MJoSHT
Malaysian Journal of Science, Health & Technology
[mjosht.usim.edu.my]

Article

Identification of Chemical Profiles of Aromatherapeutic Compounds in Commercial Fragrances and Their Potential to Modulate Emotional States

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Article Info
Article history:
Received:27 February 2025
Accepted: 15 September 2025
Published: 15 October 2025

Academic Editor:
Norsham Juliana

Malaysian Journal of Science, Health & Technology

MJoSHT2025, Volume 11, Issue No. 2
eISSN: 2601-0003

https://doi.org/10.33102/mjosht.435

***Abstract*— Aromatherapy, a holistic healing treatment that uses natural plant extracts, has been widely recognized for improving psychological well-being. This research aims to identify and quantify the key compounds in a range of commercially available fragrances and analyze their potential therapeutic effects and benefits. Using advanced chromatographic techniques and mass spectrometry, the composition of aromatherapeutic compounds in selected fragrances were determined. The findings indicate that specific aromatherapeutic compounds, such as vanilin, azulene, furanone, thujopsene, lilial, cedrol, pinene, piperonal, ethylene brassylate, butylated hydroxytoluene, and limonene, have distinct effects on emotional state. This comparative analysis highlights both similarities and differences in their chemical profiles in their potential to modulate emotional states. It underscores the potential of aromatherapy as a complementary approach to emotional well-being. The study provides valuable insights for the fragrance industry, healthcare practitioners, and consumers seeking to leverage the benefits of aromatherapy for emotional regulation.**

***Keywords*— Aromatherapy, Chromatography, Chemical Profile; Fragrance, Gas Chromatography-Mass Spectrometer (GC-MS)**

I. INTRODUCTION

In contemporary times, the use of aromatherapy as a complementary approach to promote relaxation and well-being has garnered considerable attention [1]. Aromatherapy exploits natural plant extracts and essential oils to foster physical and psychological well-being. This holistic healing treatment has garnered significant attention in recent decades for its purported ability to influence emotional states and enhance mental health[2]. With a growing interest in complementary and alternative medicine, the fragrance industry has increasingly incorporated aromatherapeutic compounds into their products to cater to consumer demand for natural and wellness-oriented solutions.

The relationship between fragrance and emotion is complex and multifaceted, involving intricate interactions between olfactory receptors and the brain's limbic system, which is responsible for emotion and memory [3]. Understanding the specific compounds in fragrances that elicit emotional responses is crucial for developing effective aromatherapy treatments. Despite the widespread use of aromatherapy, there is a need for rigorous scientific analysis to validate its benefits and optimize its application. This study aims to analyze and compare the chemical compositions of some fragrances

referred using gas chromatography-mass spectrometer (GC-MS).

Despite the subjective nature of fragrance perception, fragrances were believed to have the ability to create a serene and tranquil ambiance, thus making them ideal candidates for exploration through chemical analysis. Through GC-MS analysis, samples were collected from a local manufacturer in Malaysia called Sugarbomb Sdn. Bhd. then underwent compound analysis shedding light on the key aromatic compounds contributing to their reputed relaxation-inducing properties.

Understanding the chemical composition of these fragrances is essential for advancing our knowledge of their aromatherapeutic potential. This paper aims to explore existing research on the role of scent in enhancing relaxation and promoting holistic well-being, providing a foundation for future studies focused on leveraging fragrances for therapeutic benefits.

II. METHODOLOGY

For this study, three sample fragrances were selected based on the best-selling products from a local Malaysian perfumery company, Sugarbomb Sdn. Bhd. This approach ensures that the fragrances analyzed are popular and widely used, thereby increasing the relevance of the findings. The fragrances were chosen to provide a comprehensive analysis of the aromatherapeutic compounds present and believed to initiate various moods and emotions such as calm, confident, modest, lovable, and joyful.

Prior to conducting GC-MS analysis, each fragrance sample was preliminarily characterized based on anticipated sensory profiles informed by existing aromatherapy literature by the company. This initial classification identified three distinct fragrances which named as A, B, and C. Type A, noted for its floral and fruity notes, associated with feelings of freshness and vitality; Type B, recognized for its warm, comforting aroma reminiscent of spices and woods; and Type C, characterized by a bright, citrus-floral blend that evokes a sense of joy and upliftment. These descriptions were based on known properties of common fragrance compounds documented in aromatherapy studies. This provided a foundation for our GC-MS analysis, which later confirmed the presence of compounds linked to these sensory effects. This preliminary step established a systematic framework for categorizing the samples and guided the subsequent chemical analyzes. GC-MS analysis af all samples wasa performed with a 6890 Agilent Technologies gas chromatograph coupled to a 5975 Inert XL Agilent Technolosgies mass detector working at 70 eV ionization energy.

A. Sample Preparation

Each fragrance sample was first diluted with methanol, to ensure it fell within the optimal concentration range for GC-MS analysis. The diluted samples were then filtered using a 0.45-micron filter to eliminate any particulate matter that could interfere with the analysis [4]. Approximately 1 mL of each prepared sample was placed into a GC-MS vial for analysis. The software used to analyze the chemical compounds is the Agilent Mass Hunter.

Chromatographic separation was performed using an Agilent DB-35MS capillary column (30 m × 0.25 mm i.d.) coated with a 35%phenyl/65% dimethylpolysiloxane stationary phase (0.25 µm film thickness) [5], providing moderate polarity suitable for compounds of varying polarity. Helium (5.5 grade) was employed as the carrier gas at a constant flow rate of 1.0 mL/min. The GC oven temperature program was as follows: initial temperature of 50 °C held for 2 min, ramped at 10 °C/min to 250 °C, and maintained isothermally for 10 min. Sample injections of 1 µL were performed in split mode (10:1) at an injector temperature of 250 °C. The separated components were transferred to the MS detector for identification [6].

For the mass spectrometry (MS) phase, the electron ionization (EI) mode was used with an ionization energy of 70 eV. The mass spectrometer was set to inspect from 50 to 500 m/z to capture a wide range of fragrance compounds. The separated components from the first phase, are analyzed by the mass spectrometer (MS), which identifies and quantifies the individual molecules in the sample. The MS works by ionizing the separated molecules and measuring their mass-to-charge ratio. The ionized molecules from the separated molecules are propelled through a magnetic field after being ionized by electron impact or chemical ionization. According to their mass-to-charge ratio, the ions are split by the magnetic field, and the detector records the resulting mass spectrum, which delivers a unique "fingerprint" of the sample's chemical composition. By comparing the mass spectrum of the sample to a database of known compounds, the GC-MS can identify the specific fragrance ingredients and other components in the sample and quantify their relative amounts [7,8]. Figure 2 shows the schematic plot of the main components of the GC-MS device.

B. Data Analysis

The GC-MS data is processed using dedicated software known as Agilent Mass Hunter to analyze the chromatograms and mass spectra. The chemical compounds present in each fragrance sample are identified and quantified based on their retention times and mass spectral characteristics. Comparative analysis is performed to assess similarities and differences in the chemical compositions of the three fragrance samples.

C. Results and Reporting

The GC-MS results are interpreted to elucidate the major chemical constituents present in each fragrance sample. The significance of the detected compounds concerning the aroma profile and potential therapeutic effects of the fragrances is analyzed. Conclusions are drawn based on the findings, and their implications for fragrance development and aromatherapy are discussed.

The experimental procedures, results, and interpretations are compiled into a comprehensive report or manuscript for publication or internal documentation. Relevant details such as instrument parameters, sample preparation methods, chromatographic conditions, and compound identifications are included.

III. RESULTS

The GC-MS chromatogram analysis was performed to identify the chemical compositions of three fragrance samples: Type A, Type B, and Type C. The following results were obtained:

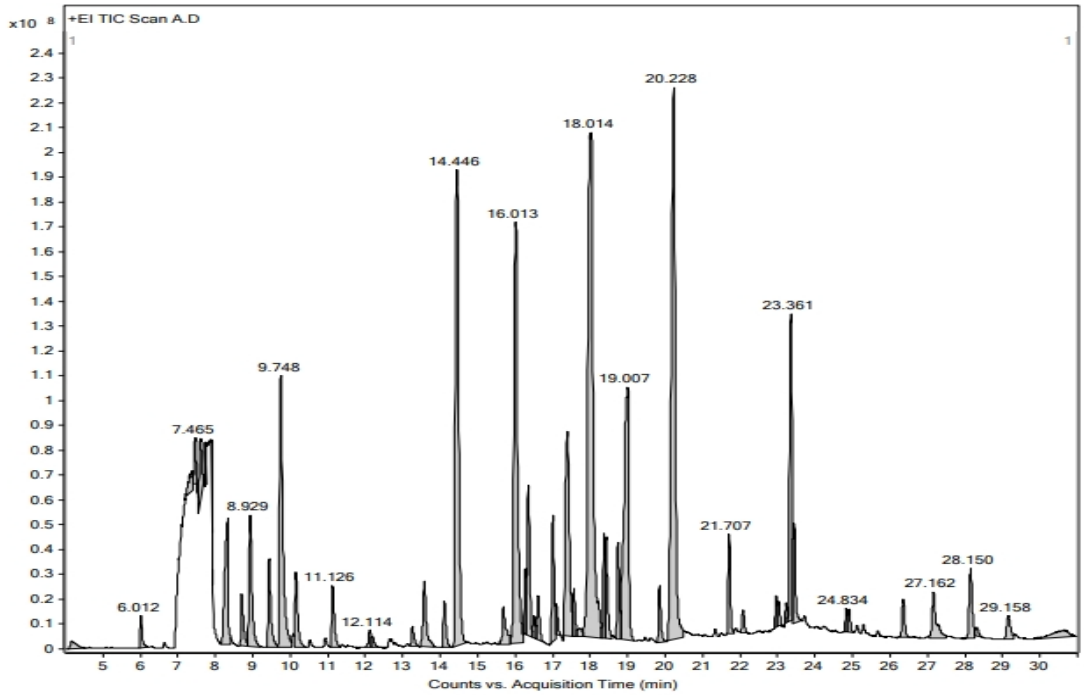


Figure. 1 Chromatogram of the Sample Type A

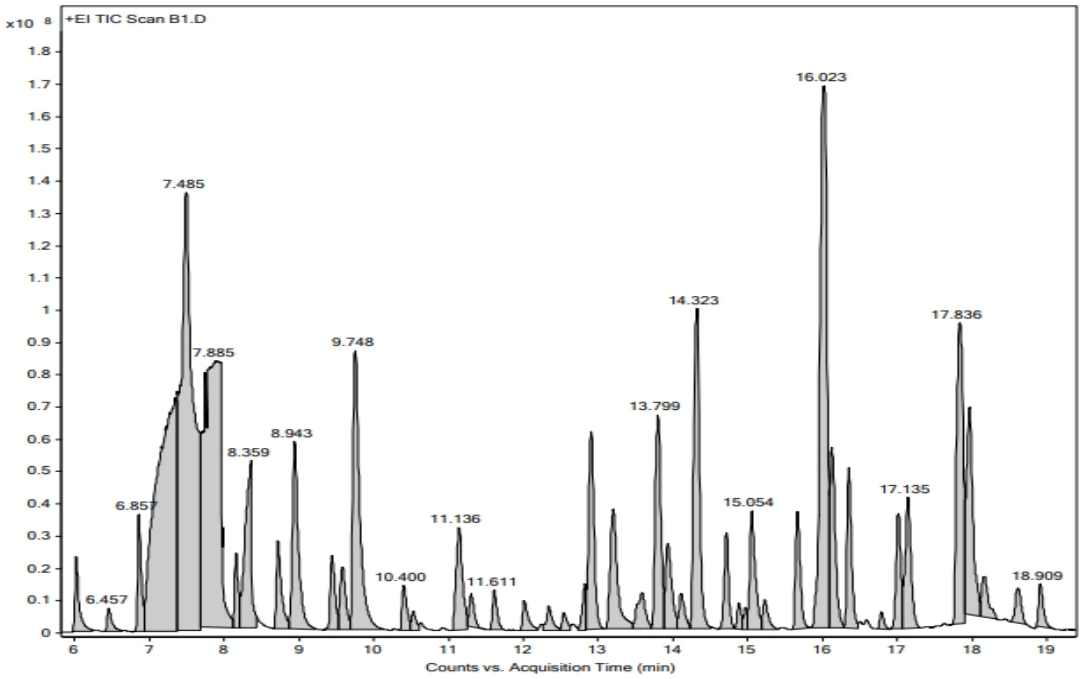
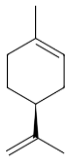
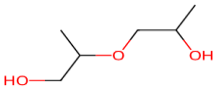
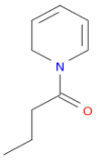
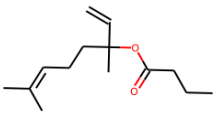
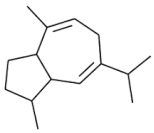
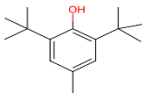
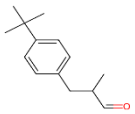
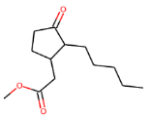
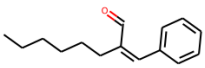
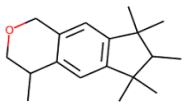
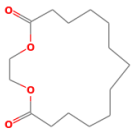


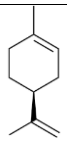
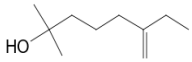
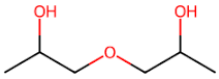
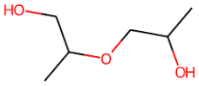
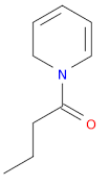
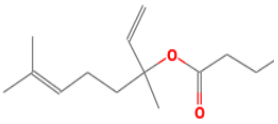
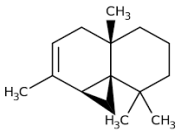
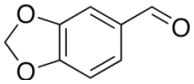
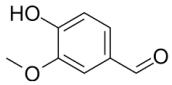
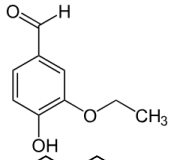
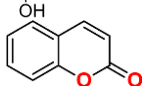
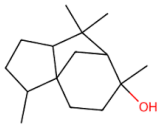
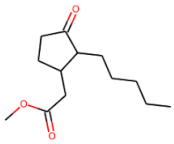
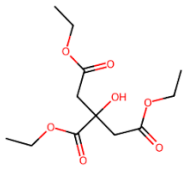
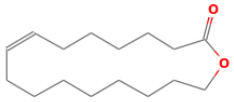
Figure 2. Chromatogram of the Sample Type B

Table I. The Chemical Compounds Found In Fragrance Type A With Its Chemical Structure, Retention Time, And Relative Abundance

Chemical Compound	Chemical Structure	Retention Time (min)	Relative Abundance (%)
Limonene		6.012	29.2
1-Propanol, 2-(2-hydroxypropoxy)-		7.901	52.1
1,2-Dihydropyridine, 1-(1-oxobutyl)		8.722	39.0
1,5-Dimethyl-1-vinyl-4-hexenyl butyrate		9.748	19.5
Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4- dimethyl-7-(1-methylethenyl)-		12.114	26.6
Butylated Hydroxytoluene		13.572	75.7
Lilial		14.446	76.8
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester		16.013	81.2
Octanal, 2-(phenylmethylene)-		16.989	95.5
Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl		18.014	19.7
Ethylene Brassylate		20.228	92.9

Sample A reveals a harmonious blend of floral and fruity notes supported by key chemical compounds identified in the GC-MS analysis. The floral character of the fragrance is primarily driven by Lilial (76.8 relative abundance), known for its lily-of-the-valley-like scent, and azulene derivatives such as octahydro-1,4-dimethyl-7-(1-methylethenyl), which contribute subtle floral or sweet herbal nuances. Complementing this, the fruity aspect is emphasized by Limonene (29.2), with its fresh, zesty aroma typical of citrus fruits, and Octanal, 2-(phenylmethylene) (95.5), which adds fruity, slightly waxy notes reminiscent of oranges. Additionally, Butylated Hydroxytoluene (75.7), primarily a preservative, may provide faintly sweet undertones, while Ethylene Brassylate (92.9), with its sweet, musky aroma, enriches both the floral and fruity elements by adding depth and warmth. Together, these compounds establish Sample A as a vibrant fragrance that balances floral elegance with fruity freshness.

TABLE 2. The Chemical Compounds Found In Fragrance TYPE B With Its Chemical Structure, Retention Time, And Relative Abundance

Chemical Compound	Chemical Structure	Retention Time (min)	Relative Abundance (%)
Limonene		6.022	26.4
2-Octanol, 2-methyl-6-methylene		6.857	15.3
2-Propanol, 1,1'-oxybis		7.351	94.1
1-Propanol, 2-(2-hydroxypropoxy)-		8.359	28.6
1,2-Dihydropyridine, 1-(1-oxobutyl)-		8.942	34.6
1,5-Dimethyl-1-vinyl-4-hexenyl butyrate		9.748	12.2
Thujopsene		12.342	46.5
Piperonal		12.905	89.2
Vanillin		13.799	66.4
Ethyl Vanillin		14.323	77.0
2H-1-Benzopyran-2-one		14.709	85.7
Cedrol		15.222	41.1
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester		16.023	77.1
Ethyl Citrate		16.122	92.4
Oxacycloheptadec-8-en-2-one		17.836	31.8

The interpretation for Sample B reveals a rich and intricate fragrance profile characterized by spicy, warm, and woody notes, supported by a diverse range of compounds identified in the GC-MS analysis. The spicy and warm character is prominently defined by Piperonal (89.2), which imparts a sweet, spicy scent reminiscent of vanilla, alongside Vanillin (66.4) and Ethyl Vanillin (77.0), both of which enhance the fragrance with their creamy, comforting sweetness. Additionally, 2H-1-Benzopyran-2-one (85.7), known for its almond-like and slightly spicy aroma, further reinforces the warmth and depth of this fragrance. The woody aspects are contributed by Thujopsene (46.5) and Cedrol (41.1), which provide cedar-like and earthy tones, grounding the scent with their natural, warm woodiness. Supporting these dominant notes, Limonene (26.4) subtly blends its citrusy brightness into the mix, enhancing the spicier elements, while Oxacycloheptadec-8-en-2-one adds a musky, sweet warmth that complements the overall profile. Ethyl Citrate (92.4) contributes a smooth, slightly fruity undertone that adds complexity and balance, seamlessly integrating the spicy, woody, and warm components. Together, these compounds create a fragrance that exudes a cozy and comforting aroma, reminiscent of spices and woods, with subtle layers of sweetness and depth.

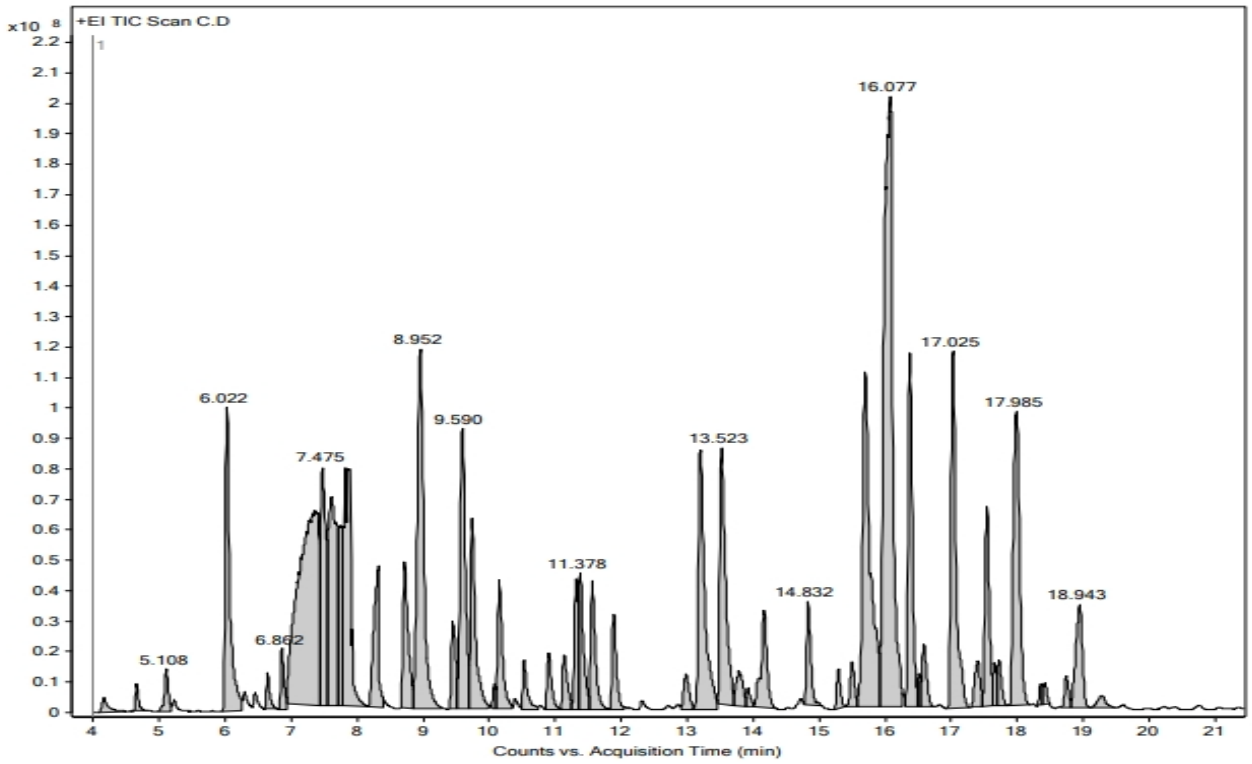


Figure 3. Chromatogram of the Sample Type C

Sample C highlights a vibrant and uplifting fragrance characterized by its citrus and floral notes, complemented by layers of sweetness, warmth, and complexity. The citrus element is primarily driven by Cyclohexene, 1-methyl-5-(1-methylethenyl)-, (R) (26.9), which provides a bright, fresh, and slightly piney scent, supported by 1R-.alpha.-Pinene (7.59), adding a crisp, uplifting touch to the fragrance. The floral character is defined by 3-Cyclohexene-1-methanol, .alpha.,.alpha.4-trimethyl- (70.6), which imparts a green, blooming freshness, and Acetic acid, phenylmethyl ester (32.7), contributing sweet, jasmine-like floral notes.Enhancing the uplifting quality, Benzeneethanol, .alpha.,.alpha.-dimethyl-, acetate (71.8) adds a fruity, lavender-like aroma, while 2(3H)-Furanone, 5-heptyldihydro (79.3) delivers a sweet, fruity richness that balances the citrus and floral components. Supporting these dominant notes, Octanal, 2-(phenylmethylene) (96.4) enhances the fragrance's brightness with its floral, aldehydic orange-like scent, and Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester (75.8) adds a smooth, musky background that rounds out the composition. Additionally, Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl provides subtle woody and musky undertones, adding depth and sophistication. Together, these compounds create a joyful and invigorating fragrance with a perfect balance of citrusy brightness, floral elegance, and layered warmth.

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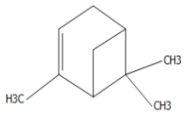
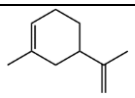
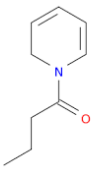
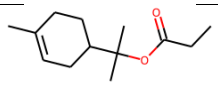
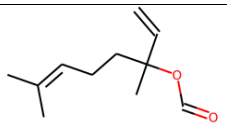
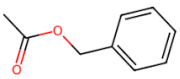
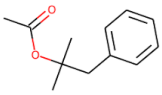
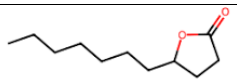
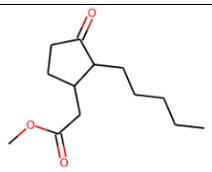
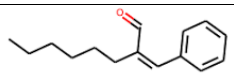
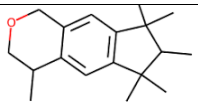
Table 3. The Chemical Compounds Found In Fragrance Type C With Its Chemical Structure, Retention Time, And Relative Abundance

CHEMICAL COMPOUND	CHEMICAL STRUCTURE	RETENTION TIME (min)	RELATIVE ABUNDANCE (%)
1R-. alpha. -Pinene		4.174	7.59
Bicyclo[3.1.0] hex-2-ene, 4-methyl-1-(1- methylethyl)-		5.108	20.4
Cyclohexene, 1-methyl-5-(1-methylethenyl)-, (R)-		6.022	26.9
1,2-Dihydropyridine, 1-(1-oxobutyl)-		8.715	32.2
3-Cyclohexene-1-methanol, alpha,.alpha.4- trimethyl-propanoate		9.446	70.6
1,6-Octadien-3-ol, 3,7-dimethyl-, formate		9.743	42.6
Acetic acid, phenylmethyl ester		9.590	32.7
Benzeneethanol, alpha.,.alpha.-dimethyl-, acetate		11.378	71.8
2(3H)-Furanone, 5-heptyldihydro		15.292	79.3
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester		16.077	75.8
Octanal, 2-(phenylmethylene)-		17.025	96.4
Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8- hexahydro-4,6,6,7,8,8-hexamethyl		17.989	49.5

IV. DISCUSSION

A. Description of variables involved in GC-MS Analysis

There are two variables involved in the analysis of GC-MS which are retention time and relative abundance. The retention time is the amount of time a particular compound spends in the chromatographic column before being detected by the detector [9]. It is the time elapsed from the injection of the sample to the detection of the compound's peak. Retention time is persuaded by various factors such as the type of column used, the nature of the sample, and the operating conditions (temperature, pressure, etc.). It is also influenced by the compound's affinity for the stationary phase and the mobile phase's flow rate. Retention time is a characteristic parameter for identifying compounds in a mixture. In the results, the retention time shown is the time when the compound is detected using a GC-MS machine.

In addition, relative abundance values obtained from the GC-MS analysis represent the proportional contribution of each compound to the overall chemical composition of the fragrance sample. These percentages are calculated based on the peak areas in the chromatogram, where the larger the peak area, the greater the compound's presence in the mixture. It is important to note that these values are semi-quantitative, meaning they provide an approximate estimation rather than an absolute quantification of the compound. This is due to variations in factors such as the compound's response to the detector and the ionization efficiency during analysis [10].

Relative abundance is particularly valuable in understanding the dominant contributors to a fragrance's profile. Compounds with higher relative abundance, such as Octanal, 2-(phenylmethylene) (96.4%) in Sample C and Ethylene Brassylate (92.9%) in Sample A, are likely to significantly influence the perceived aroma. However, compounds with lower abundance can also play critical roles, as they may have strong olfactory characteristics or synergize with other compounds to create a balanced scent [11]. For instance, 1R-.alpha.-Pinene (7.59%) in Sample C, though present in a smaller proportion, contributes to the freshness and liveliness of the citrus notes.

B. Description of Some of The Chemical Compounds Found in The Fragrance

The analysis revealed that different fragrances have unique chemical compounds contributing to their calming effects and other functionalities. The discussion will highlight several key chemical compounds identified in all these fragrances:

1) **Limonene:** Limonene is a natural compound categorized as a cyclic monoterpene, and it is found in the peels of citrus fruits, particularly in high concentrations in the peels of oranges and lemons [12]. It is one of the most common and well-known terpenes in nature. Limonene is known for its pleasant, citrusy aroma [13]. It contributes a fresh and uplifting scent reminiscent of citrus fruits. The fragrance industry often utilizes limonene as a natural fragrance compound to impart a citrus note to perfumes, colognes, and various scented products.
2) **Azulene:** Azulene derivatives occur naturally in mushrooms e.g., *Lactarius indigo*. Chamazulene can be obtained in chamomile, wormwood, or achillea oil and is known for antiallergic, antibacterial, and anti-inflammatory applications [14]. A derivative of azulene, guaiazulene (GA) has gained perception for its pleiotropic health effects, especially due to its anti-inflammatory and antioxidant properties [15]. Studies by researchers have endorsed the use of GA to manage disorders such as bacterial infections, tumours, immunomodulation, expectorants, diuretics, diaphoresis, ulcers, and dermatitis. Other than that, Azulene has a unique and pleasant herbal scent with subtle floral and fruity notes [16]. When incorporated into a perfume formulation, it can add a distinctive aroma, contributing to the overall fragrance profile. The specific scent may vary depending on the concentration and other ingredients in the perfume.
3) **Butylated Hydroxytoluene:** Butylated hydroxytoluene (BHT), is a well-known synthetic antioxidant [17]. In the process of production of essence and flavor, some synthetic phenolic antioxidants are added to prevent, or delay, the oxidation of the elements of essence, to improve stability and prolong the storage life [18]. Thus, BHT is one of the examples of the most used synthetic phenolic antioxidants. Antioxidants are used in fragrances to help protect these volatile compounds from oxidation [19]. By inhibiting the detrimental effects of oxygen exposure, antioxidants can help maintain the fragrance's original aroma and prevent it from turning rancid or losing its appeal over time.
4) **Lilial:** Lilial is a high-tonnage, low-cost perfumery ingredient with a lily-of-the-valley odor [20]. It is mainly used in home and personal care, where it is appreciated for its relatively low odour threshold of 0.45 ng/l, and its bloom and tenacity. It is a chemical compound commonly used as a perfume in cosmetic preparations and laundry powders, often under the name butylphenyl methylpropional and it is a synthetic aromatic aldehyde. Moreover, a study also shows that the used of lilial as Insect repellents are widely used to fend off nuisance mosquitoes and, more importantly, to reduce or eliminate mosquito bites in areas where viruses and other vector-borne diseases are circulating [21].
5) **Ethylene Brassylate:** Ethylene Brassylate is a synthetic musk compound commonly used in perfumery [22]. Musk compounds are valued for their ability to impart a warm, animalic, and sensual quality to fragrances [23]. Therefore, Ethylene Brassylate is used to create a musky note in perfumes that is often associated with depth, warmth, and sensuality. They can enhance the overall composition and longevity of a fragrance.
6) **Thujopsene:** Thujopsene is a natural compound found in the essential oils of various coniferous trees, such as cedar and juniper. It is a sesquiterpene hydrocarbon component that occurs in several useful coniferous woods, including *Cryptomeria japonica* and *Chamaecyparis obtuse*, belonging to the class of terpenes, and contributes a woody, earthy, and sometimes spicy aroma [24]. Thujopsene

provides a woody and earthy note to fragrances. This type of note is often used in perfumery to create a sense of depth, warmth, and connection to nature [25].

7) **Piperonal:** Piperonal also known as heliotropin is a simple aromatic aldehyde compound with a characteristic cherry-like aroma and has been widely used in the flavor and fragrance industries to exploit its vanillin- or cherry-like fragrance [26]. It also has the potential to be used as a therapeutical compound due to its diverse pharmaceutical activities, such as antitubercular, anticonvulsant, antidiabetic, anti-obesity, and antimicrobial activities. Moreover, it is an aromatic aldehyde that is solid at room temperature and has a characteristic floral fragrance [27]. This substance is utilized with fixers in the cosmetic industry, and chemical industries with substrates for synthesizing various products.
8) **Vanilin:** Vanillin, a key aromatic compound that imparts the characteristic sweet and creamy scent of vanilla is the second most popular flavoring agent after saffron and is extensively used in various applications, e.g., as a food additive in food and beverages and as a masking agent in various pharmaceutical formulations [28]. It is also considered a valuable product for other applications, such as metal plating and the production of other flavoring agents, herbicides, ripening agents, antifoaming agents, and personal and home-use products such as deodorants, air fresheners, and floor-polishing agents. The primary use of vanillin in fragrances is to provide a distinctive vanilla aroma. Moreover, Vanillin is a specialized metabolite and the main ingredient of vanilla extract that occurs in concertation of 1.0–2.0% w/w in cured vanilla beans [29]. Vanillin has different functional groups, like aldehyde, hydroxyl, and ether attached to an aromatic ring. Vanillin is either isolated from vanilla extract or is chemically synthesized from guaiacol. Besides being known for flavor and fragrance, it has diverse bioactive properties, namely anticancer, neuroprotective, antibiotic potentiation, and anti-quorum sensing.
9) **Cedrol:** Cedrol is a natural compound found in the essential oils of various coniferous trees, particularly cedarwood [30]. It is used as a woody spicy fragrance which is a valuable ingredient in the fragrance industry, contributing unique characteristics to soap, detergents, creams, lotions, and perfumes [31]. Just like Thujopsene, Cedrol is a bioactive sesquiterpene with ubiquitous distribution in the essential oils of cedar and conifers [32]. Cedar oil and its major components, β-cedrene, cedrol, and thujopsene, exert various biological activities, such as antiseptic, anti-inflammatory, antispasmodic, tonic, astringent, diuretic, sedative, insecticidal, and antifungal effects. Therefore, these compounds are used globally as traditional medicines, as well as in soaps, shampoos, fragrances, and cosmetics. Its woody scent imparts a warm, earthy, and sometimes resinous aroma, making it a popular choice for fragrances that aim to capture the essence of woodlands or forests [33].
10) **Pinene:** Pinene refers to a pair of isomeric organic compounds, alpha-pinene, and beta-pinene, that are commonly found in the essential oils of various plants, especially coniferous trees like pine [34]. Pinenes are the most abundant components in a wide range of species including tropical, Mediterranean, and coniferous plants, especially in the essential oils from the genera such as *Pinus, Eucalyptus, Rosmarinus, and Lavandula*. α-Pinene and β-pinene are also major components of commercial turpentine. Pinenes possess various pharmacological properties such as antimicrobial, hypertensive, antinociceptive, and anti-inflammatory [35]. In addition to various bioactive properties, pinenes have been used for centuries in the cosmetic industries, especially for flavor and fragrance purposes. Furthermore, Pinene is volatile and tends to evaporate relatively quickly [36]. As a result, it is often used as a top note in fragrance compositions.
11) **Furanone:** Furanones are often associated with sweet, fruity, and sometimes caramel-like notes [37]. They can contribute to the overall sweetness and complexity of a fragrance. One example of it which is 2,5-Dimethyl-4-hydroxy-3(2H)-furanone (DMHF), is an aroma compound found in various fruits and foods and used widely in the flavor and perfume industry [38]. Dilute DMHF solutions exhibit a strawberry-like flavor while DMHF concentrates have a caramel-like aroma. It's important to note that the specific furanone used in perfumery can vary, and the overall effect on a fragrance depends on their concentration and how they interact with other aromatic compounds in the formulation. Moreover, Furanone moieties establish the pharmacophores of many biologically active molecules casing various therapeutic categories such as analgesic, anti-inflammatory, anticancer, anticonvulsant, antibacterial, antifungal, antioxidant, antiulcer, and anti-tuberculosis compounds [39].

V. CONCLUSIONS

The GC-MS analysis of three commercial fragrances (Type A, B, and C) has revealed distinct chemical profiles, each characterized by a unique composition of aromatherapeutic compounds that align with their described olfactory and emotional effects. Type A, noted for its floral and fruity notes, was dominated by compounds such as Ethylene Brassylate (92.9%), contributing a sweet musky aroma, and Octanal, 2-(phenylmethylene) (95.5%), which enhances fruity and floral characteristics. These findings strongly support Type A's association with freshness and vitality.

Type B, recognized for its warm and comforting aroma reminiscent of spices and woods, was rich in compounds like Piperonal (89.2%), Vanillin (66.4%), and Cedrol (41.1%), which impart sweet, spicy, and woody qualities. These components substantiate the fragrance's ability to evoke a sense of warmth and coziness. Similarly, Type C, characterized by its bright, citrus-floral blend, exhibited high relative abundances of 2(3H)-Furanone, 5-heptyldihydro (79.3%), and Benzeneethanol,.alpha.,.alpha.-dimethyl-, acetate (71.8%), which enhance its uplifting and joyful attributes.

These chemical profiles highlight the potential of these fragrances to modulate emotional states through their olfactory properties, as many of the identified compounds are associated with specific sensory and psychological effects. Compounds such as Limonene and Vanillin, known for their roles in

enhancing mood and reducing stress, further reinforce this aromatherapeutic potential.

In conclusion, the findings provide valuable insights into the chemical composition of these fragrances and their corresponding emotional effects. These results not only validate the fragrances' claims but also underline the importance of understanding chemical profiles in designing aromatherapeutic formulations aimed at modulating emotional states. Future research should focus on linking these chemical profiles with quantitative behavioural and physiological outcomes to deepen our understanding of the role of fragrance in emotional well-being.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest regarding the publication of this paper.

ACKNOWLEDGEMENT

We extend our sincere gratitude to the Faculty of Science and Technology, Universiti Sains Islam Malaysia (USIM), the Brain & Behaviours Research Group (BBRG), and Sugarbomb Company for their invaluable support and collaboration throughout this research. Special thanks to Chem Ts Dr. Muhammad Zamir Othman from Sugarbomb Sdn. Bhd. for his guidance and industry contributions. The contributions have played a vital role in the successful completion of this study. This research was funded by the USIM grant PPPI/BM/FST/USIM/113823.

REFERENCES

[1] Vora, L. K., Gholap, A. D., Hatvate, N. T., Naren, P., Khan, S., Chavda, V. P., ... & Khatri, D. K. (2024). Essential oils for clinical aromatherapy: a comprehensive review. *Journal of Ethnopharmacology*, 118180. https://doi.org/10.1016/j.jep.2024.118180.

[2] Cui, J., Li, M., Wei, Y., Li, H., He, X., Yang, Q., ... & Qin, D. (2022). Inhalation aromatherapy via brain-targeted nasal delivery: Natural volatiles or essential oils on mood disorders. *Frontiers in Pharmacology*, *13*, 860043.https://doi.org/10.3389/fphar.2022.860043

[3] Maggioni, E. (2015). The Smell of Emotions: Olfactory Influences on Emotions and Consumer Behaviour. https://hdl.handle.net/10281/70695

[4] Hubschmann, H. J. (2015). *Handbook of GC-MS: Fundamentals and Applications*. John Wiley & Sons.

[5] Shi, T., Qi, M., & Huang, X. (2020). High-resolution performance of triptycene functionalized with polycaprolactones for gas chromatography. *Journal of Chromatography A*, *1614*, 460714. https://doi.org/10.1016/j.chroma.2019.460714.

[6] Stashenko, E., & Martínez, J. R. (2014). Gas chromatography-mass spectrometry. Advances in Gas Chromatography, 1-38.

[7] Karasek, F. W., & Clement, R. E. (2012). Basic gas chromatography-mass spectrometry: Principles and techniques. Elsevier.

[8] Sparkman, O. D., Penton, Z., & Kitson, F. G. (2011). Gas chromatography and mass spectrometry: A practical guide. Academic press.

[9] Veenaas, C., Linusson, A., & Haglund, P. (2018). Retention-time prediction in comprehensive two-dimensional gas chromatography to aid identification of unknown contaminants. *Analytical and Bioanalytical Chemistry*, *410*, 7931-7941. https://doi.org/10.1007/s00216-018-1415-x.

[10] Milman, B. L. (2015). General principles of identification by mass spectrometry. *TrAC Trends in Analytical Chemistry*, *69*, 24-33. https://doi.org/10.1016/j.trac.2014.12.009.

[11] Louw, S. (2021). Recent trends in the chromatographic analysis of volatile flavor and fragrance compounds: Annual review 2020. *Analytical Science Advances*, *2*(3-4), 157-170. https://doi.org/10.1002/ansa.202000158.

[12] Anandakumar, P., Kamaraj, S., & Vanitha, M. K. (2021). D-limonene: A multifunctional compound with potent therapeutic effects. *Journal of Food Biochemistry*, *45*(1), e13566. https://doi.org/10.1111/jfbc.13566.

[13] Vieira, A. J., Beserra, F. P., Souza, M. C., Totti, B. M., & Rozza, A. L. (2018). Limonene: Aroma of innovation in health and disease. *Chemico-Biological Interactions*, *283*, 97-106. https://doi.org/10.1016/j.cbi.2018.02.007.

[14] Bakun, P., Czarczynska-Goslinska, B., Goslinski, T., & Lijewski, S. (2021). In vitro and in vivo biological activities of azulene derivatives with potential applications in medicine. *Medicinal Chemistry Research*, *30*, 834-846. https://doi.org/10.1007/s00044-021-02701-0.

[15] Akram, W., Tagde, P., Ahmed, S., Arora, S., Emran, T. B., Babalghith, A. O., & Simal-Gandara, J. (2023). Guaiazulene and related compounds: A review of current perspective on biomedical applications. *Life Sciences*, 121389. https://doi.org/10.1016/j.lfs.2023.121389.

[16] Darrell, N. (2022). Essential oils: A concise manual of their therapeutic use in herbal and aromatic medicine. Aeon Books.

[17] Ghosh, C., Singh, V., Grandy, J., & Pawliszyn, J. (2020). Development and validation of a headspace needle-trap method for rapid quantitative estimation of butylated hydroxytoluene from cosmetics by hand-portable GC-MS. *RSC Advances*, *10*(11), 6671-6677. DOI: 10.1039/C9RA08676E.

[18] Li, X. L., Meng, D. L., Zhao, J., & Yang, Y. L. (2014). Determination of synthetic phenolic antioxidants in essence perfume by high performance liquid chromatography with vortex-assisted, cloud-point extraction using AEO-9. Chinese Chemical Letters, 25(8), 1198-1202. https://doi.org/10.1080/01496395.2018.1446983.

[19] Thiviya, P., Gamage, A., Piumali, D., Merah, O., & Madhujith, T. (2021). Apiaceae as an important source of antioxidants and their applications. *Cosmetics*, *8*(4), 111. https://doi.org/10.3390/cosmetics8040111.

[20] Schroeder, M., Mathys, M., Ehrensperger, N., & Büchel, M. (2014). γ-Unsaturated aldehydes as potential lilial replacers. *Chemistry & biodiversity*, *11*(10), 1651-1673. DOI: 10.1021/acs.orglett.9b00765.

[21] Zeng, F., Xu, P., Tan, K., Zarbin, P. H., & Leal, W. S. (2018). Methyl dihydrojasmonate and lilial are the constituents with an" off-label" insect repellence in perfumes. *PLoS One*, *13*(6), e0199386. https://doi.org/10.1016/j.ibmb.2019.103224.

[22] Soares, R. M. C. (2016). Detection of synthetic musks and UV-filters in carpobrotus edulis by QuEChERS/GC-MS.

[23] Nakano, A. K. (2019). Understanding Fragrance: From Chemistry to emotion. *Cosmetic Formulation: Principles and Practice*, 263-277.

[24] Mukai, A., Takahashi, K., Kofujita, H., & Ashitani, T. (2019). Antitermite and antifungal activities of thujopsene natural autoxidation products. *European Journal of Wood and Wood Products*, *77*, 311-317. https://doi.org/10.1007/s00107-018-1370-4.

[25] Baldovini, N., & Filippi, J. J. (2017). Natural fragrant raw materials. *Springer Handbook of Odor*, 11-12. https://doi.org/10.1007/978-3-319-26932-0_3.

[26] Jin, Z., Ro, D. K., Kim, S. U., & Kwon, M. (2022). Piperonal synthase from black pepper, piper nigrum synthesizes a phenolic aroma compound, piperonal, as a CoA-independent catalysis. *Applied Biological Chemistry*, *65*(1), 1-5. https://doi.org/10.1186/s13765-022-00691-0.

[27] Ramos, A. M., & Cremasco, M. A. (2015). Equilibrium thermodynamics and mass transfer parameters estimation of the synthesis products of piperonal from essential oil of piper hispidinervum C. DC by reversed phase liquid chromatography. *Scientia Amazonia*, *4*(1), 9. ISSN:2238.1910.

[28] Banerjee, G., & Chattopadhyay, P. (2019). Vanillin biotechnology: the perspectives and future. Journal of the Science of Food and Agriculture, 99(2), 499-506. https://doi.org/10.1002/jsfa.9303.

[29] Arya, S. S., Rookes, J. E., Cahill, D. M., & Lenka, S. K. (2021). Vanillin: A review on the therapeutic prospects of a popular flavouring molecule. *Advances in traditional medicine*, 1-17. https://doi.org/10.1007/s13596-020-00531-w.

[30] Batur, Ö. Ö., Kiran, İ., Baser, K. H. C., & Demirci, F. (2023). Fungal biotransformation of cedryl formate. *Hacettepe Journal of Biology and Chemistry*, *51*(3), 283-287. https://doi.org/10.15671/hjbc.1244894.

[31] Özşen Batur, Ö. Z. G. E., Kiran, İ., Demirci, F., & Başer, K. H. C. (2022). Fungal biotransformation of cedramber. Biocatalysis and Biotransformation, 40(4), 248-251. https://doi.org/10.1080/10242422.2021.1956908.

[32] Jeong, H. U., Kwon, S. S., Kong, T. Y., Kim, J. H., & Lee, H. S. (2014). Inhibitory effects of cedrol, β-cedrene, and thujopsene on cytochrome P450 enzyme activities in human liver microsomes. *Journal of Toxicology and Environmental Health, Part A*, *77*(22-24), 1522-1532. https://doi.org/10.1002/ffj.3496.

[33] Rhind, J. P. (2014). Listening to scent: An olfactory journey with aromatic plants and their extracts. Book of Singing Dragon.

[34] Kim, M., Sowndhararajan, K., Park, S. J., & Kim, S. (2018). Effect of inhalation of isomers,(+)-α-pinene and (+)-β-pinene on human electroencephalographic activity according to gender difference. *European Journal of Integrative Medicine*, *17*, 33-39. https://doi.org/10.1016/j.eujim.2017.11.005.

[35] Weston-Green, K., Clunas, H., & Jimenez Naranjo, C. (2021). A review of the potential use of pinene and linalool as terpene-based medicines for brain health: Discovering novel therapeutics in the flavours and fragrances of cannabis. *Frontiers in Psychiatry*, *12*, 583211. https://doi.org/10.3389/fpsyt.2021.583211.

[36] Vespermann, K. A., Paulino, B. N., Barcelos, M. C., Pessôa, M. G., Pastore, G. M., & Molina, G. (2017). Biotransformation of α-and β-pinene into flavor compounds. Applied Microbiology and Biotechnology, 101, 1805-1817. https://doi.org/10.1002/9781119434436.ch5.

[37] Haag, F., Hoffmann, S., & Krautwurst, D. (2021). Key food furanones furaneol and sotolone specifically activate distinct odorant receptors. *Journal of Agricultural and Food Chemistry*, *69*(37), 10999-11005. https://pubs.acs.org/doi/10.1021/acs.jafc.1c03314.

[38] Arihara, K., Yokoyama, I., & Ohata, M. (2019). DMHF (2, 5-dimethyl-4-hydroxy-3 (2H)-furanone), a volatile food component with attractive sensory properties, brings physiological functions through inhalation. *Advances in Food and Nutrition Research*, *89*, 239-258. https://doi.org/10.1016/bs.afnr.2019.05.001.

[39] Omanakuttan, V. K., John, J., & Hopf, H. (2021). Synthesis of 3 (2H)-furanones: A review. *European Journal of Organic Chemistry*, *2021*(2), 163-201. https://doi.org/10.1002/ejoc.202001005.