N/A	N/A	4.44	44400	Vinegar-like Flavor and Odor
Cyclohexasiloxane, Dodecamethyl	C ₁₂ H ₃₆ O ₆ Si	13.739	304.492	245	-3	3.14	31400	Odorless
1-Octadecanol	C ₁₈ H ₃₈ O	13.916	270.493	210	56-59	4.54	45400	A Mild Soapy Odor
1,1,1,5,7,7,7-Heptamethyl-3,3-bis (Trimethylsiloxy) Tetrasiloxane	C ₁₃ H ₄₀ O ₅ Si ₆	15.87	444.96	N/A	N/A	2.03	20300	Colorless to Light Yellow Transparent Liquid
1,2-Benzenedi Carboxylic Acid, Dibutyl Ester	C ₁₆ H ₂₂ O ₄	16.22	278.343	340	-35	4.11	41100	Slight, Aromatic Odor
1-Heptadecanol	C ₁₇ H ₃₆ O	16.82	256.466	309	54.0	1.6	16000	White Solid (est)
Benzoic acid, 2,5-bis(Trimethylsiloxy)-, Trimethylsilyl ester	C ₁₆ H ₃₀ O ₄ Si ₃	17.82	370.662	N/A	N/A	1.93	19300	Vinegar-like Flavor and Odor
1,1,1,5,7,7,7-Heptamethyl-3,3-bis (Trimethylsiloxy) Tetrasiloxane	C ₁₃ H ₄₀ O ₅ Si ₆	19.6	444.963	N/A	N/A	2.1	21000	Colorless to Light Yellow Transparent Liquid
1,1,1,5,7,7,7-Heptamethyl-3,3-bis (Trimethylsiloxy) Tetrasiloxane	C ₁₃ H ₄₀ O ₅ Si ₆	21.24	444.963	N/A	N/A	2.03	20300	Colorless to Light Yellow Transparent Liquid
1h-Purin-6-Amine, [(2-Fluorophenyl) Methyl]	C ₁₂ H ₁₀ FN ₅	22.79	243.241	N/A	N/A	2.23	22300	N/A
1h-Purin-6-Amine, [(2-Fluorophenyl) Methyl]	C ₁₂ H ₁₀ FN ₅	24.25	243.241	N/A	N/A	2.74	27400	N/A
1h-Purin-6-Amine, [(2-Fluorophenyl) Methyl]	C ₁₂ H ₁₀ FN ₅	25.61	243.241	N/A	N/A	3.41	34100	N/A
Cyclononasiloxane, Octadecamethyl	C ₁₈ H ₅₄ O ₉ Si ₉	26.86	667.379	N/A	N/A	3.35	33500	N/A
Cyclononasiloxane, Octadecamethyl	C ₁₈ H ₅₄ O ₉ Si ₉	27.99	667.379	N/A	N/A	3.03	30300	N/A
Tetracosamethyl-Cyclo dodecasiloxane	C ₂₄ H ₇₂ O ₁₂ Si ₁₂	29.04	889.839	518.6	N/A	5.07	50700	N/A
Cyclononasiloxane, Octadecamethyl	C ₁₈ H ₅₄ O ₉ Si ₉	30.13	667.379	N/A	N/A	3.44	34400	N/A
Total			9010.58			100	1000100	

RT – Retention Time, MW – Molecular Weight, BP – Boiling Point, MP – Melting Point.

Total No. of Carbon, Hydrogen, Oxygen, Nitrogen, Silicon, Fluorine among above identified compounds

=> C - 357, H - 833, O - 97, N - 18, SI - 72, F - 3

Total Molecular Weight Jasminum Sambac - Natural Drying Method(g/mol)

= $C * 12.011 + H * 1.0078 + O * 15.999 + N * 14.0067 + SI * 28.0855 + F * 18.998$

= $357 * 12.011 + 833 * 1.0078 + 97 * 15.999 + 72 * 28.0855 + 18 * 14.0067 + 3 * 18.998 = 9010.59 \text{ g/mol}$

Table 4. The Chemical Composition and Odour Description of Some Major Constituents of Rose Damascena – Natural Drying Method

Compound	Chemical Formulae	RT	MW	BP °C	MP °C	Area in % (% Composition of a Mixture)	PPM	Odour
Trimethylsilyl Ester	C ₂₁ H ₄₂ O ₂ Si	3.453	354.64	57	-40	3.51	35100	Fruity Odors
Tetrakis(Trimethylsilyl) Norepinephrine	C ₂₂ H ₄₂ F ₃ NO ₄ Si ₄	3.493	553.9	N/A	N/A	4.03	40300	N/A
1-Undecanol	C ₁₁ H ₂₄ O	4.291	172.31	243	19	1.35	13500	A Waxy Type Odor
1-Dodecene	C ₁₂ H ₂₄	4.333	168.32	213.8	-35.2	1.26	12600	A Mild, Pleasant Odour
Cyclo Hexasiloxane	C ₁₂ H ₃₆ O ₆ Si ₆	5.905	444.92	245	-3.00 E +00	11.13	111300	Colorless, Odorless, Non-Greasy
1-Tetradecanol	C ₁₄ H ₃₀ O	7.437	214.39	>260	38	4.74	47400	Aroma of Cooked and Raw Beef
1,1,1,3,3,5,7,7-Nonamethyl-5-	C ₁₅ H ₃₂ O ₃ Si ₄	8.680	372.75	N/A	N/A	6.31	63100	N/A

Compound	Chemical Formulae	RT	MW	BP °C	MP °C	Area in % (% Composition of a Mixture)	PPM	Odour
2,4-Ditert-Butylphenyl	C ₄₂ H ₆₃ O ₃ P	9.342	646.92	~609.8	58-61	0.97	9700	A Distinct Phenolic Odour
1h-3a, 7-Methanoazulene	C ₁₅ H ₂₄	10.698	204.35	264.00	N/A	0.5	5000	N/A
1-Hexadecene	C ₁₆ H ₃₂	10.768	224.43	285	4	3.87	38700	Mild Hydrocarbon Odor
Hexadecamethyl-	C ₁₆ H ₄₈ O ₆ Si ₇	11.365	533.1	N/A	N/A	4.62	46200	N/A
Orthosilicate	O ₄ Si ₄	13.740	92.08	N/A	N/A	3.61	36100	N/A
1-Octadecanol	C ₁₈ H ₃₈ O	13.917	270.49	336	59.8	2.17	21700	Unpleasant, 'Garlic-like' Odor
Neophytadiene	C ₂₀ H ₃₈	14.554	278.52	345.00	N/A	1.14	11400	Almost Odorless
1h-purin-6-amine	C ₅ H ₅ N ₅	15.872	137.12	373.4	286 - 290	2.61	26100	Appearance White powder
1,2-Benzenedi Carboxylic Acid	C ₈ H ₆ O ₄	16.227	166.13	289	167	2.75	27500	A Slight Odor
1-Octadecene	C ₁₈ H ₃₆	16.803	252.48	315	17 - 18	1.3	13000	Odor Mild Hydrocarbon Odor
Tetracosamethyl	C ₂₄ H ₇₂ O ₁₂ Si ₁₂	17.824	889.84	518.6±33.0	N/A	2.56	25600	A Synthetic Woody Odorant
1-Heptadecanol	C ₁₇ H ₃₆ O	19.448	256.47	309	54.0	0.54	5400	White Solid (est)
1h-purin-6-amine, [(2-fluorophenyl)methyl]	C ₁₂ H ₁₀ FN ₅	19.598	243.24	N/A	245 - 246	2.9	29000	N/A
1h-purin-6-amine, [(2-fluorophenyl)methyl]	C ₁₂ H ₁₀ FN ₅	21.238	243.24	N/A	245 - 246	3.09	30900	N/A
Bis(2-ethylhexyl) ester of Hexanedioic Acid	C ₂₂ H ₄₂ O ₄	21.789	370.57	417	-67.8	0.52	5200	Straw-colored Liquid with a Mild Odor
1h-purin-6-amine, [(2-fluorophenyl)methyl]	C ₁₂ H ₁₀ FN ₅	22.790	243.24	N/A	245 - 246	3.75	37500	N/A
1h-purin-6-amine, [(2-fluorophenyl)methyl]	C ₁₂ H ₁₀ FN ₅	24.246	243.24	N/A	245 - 246	4.49	44900	N/A
1h-purin-6-amine, [(2-fluorophenyl)methyl]	C ₁₂ H ₁₀ FN ₅	25.609	243.24	N/A	245 - 246	4.86	48600	N/A
Cyclononasiloxane, Octadecamethyl	C ₁₈ H ₅₄ O ₉ Si ₉	26.856	667.38	415.7	-27	5.29	52900	N/A
Dodecane, 1,1'-oxybis-	C ₂₄ H ₅₀ O	27.205	354.65	497.79	32	1.25	12500	Suffocating Odor
Cyclononasiloxane, octadecamethyl	C ₁₈ H ₅₄ O ₉ Si ₉	27.992	667.4	N/A	N/A	5.06	50600	N/A
Cyclononasiloxane, octadecamethyl	C ₁₈ H ₅₄ O ₉ Si ₉	29.038	667.4	N/A	N/A	6.02	60200	N/A
Tetracosamethyl-Cyclo dodecasiloxane	C ₂₄ H ₇₂ O ₁₂ Si ₁₂	30.128	889.84	518.6	N/A	3.8	38000	Almost white, Odourless
Total			10023.5			100	1000000	

RT – Retention Time, MW – Molecular Weight, BP – Boiling Point, MP – Melting Point

Total No. of Carbon, Hydrogen, Oxygen, Silicon, Phosphorus, Nitrogen, Fluorine among above identified compounds, => C - 430, H - 1004, O - 88, Si - 68, F - 5, N - 31, P - 1

Total Molecular Weight Rose Damascena – Natural Drying Method(g/mol)

$$= C * 12.011 + H * 1.0078 + O * 15.999 + SI * 28.0855 + P * 30.973762 + N * 14.0067 + F * 18.998$$

$$= 430 * 12.011 + 1004 * 1.0078 + 88 * 15.999 + 68 * 28.0855 + 1 * 30.973762 + 31 * 14.0067 + 5 * 18.998$$

$$= 10023.48 \text{ g/mol}$$

7. Interpreting the Results

The procedure of Solid-Phase technique and Natural Drying Method allows reliable identification of major chemical compounds; Eicosane, Heneicosane, 9-Tricosene, Tetracosane, Pentadecane, Octadecane, Heptadecane, Farnesol, volatiles from Jasminum Sambac and Eicosane, Pentacosane, Heneicosane, Tetracosane, Nonadecane, Octadecane, gamma-Sitosterol, volatiles from Rosa Damascena through SPE is detected. The Natural Drying method results, 1-Undecanol, 1-Tetradecanol, 1-Hexadecene, 1-Octadecanol, 1-Heptadecanol etc., through J.Sambac and Trimethylsilyl Ester, 1-Undecanol, 1-Tetradecanol, 1-Hexadecene, 1-Octadecanol, Neophytadiene etc.,

through R.Damascena. The results (Table 5) demonstrate that the described Solid State Extraction and Natural Drying through GC-MS analysis procedure could be reliably applied for the identification of chemical compounds of Indian Jasmine and Rose Flower.

Table 5. Comparison of Reliable Identification of Compounds through SPE and ND Method

	Total Molecular Weight in g/mol	Total PPM
Jasminum Sambac - SPE	9756.62	1000200
Jasminum Sambac - ND	9010.58	1000100
Rosa Damascena - SPE	6224.19	999900
Rosa Damascena - ND	10023.48	1000000

8. Conclusion

To calculate the densities of odour compounds, the calibration curves of odour compounds were constructed by GC-MS measurement. In this study, we found that the set of chemical compounds identified via the Solid-PE and Natural Drying Methods differ. The e-nose digital signals are based on the concentration of the odour. Further, the concentration is converted into PPM. The PPM found for each chemical compound in tabular columns 1 and 2 for both samples are further used to compare with the e-nose classification of odour. The dryness of floral flowery appears to be pivotal in ensuring the physical, chemical, and sensory qualities of the final products. The drawback we faced while implementing our sampling through the SPE method was due to additional water content in a given sample, and over-moisture may have a significant impact on the physical, chemical properties and set of volatile compounds identified. Moreover, all of the sample's constituents must be volatile in the gas chromatograph. Since Volatility is based on the boiling point, the results have significant differences in set of volatile compounds identified between SPE and ND Methods. The effects of different identification processes on the Chemical Compounds of J.Sambac and R.Damascena could be further analyzed based on factors, such as Sensory Evaluation, Process/Methodology differences, and so on.

Acknowledgments

I would like to express my gratitude to Dr. Ramaswamy Babu Rajendran, Professor, School of Environmental Sciences, Bharathidasan University, Tiruchirappalli, TamilNadu, India, who have been supportive for provided me abundance knowledge on Gas Chromatography and Related Techniques. Each of the members of my department has provided me extensive personal and professional guidance and taught me a great deal about both scientific research and life in general.

Competing Interests

I/We certify that we have NO affiliations with or involvement in any organization or entity with any financial interest or non-financial interest in the subject matter or materials discussed in this manuscript. I/We

have no conflicts of interest to disclose. The above information is true and correct, up to our knowledge.

List of Abbreviations

Solid Phase Extraction (SPE)

Natural Drying (ND)

Parts Per Million (PPM)

Gas Chromatography-Mass Spectrometry (GC-MS)

References

- [1] Shuyan Wang et.al., "Comparison of Volatiles in Different Jasmine Tea Grade Samples Using Electronic Nose and Automatic Thermal Desorption-Gas Chromatography-Mass Spectrometry Followed by Multivariate Statistical Analysis", *Molecules* 2020, 25, 380.
- [2] Scott E. Van Bramer, *An Introduction to Mass Spectrometry*, Department of Chemistry, Widener University, Chester, PA 19013, September 2 1998
- [3] Steven J. Lehotay et.al., "Application of gas chromatography in food analysis", *Trends in Analytical Chemistry*, Vol. 21, Nos. 9+10, 2002.
- [4] Leopold Jirovetz et.al., "Chemical Composition, Olfactory Evaluation and Antimicrobial Activities of *Jasminum grandiflorum* L. Absolute from India", *Natural Product Communications*, Vol. 2 (4), 407-412, 2007.
- [5] Krasimir E. Rusanov et al., "Comparative GC/MS Analysis of Rose Flower and Distilled Oil Volatiles of The Oil Bearing Rose *Rosa Damascena*", *Biotechnology & Biotechnological Equipment*, 25:1, 2210-2216.
- [6] T.C. Sasedharen, B. Santhi, "Odour Classification by Electronic Nose", *European Journal of Scientific Research*, ISSN 1450-216X / 1450-202X Vol. 98 No 4 March, 2013.
- [7] Gan-Lin Chen et.al., "Comparison of Different Drying Methods for Asparagus [*Asparagus cochinchinensis* (Lour.) Merr.] Root Volatile Compounds as Revealed Using Gas Chromatography Ion Mobility Spectrometry", *Frontiers in Nutrition*.
- [8] Hyun-Jung Kim et al. "Determination of floral fragrances of *Rosa hybrida* using solid-phase trapping-solvent extraction and gas chromatography-mass spectrometry", *Journal of Chromatography A*, 902, 389-404, 2000.
- [9] Ranchana et al. "Analysis of Volatile Compounds from the Concrete of *Jasminum Multiflorum* Flowers", *International Journal of Current Microbiology and Applied Sciences*, ISSN: 2319-7706, Volume 6 Number 11, pp. 2229-2233, 2017.
- [10] Nurlaila Ismail et al. "Analysis of Chemical Compounds of Agarwood Oil based on Headspace-Solid Phase Microextraction combined with Gas Chromatography Mass-Spectrometry", *IEEE 9th International Colloquium on Signal Processing and its Applications*, 8-10 Mac. 2013, Kuala Lumpur, Malaysia, 2013.
- [11] Takuma Kitamoto et al. "Quantitative Analysis of Aroma Components by Gas Chromatography-Mass Spectrometry and its Subjective Evaluation for Olfactory Media Content", *IEEE*, 2018.



© The Author(s) 2022. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).