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COMPARISON OF GC-MS INTRODUCING TECHNIQUES FOR 2-PHENYLETHANOL DETECTION FROM YEAST

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Abstract

2-Phenylethanol (2-PE) can be produced by microorganisms, especially Saccharomyces cerevisiae. Gas Chromatography-Mass Spectrometer (GC-MS) has been used to analyze volatile producing microorganisms. The Gas Syringe-Static Headspace (GS-SHS), Thin Film-Solid Phase Micro Extraction (TF-SPME), Headspace Sorptive Extraction (HSSE), Dynamic Headspace (DHS), and Direct Thermal Desorption (DTD) were used to introduce Saccharomyces cerevisiae LV-007 cultured medium to GC-MS for 2-PE qualitative and quantitative analyses. The numbers

of detected volatiles from introducing techniques of GS-SHS, TF-SPME, HSSE, DHS, and DTD were 8, 26, 15, 27, and 16, respectively by qualitative analysis. After 2-PE and viable cell quantifications from LV-007 of various introducing techniques, DTD showed the highest 2-PE ratio of 237.37×10-6 μg/ml·CFU. The DTD technique also used short time of 30 min to analyze sample.

Keywords:
2-Phenylethanol, Gas Chromatography-Mass Spectrometry, Introducing Techniques, Direct Thermal Desorption

1. Introduction

2-Phenylethanol or Phenylethyl alcohol (2-PE) is an aromatic alcohol with rose scent. This compound has been applied in many goods, such as cosmetics, foods, and cleaning agents, etc. In present, 2-PE can be produced by rose distillation, chemical synthesis, and microorganisms. Chemical synthesis causes environmental effects, while distillation spends high cost (Mitri et al., 2022).

The volatile producing yeasts have been studied to collect volatile compounds and increased agricultural waste values (Bernardino et al., 2024). 2-PE is not only produced by some bacteria and molds, but it also biosynthesized by yeasts, for example, Saccharomyces cerevisiae and Pichia kudriavzevii (Chreptowicz et al., 2017).

GC-MS is an analytical instrument to identify and quantify the volatile compounds, especially in foods and beverages (Xu et al., 2016). However, there are many techniques to introduce volatile compounds from headspace of food and beverage samples for GC-MS.

Gas Syringe-Static Headspace (GS-SHS) is a simple static technique. By this technique, volatiles from headspace of sample are directly injected into GC-MS by a gastight syringe. While Thin Film-Solid Phase Micro-Extraction (TF-SPME) and Headspace Sorptive Extraction (HSSE), headspace volatiles are absorbed by absorbents, then they are thermally desorbed and transferred into GC-MS (Kremser et al., 2016). Dynamic Headspace (DHS), volatile compounds are purged by inert gas, and then trapped by absorbent. Thermal desorption unit (TDU) is used to release volatiles from absorbents into GC-MS (Hodgson et al., 2000). By Direct Thermal Desorption (DTD), food sample is directly placed in TDU of GC-MS. Their volatiles are purged and transferred into GC-MS column by carrier gas (Lerch & Hässelbarth, 2014). The aims of this study were to qualitatively analyze 2-PE from a reference yeast of Saccharomyces cerevisiae (LV-007) by GC-MS with 5 introducing techniques of GS-SHS, TF-SPME, HSSE, DHS, and DTD, and to compare quantified 2-PE of LV-007 from various introducing techniques with GC-MS.

2. Material & Methods

2.1 2-PE producing yeast strain

Saccharomyces cerevisiae LV-007 was used as a reference strain of 2-PE producing yeast. This strain was isolated from a local Thai dessert fermented rice cake; Ka-nom-tooay-foo (Phithakpol et al., 1995) by our laboratory staffs, and it represented a strongly rose scent and fruity

aroma on potato dextrose agar (PDA) (HIMEDIA, India). After LV-007 stock culture thawing, suspension was streaked on PDA, and incubated at 30°C for 24 h to activate strain.

2.2 Sample preparation for qualitative analysis by GC-MS

To prepare slant agars, 4 ml sterile PDA liquid was placed into 20 ml sterile headspace vial with septum-screwed cap. The LV-007 single colony was streaked onto PDA surface, and incubated at 30°C for 24 h. This cultured LV-007 in headspace vial was then qualitatively analyzed by GC- MS with GS-SHS, TF-SPME, HSSE, and DHS sample introducing techniques. For DTD introducing technique, 35 µl sterile PDA liquid was gently loaded into a sterile glass micro-vial for TDU (GERSTEL, Germany). After agar solidification, LV-007 was stamped on agar surface by in-house micro-loop, and incubated with the same conditions. This experiment, mixture of C8-C20 standard alkanes (Sigma-Aldrich, USA) were analyzed their retention times for retention indexes (RI) calculation.

2.3 Sample preparation for quantitative analysis by GC-MS

Standard 2-PE (Sigma-Aldrich, USA) was prepared with concentrations from 0.102-10200 µg/ml. The GC-MS with 5 introducing techniques was used to analyze 2-PE standard solutions.

LV-007 inoculum with 1% was loaded into potato dextrose broth (PDB) (HIMEDIA, India). After cultivation at 30°C for 24 h, 4 ml LV-007 cultured broth was loaded in a headspace vial with septum-screwed cap for GC-MS quantitative analysis with TF-SPME, HSSE, and DHS sample introducing techniques. While 35 µl LV-007 cultured broth was filled into a glass micro-vial for DTD introducing technique. These samples were immediately analyzed by GC-MS. The triplicate experiments were performed.

2.4 Introducing Technique Conditions

2.4.1 Gas Syringe-Static Headspace (GS-SHS)

The cultured sample was placed into SHS heating box of the robotic autosampler (MPS Robotic, GERSTEL, Germany) at 40°C for 20 min. Volatile headspace with 1000 µl was injected into GC-MS by gastight syringe with speed of 50 µl/s.

2.4.2 Thin Film-Solid Phase Micro-Extraction (TF-SPME)

A thin film of polydimethyl siloxane-divinyl benzene (PDMS-DVB) with 96 mm2 and 450 μm thickness (GERSTEL, Germany) was hanged onto headspace of the cultured sample at 40°C for 20 min. After volatiles absorption onto thin film, it was placed in a thermal desorption glass tube (GERSTEL, Germany), and placed into TDU for thermal desorption.

2.4.3 Headspace Sorptive Extraction (HSSE)

TwisterTM with 10 mm length and 0.5 mm film thickness PDMS (GERSTEL, Germany) was used and performed with the same procedures of TF-SPME.

2.4.4 Dynamic Headspace (DHS)

The cultured sample was pre-heated in DHS heating box (MPS Robotic, GERSTEL, Germany) at 40°C for 20 min. The volatiles were purged by 10 ml/min He gas, and trapped by Tenax TATM sorbent with 35 m2/g (GERSTEL, Germany). Dry purge was performed with the same He gas flow rate for 4 min before placed into TDU.

2.4.5 Direct Thermal Desorption (DTD)

The LV-007 cultured sample in a glass micro-vial was loaded in a thermal desorption glass tube, and then placed into TDU.

2.5 Thermal Desorption Unit (TDU) and GC-MS conditions

TDU condition: TDU (GERSTEL, Germany) was programmed as spitless mode by holding at 30°C for 1 min, then ramping to 60°C with 60°C/min, holding for 5 min with flow 1 ml/min He gas. The volatiles were trapped by cooled injection system (CIS) at -30°C before transferred to GC column.

GC-MS conditions: Volatiles were analyzed by GC-MS (Agilent 8890 GC; Agilent Technologies (Shanghai) Co., Ltd. Shanghai, P.R. China, and 5977B MSD; Agilent Technologies, Inc. CA, USA). HP-5MS column (50 m × 250 μm × 0.25 μm, Agilent, USA) was used with 1 ml/min He carrier gas flow. GC oven was held at 35°C for 4 min, raised to 160°C with 16°C/min, and raised to 250°C at 25°C/min held for 5 min. The interphase temperature of MS was 250°C. Molecule ionization by electron impact with 70 eV, and mass analyzer was quadrupole with scanning range of 30-350 m/z.

2.6 Comparison of quantified 2-PE of LV-007 from various introducing techniques

Because of the different cultured broth volume of DTD, 2-PE ratio was calculated by following equation for comparison detectable 2-PE from different introducing techniques.

$$2-PE\ ratio = \frac{2-PE\ concentration}{Amount\ of\ yeast} \quad (1)$$

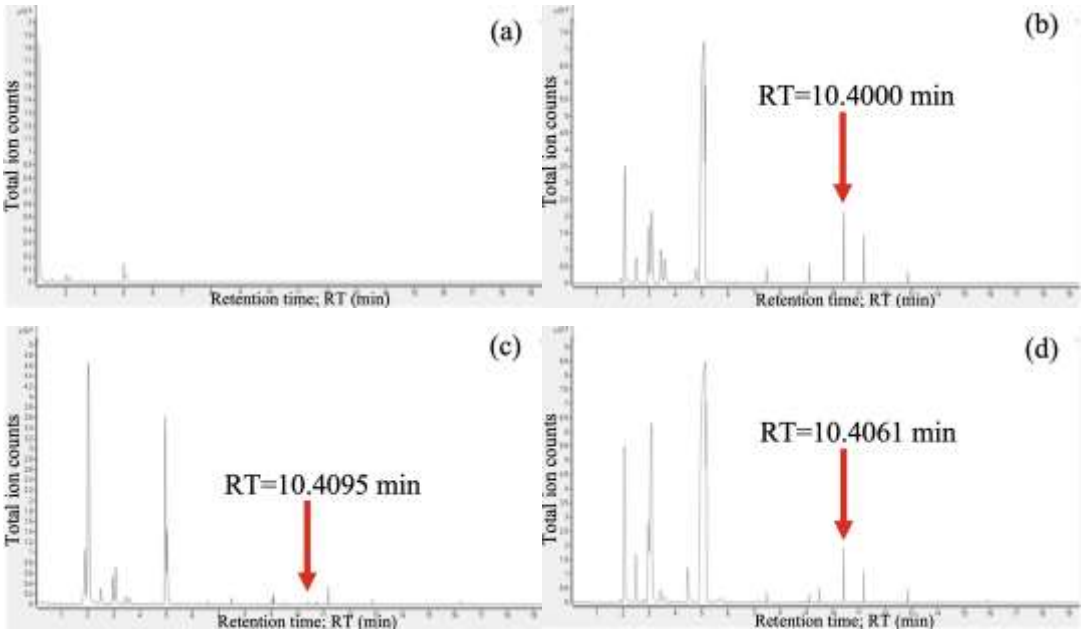
2.7 LV-007 viable yeast cells determination

Before loading cultured broth into the glass wares of each introducing technique, LV-007 was individually cultured in 100 ml PDB at 30°C for 24 h, and determined viable yeast cells by 10-fold serial dilution method.

3. Results & discussions

3.1 2-PE qualitative analysis

2-PE from LV-007 yeast was detected at retention time about 10.4 min, and identified by GC-MS with introducing techniques of TF-SPME, HSSE, DHS, and DTD, except GS-SHS (Figure 1). GS-SHS was not suitable for high molecular weight and low vapor pressure liked 2-PE, which were 122.16 g/mol and 0.0868 mmHg at 25°C, respectively (National Center for Biotechnology Information). Not only 2-PE was produced by reference yeast strain, but other volatiles were also delivered by LV-007 strain (Table 1). The numbers of detected volatiles from introducing techniques of GS-SHS, TF-SPME, HSSE, DHS, and DTD were 8, 26, 15, 27, and 16, respectively.



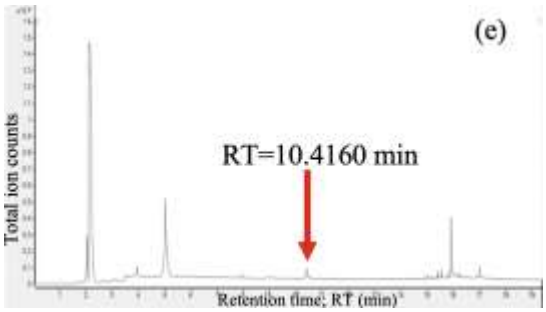


Figure 1: *Chromatogram of LV-007 yeast on PDA by 5 introducing techniques of GS-SHS (a), TF-SPME (b), HSSE (c), DHS (d), and DTD (e).*

3.2 Quantitative analysis of 2-PE and viable LV-007

To determine 2-PE concentrations from various introducing techniques, standard curves were performed (Figure 2). Viable LV-007 of each introducing technique were also determined. The comparison detectable 2-PE from different introducing techniques in term of 2-PE ratio was calculated. The direct thermal desorption (DTD) showed the highest 2-PE ratio with 237.37 ×10-6 μg/ml·CFU (Table 2), while TF-SPME, HSSE, and DHS were 5.48×10-6, 0.77×10-6, and 4.37 ×10-6 μg/ml·CFU, respectively. DTD introducing technique used very small amount sample of 35 μl (Velasco González de Peredo et al., 2023), but others were 4000 μl. Not only small sample volume of DTD, detectable 2-PE was also increased by direct purging volatiles to column.

Table 1: *Volatile compounds of LV-007 yeast by GS-SHS, TF-SPME, DHS, HSSE, and DTD introducing techniques*

Peak No.	Compound names	Retention index (RI)					Aroma descriptions	RI references*
		GS-SHS	***TF-SPME***	***HSSE***	***DHS***	***DTD***		
1	(2-Aziridinylethyl) amine	N.D.	N.D.	N.D.	N.D.	<805.73	-	-
2	Glycidol	N.D.	<806.12	N.D.	<810.12	<805.73	Odorless[1]	-
3	Ethanol	<882.12	<806.12	<880.24	<810.12	<805.73	Alcoholic[2]	-
4	Pentane	N.D.	<806.12	N.D.	N.D.	N.D.	Gasoline[1]	-
5	Isobutylene epoxide	N.D.	N.D.	<880.24	N.D.	N.D.	-	-
6	2-Methyl-propanal	<882.12	<806.12	N.D.	N.D.	N.D.	Pungent floral odor[2]	-
7	2-Hydroxy-propanoic acid, propyl ester	N.D.	N.D.	N.D.	N.D.	<805.73	Sweet pineapple, winey[2]	-
8	3-Methyl-2-butanone	N.D.	N.D.	<880.24	N.D.	N.D.	Pleasent[1]	-
9	Ethyl Acetate	<882.12	<806.12	<880.24	<810.12	N.D.	Fruity, sweet, grape[2]	-
10	2-Methyl-1-propanol	<882.12	<806.12	<880.24	N.D.	<805.73	Winery[2]	-
11	3-Methyl-butanal	<882.12	<806.12	<880.24	<810.12	N.D.	Fruity, peach[2]	-
12	Acetic acid, methoxy-, anhydride	N.D.	N.D.	N.D.	N.D.	<805.73	Acidic-like[2]	-
13	2-Methyl-butanal	N.D.	<806.12	<880.24	<810.12	N.D.	Cocoa[2]	-
14	Cyclopropyl methyl carbinol	N.D.	N.D.	N.D.	N.D.	<805.73	-	-
15	Acetic acid	N.D.	N.D.	N.D.	<810.12	<805.73	Sour, vinegar[2]	-
16	Ethyl ester propanoic acid	N.D.	<806.12	N.D.	N.D.	N.D.	Sweet fruity[2]	-
17	3-Methyl-1-butanol	<882.12	<806.12	<880.24	<810.12	<805.73	Banana, fruity, alcoholic[2]	-

Table 1 (continued): *Volatile compounds of LV-007 yeast by GS-SHS, TF-SPME, DHS, HSSE, and DTD introducing techniques*

Peak No.	Compound names	Retention index (RI)					Aroma descriptions	RI references*
		GS-SHS	*TF-SPME*	*HSSE*	*DHS*	*DTD*		
18	2-Methyl-1-butanol	N.D.	<806.12	<880.24	<810.12	N.D.	Alcoholic[2]	-
19	2-Methyl-propanoic acid, ethyl ester	N.D.	<806.12	N.D.	N.D.	N.D.	Fruity, alcoholic[2]	-
21	2-Methyl-propanoic acid	N.D.	<806.12	N.D.	<810.12	N.D.	Acidic sour cheesy[2]	-
22	Isobutyl acetate	<882.12	<806.12	<880.24	<810.12	N.D.	Sweet fruity, banana[2]	-
23	Butanoic acid, ethyl ester	N.D.	806.12	N.D.	810.28	805.73	Sweet fruity[2]	802
24	3-Methyl-1-pentanol	N.D.	N.D.	N.D.	843.47	N.D.	Cocoa, winey[2]	843
25	2-Methyl-butanoic acid	N.D.	863.04	N.D.	846.83	N.D.	Acidic, fruity, dairy[2]	846
26	2-Furanmethanol	N.D.	867.78	N.D.	N.D.	N.D.	Caramel, burnt[1]	864
27	3-Methyl-1-butanol, acetate	882.12	881.02	880.24	883.00	N.D.	Banana, fruity[1]	-
28	2-Methyl-1-butanol, acetate	N.D.	883.39	882.61	885.18	N.D.	Ripe sweet banana[2]	880
29	Hexanoic acid	N.D.	N.D.	N.D.	980.20	N.D.	Sour cheesy[2]	981
30	Hexanoic acid, ethyl ester	N.D.	999.45	N.D.	1000.18	999.22	Sweet, green, banana[2]	996
31	cis-7-Decen-1-al	N.D.	1033.45	N.D.	N.D.	N.D.	-	-
32	Benzene acetaldehyde	N.D.	1050.07	N.D.	1050.08	N.D.	Honey, sweet, floral[2]	1049
33	1-Octanol	N.D.	N.D.	N.D.	1071.86	N.D.	Waxy, citrus[2]	1068
34	2-Phenyl ethanol	N.D.	1119.48	1119.82	1115.32	1120.47	Floral, rose, sweet[2]	1116

Table 1 (continued): *Volatile compounds of LV-007 yeast by GS-SHS, TF-SPME, DHS, HSSE, and DTD introducing techniques*

Peak No.	Compound names	Retention index (RI)					Aroma descriptions	RI references*
		GS-SHS	***TF-SPME***	***HSSE***	***DHS***	***DTD***		
35	Octanoic acid, ethyl ester	N.D.	1195.78	1195.80	1195.79	N.D.	Waxy, fruity[2]	1196
36	Acetic acid, octyl ester	N.D.	N.D.	N.D.	1210.20	N.D.	Floral, waxy[2]	1215
37	Hexanoic acid, anhydride	N.D.	N.D.	N.D.	1253.31	N.D.	-	-
38	Acetic acid, 2-phenylethyl ester	N.D.	1263.55	N.D.	1263.20	N.D.	Floral, rose, sweet[2]	1256
39	Decanoic acid, ethyl ester	N.D.	1395.03	N.D.	1394.62	N.D.	Waxy, fruity[2]	1392
40	2-Methyl-propanoic acid, 2-phenylethyl ester	N.D.	N.D.	N.D.	1657.25	N.D.	Floral, rose, honey[2]	-
41	1-Hexadecanol	N.D.	N.D.	N.D.	N.D.	1885.02	Waxy, greasy, oily[2]	1883
42	cis-7-Hexadecenoic acid	N.D.	N.D.	N.D.	N.D.	1937.18	-	-
43	n-Hexadecanoic acid	N.D.	N.D.	N.D.	1951.59	1954.00	Waxy, fatty [2]	1962
44	Dibutyl phthalate	N.D.	N.D.	N.D.	N.D.	1970.24	-	1967
45	Isopropyl palmitate	N.D.	N.D.	>1195.80	N.D.	N.D.	Oily[2]	-

N.D.= Not detected

*= Retention index from NIST database (National Institute of Standards and Technology).

[1]= Odor descriptions were obtained from The Good Scents Company (The Good Scents Company).

[2]= Odor descriptions were obtained from PubChem (National Center for Biotechnology Information).

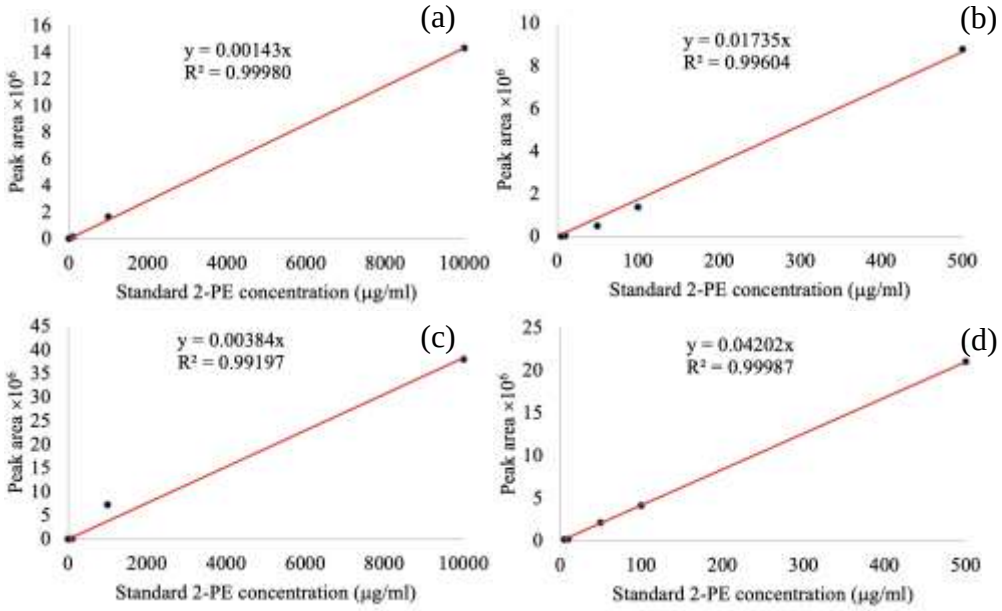


Figure 2: *2-PE standard curve from introducing techniques of TF-SPME (a), HSSE (b), DHS (c), and DTD (d).*

Table 2: *Viable LV-007, 2-PE concentrations, and 2-PE ratio from various introducing techniques*

Introducing techniques	Viable yeast × 10^6 (CFU/ml)	Cultured broth volume in glassware (µl)	Amount yeast in sample × 10^6 (CFU)	2-PE concentration (µg/ml)	2-PE Ratio × 10^{-6} (µg/ml·CFU)
TF-SPME	6.33±0.35	4000	24.12±1.40	132.88±35.22	5.48±1.32
HSSE	9.67±0.65	4000	38.66±2.60	24.49±2.61	0.77±0.10
DHS	6.33±0.50	4000	24.12±2.01	105.55±13.01	4.37±0.32
DTD	7.83±0.31	35	0.27±0.07	61.96±2.44	237.37±61.61

3.3 Comparison of time-consuming sample preparations of introducing techniques and GC-MS analysis

To analyze volatiles from LV-007 yeast, GS-SHS, TF-SPME, and HSSE techniques required totally 50 min for sample pre-heating and GC-MS analysis (Table 3). The highest time-consuming of 55 min was DHS. This technique required times not only for sample pre-heating, but dry purging of 5 min was also important step. The simplest sample preparation and shortest time requirement was DTD technique. DTD required only 30 min to achieve chromatogram. This was the advantage of DTD for analysis of microbial volatiles from large sample amounts.

Table 3 *Time requirement for each introducing technique*

Introducing techniques	**Time-consuming per sample (min)**			
	Sample pre-heating	***Absorbent drying***	***GC-MS analysis***	***Total***
GS-SHS	20	-	30	50
TF-SPME	20	-	30	50
HSSE	20	-	30	50
DHS	20	5	30	55
DTD	-	-	30	30

4. Conclusion

GC-MS with introducing techniques of TF-SPME, HSSE, DHS, and DTD were able to qualitatively analyze volatiles and quantify 2-PE from S. cerevisiae LV-007. DTD was predominated by the highest 2-PE ratio, the shortest analysis time, and the simplest sample preparation. By these advantages of DTD, it might be used to apply in the further of screening of volatiles producing wild microorganisms by GC-MS to spend short analysis time and avoid health risk by airborne pathogens of panelists.

References

Bernardino, A. R. S., Torres, C. A. V., Crespo, J. G., & Reis, M. A. M. (2024). Biotechnological 2-Phenylethanol Production: Recent Developments. Molecules, 29(23), 5761.

Chreptowicz, K., Sternicka, M. K., Kowalska, P. D., & Mierzejewska, J. (2018). Screening of yeasts for the production of 2-phenylethanol (rose aroma) in organic waste-based media. Letters in applied microbiology, 66(2), 153–160. doi: 10.1111/lam.12835

Hodgson, S. C., Casey, R. J., Orbell, J. D., & Bigger, S. W. (2000). Use of a Dynamic Headspace GC-MS Method for the Study of Volatile Organic Compounds in Polyethylene Packaging. An Undergraduate Experiment in Polymer Analysis. Journal of Chemical Education, 77(12), 1631. doi: 10.1021/ed077p1631

Kremser, A., Jochmann, M. A., & Schmidt, T. C. (2016). Systematic comparison of static and dynamic headspace sampling techniques for gas chromatography. Analytical and Bioanalytical Chemistry, 408(24), 6567-6579. doi: 10.1007/s00216-016-9843-y

Lerch, O., & Hässelbarth, A. (2025, December 10). Analysis of aroma compounds in edible oils by direct thermal desorption GC/MS using slitted microvials. Retrieved from https://www.gerstelus.com/applications/analysis-of-aroma-compounds-in-edible-oils-by-direct-thermal-desorption-gcms-using-slitted-microvials

Mitri, S., Koubaa, M., Maroun, R. G., Rossignol, T., Nicaud, J.-M., & Louka, N. (2022). Bioproduction of 2-Phenylethanol through Yeast Fermentation on Synthetic Media and on Agro-Industrial Waste and By-Products: A Review. Foods, 11(1), 109.

National Center for Biotechnology Information, PubChem, & National Library of Medicine. (2025, December 10). PubChem. Retrieved from https://pubchem.ncbi.nlm.nih.gov/

National Institute of Standards and Technology. (2025, December 10). NIST Chemistry WebBook (Standard Reference Database No. 69). Retrieved from https://webbook.nist.gov/chemistry/

Phithakpol, B., Varanyanond, W., Reungmaneepaitoon, S., & Wood, H. I. (1995). Traditional fermented foods of Thailand (pp. 125). Kuala Lumpur: Institute of Food Research and Product Development. Kasetsart University.

The Good Scents Company. (2025, December 10). The Good Scents Company — Information on aroma chemicals, essential oils, and fragrance materials. Retrieved from https://www.thegoodscentscompany.com/

Xu, C.-H., Chen, G.-S., Xiong, Z.-H., Fan, Y.-X., Wang, X.-C., & Liu, Y. (2016). Applications of solid-phase microextraction in food analysis. TrAC Trends in Analytical Chemistry, 80, 12-29. doi: 10.1016/j.trac.2016.02.022

Ye, J., Tian, S., Lv, L., Ding, Y., Xu, J., Zhang, J., & Li, L. (2021). Production and purification of 2-phenylethanol by Saccharomyces cerevisiae using tobacco waste extract as a substrate. Lett Appl Microbiol, 73(6), 800-806. doi: 10.1111/lam.13575