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Chemical Profiling of Electronic Cigarette Liquids from the Klang Valley: GC–MS Analysis and Decision Tree Identification of Flavour Markers

(Profil Kimia Cecair Rokok Elektronik dari Lembah Klang: Analisis GC–MS dan Pengenalpastian Pokok Keputusan Penanda Perisa)

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Abstract

This study sought to characterise the chemical composition of electronic cigarette liquids (e-liquids) available on the Klang Valley market, with a focus on identifying toxic compounds and understanding the key factors that determine flavour categories. The work addresses growing public health concerns regarding the proliferation of unregulated vaping products. Two hundred e-liquid samples collected from the Klang Valley were analysed using Gas Chromatography-Mass Spectrometry (GC-MS) to identify and quantify their chemical constituents. Decision Tree Analysis (DTA) was then applied to investigate associations between specific toxic compounds and different flavour profiles. Nicotine was detected in 196 of 200 samples (98.0%), with a mean relative concentration of 48.79% (SD 20.69; range 4.99–92.67) based on GC–MS peak-area estimation. GC–MS profiling identified 459 compounds in total, including 11 chemicals of potential toxicological concern. Decision Tree Analysis identified ethyl vanillin as the most significant variable for flavour classification ($\chi^2 = 80.688$, $df = 3$, $p < 0.001$), with concentrations above 0.07154% more commonly associated with coffee, dessert, nut and tea profiles. Concentrations below 0.07154% were primarily linked to sweet, fruity flavours, whereas higher levels were characteristic of richer, dessert-like profiles. These findings indicate that the Klang Valley e-liquid market is heavily dominated by nicotine-containing products and flavour additives, with ethyl vanillin being a particularly prevalent flavouring agent. Of particular concern is the widespread presence of ethyl vanillin, as flavour aldehydes may undergo thermal transformation during vaping and contribute to inhalation exposure to potentially harmful degradation products. This underscores an urgent need for evidence-based regulatory standards, including limits on specific flavour additives to mitigate potential inhalation health risks.

Keywords: Electronic cigarette, e-liquid, GC-MS, decision tree analysis, ethyl vanillin, nicotine

Abstrak

Kajian ini menangani kebimbangan kesihatan awam yang semakin meningkat mengenai percambahan produk vape yang tidak dikawal selia. Dua ratus sampel e-cecair yang dikumpulkan dari Lembah Klang dianalisis menggunakan Kromatografi Gas-Spektrometri Jisim (GC-MS) untuk mengenal pasti dan mengukur kandungan kimianya. Analisis Pokok Keputusan (DTA) kemudiannya digunakan untuk menyiasat perkaitan antara sebatian toksik tertentu dan profil perisa yang berbeza. Nikotin dikesan dalam 196 daripada 200 sampel (98.0%), dengan kepekatan relatif purata 48.79% (SD 20.69; julat 4.99–92.67) berdasarkan anggaran kawasan puncak GC-MS. Profil GC-MS mengenal pasti 459 sebatian secara keseluruhan, termasuk 11 bahan kimia yang berpotensi membimbangkan toksikologi. Analisis Pokok Keputusan mengenal pasti etil vanilin sebagai pembolehubah paling ketara untuk pengelasan perisa ($\chi^2 = 80.688$, $df = 3$, $p < 0.001$), dengan kepekatan melebihi 0.07154% lebih kerap dikaitkan dengan profil kopi, pencuci mulut, kacang dan teh. Kepekatan di bawah 0.07154% terutamanya dikaitkan dengan perisa manis dan buah-buahan, manakala tahap yang lebih tinggi adalah ciri profil yang lebih kaya dan seperti pencuci mulut. Penemuan ini menunjukkan bahawa pasaran e-cecair Lembah Klang banyak didominasi oleh produk yang mengandungi nikotin dan bahan tambahan perisa, dengan etil vanilin menjadi agen perisa yang sangat lazim. Kebimbangan khusus ialah kehadiran etil vanilin yang meluas, kerana aldehid perisa mungkin mengalami transformasi haba semasa vape dan menyumbang kepada pendedahan penyedutan kepada produk degradasi yang berpotensi berbahaya. Ini menggariskan keperluan mendesak untuk piawaian kawal selia berasaskan bukti, termasuk had ke atas bahan tambahan perisa tertentu untuk mengurangkan potensi risiko kesihatan penyedutan.

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Kata kunci: Rokok elektronik, e-cecair, GC-MS, analisis pokok keputusan, etil vanilin, nikotin

INTRODUCTION

The global use of electronic cigarettes (e-cigarettes) has surged, becoming a prevalent phenomenon across various age groups, particularly among adult men (Chong et al. 2020). In Malaysia, this trend is alarmingly common among youth and adolescents (Ab Rahman et al. 2019; Ching Sin Siau et al. 2025). The 2022 National Health and Morbidity Survey (NHMS) estimated 1.1 million e-cigarette users in Malaysia, with the highest prevalence among those aged 20-24. The prevalence was increasing in trend, starting with 9.8% in 2017 to 14.9% in 2022 (Institut Kesihatan Umum Malaysia 2022). The accessibility and unregulated sale of diverse e-liquid flavours fuel concerns regarding product misuse, safety standards, and potential health risks (Wartawan Bisnes Berita Harian 2024). In Malaysia, the lack of standardised regulations for e-liquid composition and labelling has led to a market filled with products of unknown and potentially harmful chemical profiles. This study addresses this gap by providing a chemical survey of locally available e-liquids.

E-liquids typically contain a base of propylene glycol (PG) and vegetable glycerine (VG), nicotine, and flavourings. While PG and VG are generally recognized as safe (GRAS) for ingestion, their thermal degradation during aerosolisation can generate toxic compounds such as formaldehyde, acetaldehyde, and acrolein (Farsalinos & Gillman 2017; Shields et al. 2017). Furthermore, flavour chemicals, though safe for consumption, have unknown and potentially adverse effects when inhaled (Tierney et al. 2016). Certain flavourings like diacetyl, cinnamaldehyde, and pulegone have been associated with respiratory irritation, cytotoxicity, and carcinogenicity (Behar et al. 2016; Jabba & Jordt 2019; Omaiye et al. 2019). Although several flavouring chemicals and thermal degradation products have been reported in e-liquids and aerosols, inhalation-specific exposure limits remain unavailable for many of these compounds. This creates a particular challenge for risk assessment, as substances considered acceptable for oral consumption may not be safe when heated and inhaled.

The link between E-cigarette or Vaping Product Use-Associated Lung Injury (EVALI) and toxic compounds in e-liquids underscores the critical need for research into their chemical composition (Kalininskiy et al. 2019). In Malaysia, the regulatory landscape is evolving, but a significant gap remains in the empirical surveillance of e-liquid constituents sold on the market.

Among flavouring agents, ethyl vanillin warrants closer attention. Although widely used as a food flavouring, its safety profile for inhalation remains insufficiently characterised. Experimental work has shown that several flavouring chemicals used in e-liquids, including aldehydic compounds, may impair cellular viability and function. Rickard et al. reported cytotoxic responses in liver-cell models following exposure to selected e-cigarette flavouring chemicals (Rickard et al. 2021) while Jabba et al. demonstrated that flavour aldehydes can react with e-liquid solvents to form adducts with altered toxicological properties (Jabba et al. 2020). These findings suggest that the toxicological behaviour of flavouring compounds cannot be inferred solely from their food-use status and highlight the need for compound-specific surveillance in inhalation products.

This study aims to address this gap by: 1) identifying the primary formulations of e-liquids in Klang Valley, 2) detecting the presence of toxic and prohibited substances using GC-MS, and 3) utilising Decision Tree Analysis to identify the key chemical compounds associated with different flavour categories. The findings will provide crucial data to inform evidence-based regulatory policies for the e-cigarette industry in Malaysia and similar markets. Given the complexity and variability of e-liquid matrices, and the unavailability of certified reference standards for many flavour compounds, a semi-quantitative GC-MS approach was employed. This allowed for broad chemical profiling and detection of toxicants, with quantitative focus placed on nicotine and major flavour markers where standards were accessible.

METHODOLOGY

Sample Collection

A total of 200 refillable e-liquid samples were purchased from eight vendors across the Klang Valley, Malaysia. Sampling was purposive rather than strictly random, with efforts made to capture the range of products commonly available to consumers at the point of sale. Products were selected to represent variation in brand, labelled flavour, nicotine indication, PG/VG ratio where stated, packaging style, and retail price. Samples were priced between RM15 and RM40 (approximately USD4–10). Each sample was assigned a unique identification code based on postal code, month of purchase, and sample number.

Preliminary Analysis

Each sample underwent preliminary characterisation. The flavour aroma and category were determined by four independent analysts through orthonasal evaluation and confirmed against the labelled flavour on the packaging. Categories were classified as: 1) Alcoholic beverages/Cordial/Candy/Fruit, 2) Coffee/Dessert/Nut/Tea, 3) Menthol/Mint, and 4) Spices/Tobacco/Others (Krüsemann et al. 2020). Information on brand, flavour name, PG/VG ratio, and labelled nicotine concentration was recorded.

Sample Preparation

Each e-liquid sample was homogenised using a shaker at 1800 rpm for 1 minute. A 10 µL aliquot of the sample was then diluted with 1000 µL of methanol in a GC vial and homogenised again for 1 minute prior to instrumental analysis.

GC-MS Analysis

Analysis was performed using a Shimadzu Nexis GC-2030 gas chromatograph coupled with a GCMS-QP2020 NX mass spectrometer, equipped with an AOC-20i+s auto sampler/injector. The GC-MS analysis was performed using the following parameters (Abdull Manap et al. 2024). Separation was achieved using a column oven temperature of 50.0 °C. Samples were introduced via a splitless injection mode with the injector port maintained at 280.00 °C. The carrier gas pressure was set at 28.0 kPa, with a total flow of 40.9 mL/min, a column flow of 1.80 mL/min, and a resulting linear velocity of 48.7 cm/sec. The mass spectrometer interface temperature was set to 280.00 °C and the ion source temperature to 230.00 °C. A solvent cut time of 8.00 min was applied to protect the detector. Data acquisition in full scan mode (Q3 Scan) commenced at 8.50 min and ended at 35.00 min, with a scan range of *m/z* 40.00 to 600.00. The event time was 0.150 sec with a scan speed of 5000. The detector gain was set to 1.00 kV, relative to the tuning result, with a threshold of 0. Compound identification was achieved by comparing mass spectra and retention times with the NIST 17 library. Semi-quantitative analysis was performed using chromatographic peak area normalisation following compound identification by library matching and retention behaviour. For each detected compound, the integrated peak area from the total ion chromatogram was expressed as a percentage of the total integrated peak area of the sample chromatogram. These values were used as relative abundance estimates rather than absolute concentrations. Identification was based on mass spectral matching and retention time consistency; quantification of non-nicotine compounds was not performed by selected ion calibration because certified reference standards were not available for most flavour constituents. Nicotine was analysed separately using an external calibration approach with a certified nicotine reference standard. A series of nicotine calibration solutions was prepared in methanol, and the calibration curve was generated from GC–MS peak responses under the same analytical conditions as the samples. Nicotine concentrations were then estimated by comparison with the calibration curve. No internal standard was used in the present study. Nicotine values are presented as estimated concentrations, whereas all other detected compounds were interpreted semi-quantitatively as relative peak-area percentages (Hamzah et al. 2025).

Limitations in Quantitative Analysis

Because certified reference standards were unavailable for most flavouring compounds and no internal standards were used for these analytes, full quantitative analysis was not possible. Consequently, non-nicotine compounds were interpreted using relative peak-area percentages only. Nicotine was the only target analyte assessed using external calibration. This distinction is important when interpreting the reported prevalence and abundance of flavour-related compounds, including ethyl vanillin.

Data Analysis

Descriptive statistics were used to summarise the PG/VG ratios, nicotine presence, and the concentrations of detected toxic compounds. Decision Tree Analysis (DTA) was performed using IBM SPSS Statistics version 22. The dependent variable was the flavour category (1-4), and the independent variables were the concentrations of the 11 detected toxic compounds. The DTA algorithm was used to identify the compound that best differentiated the flavour categories based on statistical significance (χ^2 test).

RESULTS

E-liquid Formulation

The analysis of labelled ingredients revealed that 83% of the samples contained a 50:50 PG/VG ratio (Figure 1). The remaining samples had ratios skewed towards higher VG content (e.g., 30:70, 40:60), typically associated with larger aerosol cloud production.

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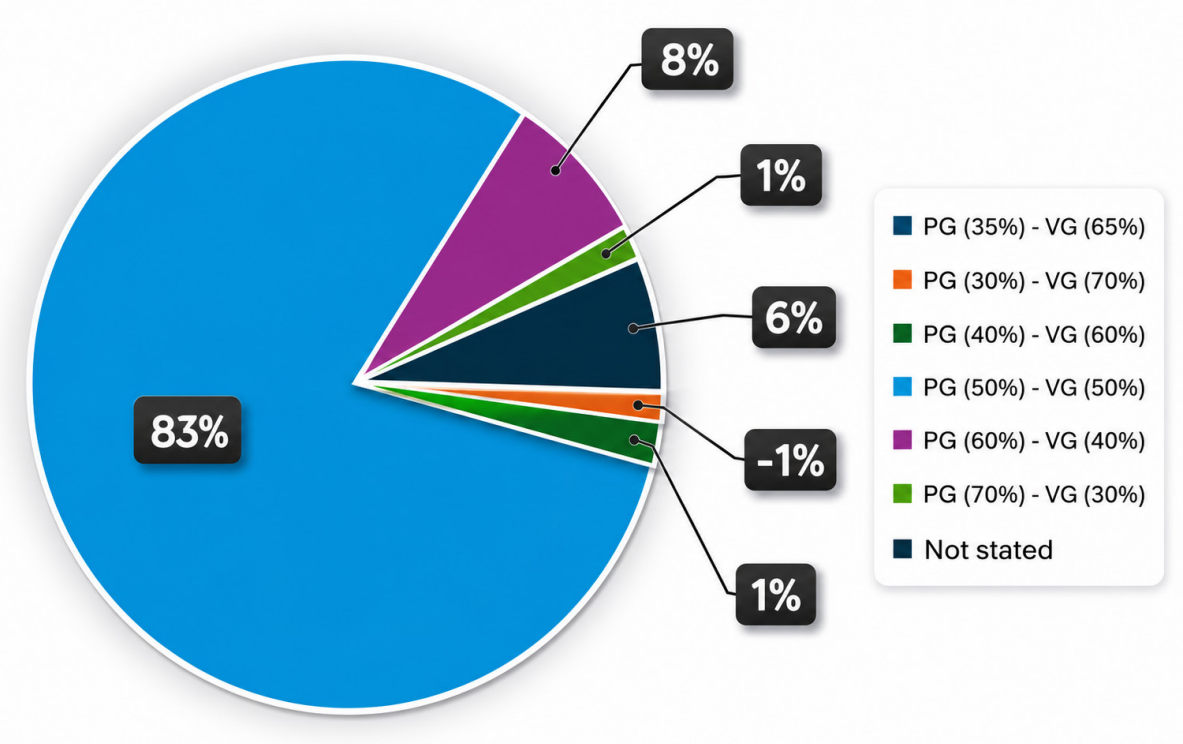

FIGURE 1. PG/VG ratio in e-liquid samples

Nicotine Content

GC–MS analysis confirmed the presence of nicotine in 196 of the 200 samples analysed (98.0%) (Figure 2). Estimated nicotine concentrations varied widely across products, ranging from 4.99 to 92.67%, with a mean of 48.79% and a standard deviation of 20.69. This finding indicates substantial variability in nicotine content across commercially available e-liquids, despite frequently ambiguous or non-standardised product labelling (Figure 3).

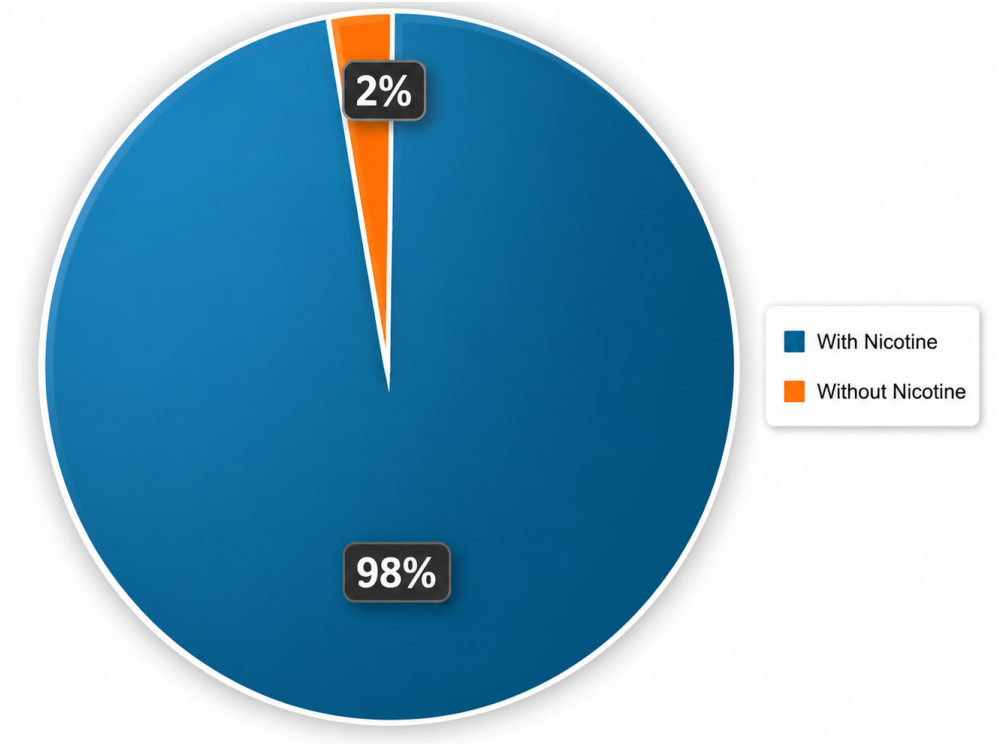

FIGURE 2. GC-MS analysis confirmed the presence of nicotine in 196 out of 200 samples (98%)

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FIGURE 3: Ambiguous labelling using colour codes and symbols. The red arrow indicates the nicotine level, a detail only the seller understands

Identification of Chemical Compounds

GC-MS analysis detected a total of 459 compounds across all samples, encompassing alcohols, aldehydes, ketones, esters, acids, and nitrogen-containing compounds.

Toxic Compounds

Eleven chemicals of potential toxicological concern were identified in the sample set (Table 1). This included nicotine and several flavour-related compounds for which inhalation safety data remain limited or context-dependent. Nicotine was the most prevalent detected compound. Among flavour-related constituents, ethyl maltol, vanillin, and ethyl vanillin were the most frequently observed. Other toxic compounds like benzaldehyde, cinnamaldehyde, and pulegone were detected in fewer than five samples.

TABLE 1: Descriptive statistics of detected toxic compounds expressed as relative peak area percentage (%) from GC-MS analysis

Compound	N	Minimum (%)	Maximum (%)	Mean (%)	Std. Deviation
Nicotine*	196	4.9922	92.6662	48.7876	20.6864
Ethyl Maltol	159	0.0192	18.8703	3.4866	3.6722
Vanillin	139	0.0205	31.4969	3.1509	4.6559
Ethyl Vanillin	86	0.0243	15.4476	2.7425	3.4488
Furfural	7	0.0250	0.5672	0.1611	0.1852
Cinnamaldehyde	4	0.2670	0.4662	0.3706	0.1071
Benzaldehyde	3	0.0523	0.2804	0.1360	0.1256
Menthol	4	0.0000	0.2873	0.1043	0.1365
Pulegone	2	0.0541	0.3171	0.1856	0.1860
Eugenol	1	0.1868	0.1868	0.1868	-
5-Hydroxymethylfurfural	1	0.0209	0.0209	0.0209	-

*Nicotine concentrations are reported as relative peak area percentages. Although not absolute quantitation without internal standard correction, these values reflect the high and variable nicotine content in market samples.

Decision Tree Analysis (DTA)

The flavour category distribution was: Category Alcoholic beverages/Cordial/Candy/Fruit (63.0%), Category Coffee/Dessert/Nut/Tea (33.0%), Category Menthol/Mint (2.5%), and Category Spices/Tobacco/Others (1.5%). The DTA model identified ethyl vanillin concentration as the most significant splitting variable ($\chi^2 = 80.688$, df = 3, $p < 0.001$) at a threshold of 0.07154% (Figure 4).

Node 1 (Ethyl Vanillin ≤ 0.07154%): 120 samples. Of these, 85% were classified as Category Alcoholic beverages/Cordial/Candy/Fruit.

Node 2 (Ethyl Vanillin > 0.07154%): 80 samples. Of these, 68.8% were classified as Category 2 Coffee/Dessert/Nut/Tea.

The DTA does not identify the most abundant or most frequently detected compound overall. Rather, it identifies the variable that best separates flavour categories statistically within the dataset. Although ethyl maltol and vanillin were more prevalent across all samples, ethyl vanillin provided the strongest discriminatory threshold for distinguishing between broader fruity/candy-type profiles and richer dessert-related profiles (Figure 4).

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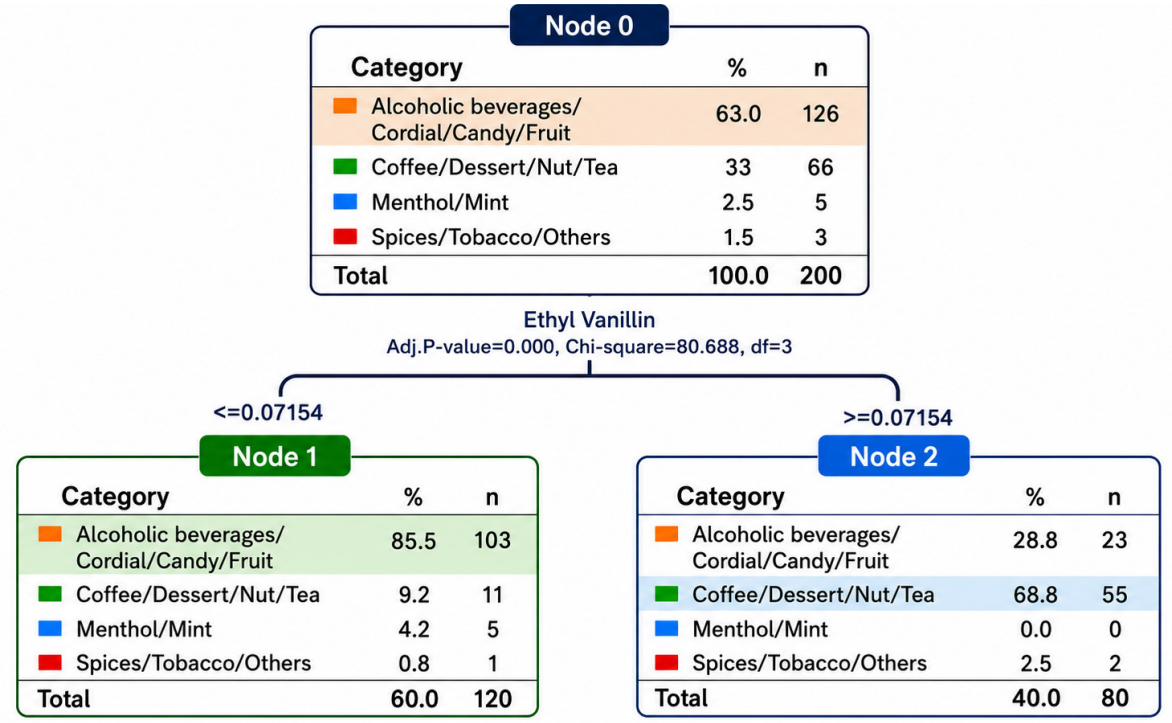

FIGURE 4. The DTA model identified ethyl vanillin concentration as the most significant splitting variable (χ^2 = 80.688, df = 3, $p < 0.001$) at a threshold of 0.07154%

DISCUSSION

While this study employed a semi-quantitative GC-MS approach due to the lack of available standards for many flavourants, the relative abundance data provide a useful indication of compound prevalence and comparative concentration trends within the sampled products in the Klang Valley. The high detection frequency and relative levels of nicotine and ethyl vanillin are of particular concern. This study provides a comprehensive chemical profile of e-liquids readily available in the Klang Valley market, revealing two major public health concerns: the near-universal and often high-concentration presence of nicotine, and the dominant use of ethyl vanillin as a key flavour-defining compound with significant toxicological potential upon inhalation (Abdull Manap et al. 2021; Mohd Aris et al. 2022).

The detection of nicotine in 98% of samples, with an alarmingly high average concentration of 48.79 mg/g, underscores a possible critical failure in consumer protection and regulatory oversight. This finding is particularly concerning given the prevalent use of ambiguous colour codes and symbols for nicotine strength (Figure 2), a practice that obscures the addictive potency of these products. Such obfuscation poses a direct threat to public health, potentially facilitating nicotine addiction among youth and non-smokers who may initiate use unaware of the high dosage they are consuming (Yingst et al. 2019). The discrepancy between the often vague labelling and the actual, potent nicotine content highlights an urgent need for regulations mandating clear, accurate, and standardized nicotine disclosure on all e-liquid products.

The GC-MS analysis identified a complex mixture of compounds, including eleven known toxicants. However, the Decision Tree Analysis (DTA) revealed a particularly insightful finding: ethyl vanillin concentration was the most statistically significant variable for classifying e-liquid flavours. This is toxicologically noteworthy because ethyl vanillin, while generally recognized as safe for ingestion (GRAS), is a synthetic compound chosen over natural vanillin for its superior potency, being approximately 2-4 times stronger in aroma and flavour (Vilela et al. 2019). This potency makes it a cost-effective agent for creating intense sweet, creamy, and vanilla notes, explaining its prevalence in dessert and candy-themed e-liquids. The DTA quantitatively confirms this, showing that concentrations above 0.07154% primarily define the Coffee/Dessert/Nut/Tea category, while lower levels are characteristic of Alcoholic beverages/Cordial/Candy/Fruit flavours. This positions ethyl vanillin not merely as an additive, but as a primary driver of product identity in the Klang Valley market.

The predominance of ethyl vanillin is concerning due to its potential behaviour under the thermal stress of vaping. When heated, flavour compounds can decompose into harmful degradation products. Specifically, compounds with aldehyde and phenolic structures, like ethyl vanillin, are known precursors to toxic carbonyl compounds

such as formaldehyde, acetaldehyde, and acrolein (Erythropel et al. 2019). More alarmingly, the pyrolysis of vanillin derivatives can yield reactive phenols like guaiacol and catechol, which are associated with airway irritation and cytotoxicity (Klager et al. 2017; Omaiye et al. 2019). Ethyl vanillin was present in 86 samples and showed a broad range of relative abundance values in the chromatographic data. Although the present study did not perform absolute quantification of ethyl vanillin, its repeated detection and its role in flavour classification suggest that it is an important constituent of many commercially available products. This is relevant from a toxicological perspective because flavour aldehydes may undergo thermal transformation during vaping, yet their inhalation safety remains insufficiently characterised. The chronic inhalation of these thermal degradation products is linked to respiratory inflammation, epithelial damage, and an increased risk of cardiovascular and pulmonary diseases (Clapp et al. 2017). Ethyl vanillin, like many food-grade flavouring agents, is generally regarded as safe for ingestion; however, this designation cannot be assumed to apply to inhalation exposure, particularly following heating and aerosol generation.

Interestingly, despite the well-documented risks of certain flavourants, other known toxicants like diacetyl, cinnamaldehyde, and pulegone were detected in fewer than five samples. This low prevalence may reflect a market response to widespread publicity surrounding popcorn lung and other flavourant-related illnesses, leading manufacturers to reformulate away from these notorious compounds (Allen et al. 2016). Alternatively, it may indicate distinct regional flavour preferences in the Klang Valley market, shifting the primary toxicological concern from these compounds to the high-volume use of others, such as ethyl vanillin. This finding underscores the importance of localised market surveillance, as risk profiles can vary significantly by region and over time.

This study has limitations. The sampling was focused on the Klang Valley, which may not be fully representative of the entire Klang Valley market. Furthermore, the analysis was performed on the e-liquid itself; future research should analyse the aerosol generated from these liquids to determine the specific transfer efficiency of ethyl vanillin and quantify the actual yield of its thermal degradation products that a user would inhale. These findings provide evidence-based support for the urgent development and enforcement of Klang Valley regulations governing e-liquid composition, labelling, and sales, particularly to protect youth from high-nicotine products and unassessed flavorant exposures.

CONCLUSION

This study demonstrates that the Klang Valley e-liquid market is dominated by products containing nicotine and a wide array of flavour chemicals. Ethyl vanillin was identified as a significant flavour-related marker associated with major flavour categories that defines key product categories. Given the potential for flavour aldehydes and related compounds to undergo thermal transformation during vaping, the widespread presence of ethyl vanillin supports the need for further aerosol-based toxicological assessment. These findings strongly support the urgent implementation and enforcement of stricter regulatory measures. Recommendations include mandatory disclosure of all ingredients and accurate nicotine concentrations on labels, establishment of maximum concentration limits for specific flavour additives, particularly ethyl vanillin, continuous monitoring and surveillance of the market using advanced analytical techniques like GC-MS and public health campaigns to educate users, especially youth, about the potential risks of inhaling flavour chemicals.

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