**Supplementary Material**

**Volatile Characterization of Crude and Refined Walnut Oils from Aqueous Enzymatic Extraction by GC-IMS and GC-MS**

Jiankang Denga,c,d 1, Huibo Zhaob,e 1, Bing Qib,e , Di Wangb,e, Yanbing Wub, Shengxing Daib, Junxia Xia\*b,e , Min Lub,d, Kuizhang Yaob,d,e, Aijin Maa,b, Yingmin Jia\*a,b

a. School of Food and Health, Beijing Technology and Business University, Beijing100048, China;

b. Hebei Yangyuan Zhihui Beverage Co., Ltd. Hengshui 053000, China;

c. College of Life Science, Hengshui University, Hengshui 053000, China;

d. Hebei Key Laboratory of Walnut Nutritional Function and Processing Technology, Hengshui 053000, China;

e. Hebei Technology Innovation Centre of Walnut Beverage, Hengshui 053000, China;

***1 Contributed equally to this study.*** \****Corresponding author*：**

***Yingmin Jia ,*** *jiayingmin@btbu.edu.cn; School of Food and Health,Beijing Technology and Business University, No.33 Fu Cheng Road, Beijing 100048, People’s Republic of China*

***Junxia Xia****, phone number: +86 03182089919, Email:yangyuanshengjibu@hbyangyuan.com. Address:Hebei Yangyuan Zhihui Beverage Co., Ltd., New Zone 6 Road Fuyang 4 Road, North District of Hebei Hengshui Economic Development Zone , Hengshui053000, China.*

**Table S1 Comparative study of oil yield, water content, AV, and PV in CWO and RWO obtained by AEE**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Samples | Oil yeild (%) | Water content (%) | AV (mg/g) | PV (g/100 g) |
| C1 | Niangqing | 85.2±1.3a | 0.22±0.01a | 0.19±0.005a | 0.09±0.003a |
| C2 | Tongziguo | 88.2±1.2b | 0.21±0.02a | 0.18±0.008a | 0.16±0.006b |
| C3 | Macha | 89.1±1.6b | 0.19±0.02a | 0.94±0.06b | 0.08±0.008a |
| C4 | Boluoguo | 90.2±2.5b | 0.21±0.01a | 0.65±0.09c | 0.21±0.01c |
| C5 | Jidanpi | 86.7±1.1a | 0.10±0.01b | 0.36±0.04d | 0.21±0.03c |
| C6 | Dapao | 86.5±1.1a | 0.03±0.001c | 0.37±0.08d | 0.20±0.02c |
| C7 | Santai | 85.2±2.2a | 0.11±0.03b | 0.26±0.03a | 0.10±0.01a |
| CWO |  | 87.3±2.2 | 0.15±0.07 | 0.42±0.26 | 0.15±0.06 |
| R1 | Niangqing |  | 0.09±0.01a | 0.07±0.005a | 0.16±0.004a |
| R2 | Tongziguo |  | 0.08±0.01a | 0.004±0.001b | 0.19±0.01b |
| R3 | Macha |  | 0.09±0.02a | 0.05±0.006c | 0.11±0.003c |
| R4 | Boluoguo |  | 0.09±0.002a | 0.09±0.006d | 0.19±0.03b |
| R5 | Jidanpi |  | 0.07±0.008b | 0.09±0.005d | 0.12±0.01c |
| R6 | Dapao |  | 0.03±0.001c | 0.01±0.001e | 0.13±0.01c |
| R7 | Santai |  | 0.08±0.001a | 0.05±0.001c | 0.16±0.02a |
| RWO |  |  | 0.08±0.02 | 0.05±0.03 | 0.15±0.02 |

Values are means±standard deviation. The superscript letters indicate the statistical difference at a threshold of p<0.05.

**Table S2 Identification of volatile compounds in CWO and RWO by HS-SPME-GC-MS**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| NO. | Compoundx | CAS | Formula | MW | Odor descriptions | References |
| 1 | α-Farnesene | 502-61-4 | C15H24 | 204.4 | Citrus, herbal, lavende, neroli, green | (Guo and Ho et al., 2021) |
| 2 | α-Pinene | 80-56-8 | C10H16 | 136.2 | Fresh, camphor, sweet, pine, earthy, woody | (Schreiner and Bauer et al., 2018) |
| 3 | β-Bisabolene | 495-61-4 | C15H24 | 204.4 | Balsamic, woody |  |
| 4 | 3-Methylbutyl acetate | 123-92-2 | C7H14O2 | 130.2 | Sweet, fruity, banana, solvent | (Ledauphin and Guichard et al., 2003) |
| 5 | 2-Hexyl-1-decanol | 2425-77-6 | C16H34O | 242.4 |  |  |
| 6 | 1-Heptanol | 111-70-6 | C7H16O | 116.2 | Musty, leafy, violet, herbal, green, sweet, woody, peony | (Guo and Ho et al., 2021) |
| 7 | 1-Hexanol | 111-27-3 | C6H14O2 | 102.2 | Ethereal, fusel oil, fruity, alcoholic, sweet, green | (Guo and Ho et al., 2021) |
| 8 | 2-Ethyl-hexanol | 104-76-7 | C8H18O | 130.2 | Citrus, fresh, floral, oily, sweet | (Xi and Zhang et al., 2024) |
| 9 | 1-Octanol | 111-87-5 | C8H18O | 130.2 | Waxy, green, orange, rose, mushroom | (Xi and Zhang et al., 2024) |
| 10 | 2-Butyl-1-octanol | 3913-02-8 | C12H26O | 186.3 |  |  |
| 11 | 1-Octen-3-ol | 3391-86-4 | C8H16O | 128.2 | Mushroom, earthy, green, oily, fungal | (Guo and Ho et al., 2021) |
| 12 | 1-Octen-3-one | 4312-99-6 | C8H14O | 126.1 | Herbal, mushroom, earthy, musty, dirty | (Schreiner and Bauer et al., 2018) |
| 13 | 1-Pentanol | 71-41-0 | C5H12O | 88.2 | Fusel, oil, sweet, balsam | (Xi and Zhang et al., 2024) |
| 14 | 1-Tetradecanol | 112-72-1 | C14H30O | 214.4 | Fruity, waxy, orris, coconut | GSC |
| 15 | 1-Undecanol | 112-42-5 | C11H24O | 172.3 | Fresh, waxy, rose, soapy, clean, clothes, floral, citrus | GSC |
| 16 | 2,3-Heptanedione | 96-04-8 | C7H12O2 | 128.2 | Butter, cheese, oily, fresh, yogurt | GSC |
| 17 | (E,E)-2,4-Decadienal | 1050222-52-0 | C10H16O | 152.2 | Oily, cucumber, fatty, fried | (Guo and Ho et al., 2021) |
| 18 | 2,4-Dimethyl-1-heptene | 19549-87-2 | C9H18 | 126.2 |  |  |
| 19 | (E,E)-2,4-Heptadienal | 4313-03-5 | C7H10O | 110.2 | Fatty, green, oily, aldehydic, vegetable, cake, cinnamon | (Guo and Ho et al., 2021) |
| 20 | (E,E)-2,4-Nonadienal | 5910-87-2 | C9H14O | 138.2 | Fatty, melon, waxy, green, violet, leaf, cucumber, tropical fruit, chicken, fat | (Schreiner and Bauer et al., 2018) |
| 21 | 2,6,6-Trimethyl-2-cyclohexene-1,4-dione | 1125-21-9 | C9H12O2 | 152.2 | Musty, woody, sweet, tea, tobacco, leaf | (Guo and Ho et al., 2021) |
| 22 | (E)-2-Decenal | 3913-81-3 | C10H18O | 154.3 | Waxy, fatty, earthy, green, cilantro, mushroom, aldehydic, fried, chicken, fat, tallow | (Guo and Ho et al., 2021) |
| 23 | 2-Heptanone | 110-43-0 | C7H14O | 114.2 | Fruity, spicy, sweet, herbal, coconut, woody | (Xi and Zhang et al., 2024) |
| 24 | (E)-2-Hepten-1-ol | 33467-76-4 | C7H14O | 114.2 | Pungent, fatty, plastic, green | GSC |
| 25 | (E)-2-Heptenal | 18829-55-5 | C7H12O | 112.2 | Pungent, green, vegetable, fresh, fatty | (Xi and Zhang et al., 2024) |
| 26 | (E)-2-Hexenal | 6728-26-3 | C6H10O | 98.1 | Green, banana, aldehydic, fatty, cheesy | (Guo and Ho et al., 2021) |
| 27 | 2-Nonanone | 821-55-6 | C9H18O | 142.2 | Fresh, sweet, green, weedy, earthy, herbal | GSC |
| 28 | 2-Octanone | 111-13-7 | C8H16O | 128.2 | Earthy, weedy, natural, woody, herbal | GSC |
| 29 | (E)-2-Octen-1-ol | 18409-17-1 | C8H16O | 128.2 | Green, citrus, vegetable, fatty | (Xi and Zhang et al., 2024) |
| 30 | (E)-2-Octenal | 2548-87-0 | C8H14O | 126.2 | Fresh, cucumber, fatty, green, herbal, banana, waxy, green leaf | (Schreiner and Bauer et al., 2018) |
| 31 | 1-Ethoxy-4,4-dimethyl-2-pentene | 55702-60-8 | C9H18O | 142.2 |  |  |
| 32 | (E)-3-Methyl-2-undecene | 74630-47-0 | C12H24 | 168.3 |  |  |
| 33 | 3,5-Octadien-2-one | 30086-02-3 | C8H12O | 124.2 | Fruity, green, grassy | GSC |
| 34 | 2-Methyl-3-heptanone | 13019-20-0 | C8H16O | 128.2 | Fruity, green, leafy | GSC |
| 35 | 2,5-Dimethyl-3-hexanone | 1888-57-9 | C8H16O | 128.2 |  |  |
| 36 | 3-Octen-2-one | 1669-44-9 | C8H14O | 126.2 | Earthy, spicy, herbal, sweet, mushroom, hay, blueberry | GSC |
| 37 | 2,7-Dimethyl-4,5-octanediol | 154468-18-5 | C10H22O2 | 174.3 |  |  |
| 38 | 4-Ethylcyclohexanol | 4534-74-1 | C8H16O | 128.2 |  |  |
| 39 | (E)-6,10-Dimethylundeca-5,9-dien-2-one | 689-67-8 | C13H22O | 194.3 | Fresh, rose, leaf, floral, green, magnolia, aldehydic, fruity | GSC |
| 40 | 6-Methyl-5-hepten-2-one, | 110-93-0 | C8H14O | 126.2 | Citrus, green, musty, lemongrass, apple | (Guo and Ho et al., 2021) |
| 41 | Acetophenone | 98-86-2 | C8H8O | 120.2 | Sweet, pungent, hawthorn, mimosa, almond, acacia, chemical | (Guo and Ho et al., 2021) |
| 42 | Anisole | 100-66-3 | C7H8O | 108.1 | Phenolic, gasoline, ethereal, anise |  |
| 43 | Benzaldehyde | 100-52-7 | C7H6O | 106.1 | Strong, sharp sweet bitter almond cherry | (Guo and Ho et al., 2021) |
| 44 | 1,3-Bis(1,1-dimethylethyl)-benzene | 15181-11-0 | C15H24 | 204.4 |  |  |
| 45 | 1-Ethenyl-4-ethyl-benzene | 3454-07-7 | C10H12 | 132.2 |  |  |
| 46 | 1-Ethyl-2-methyl-benzene | 611-14-3 | C9H12 | 120.2 |  |  |
| 47 | 1-Ethyl-3-methyl-benzene | 620-14-4 | C9H12 | 120.2 |  |  |
| 48 | Benzeneacetaldehyde | 122-78-1 | C8H8O | 120.2 | Green sweet floral hyacinth clover honey cocoa | (Guo and Ho et al., 2021) |
| 49 | Benzofuran | 271-89-6 | C8H6O | 118.1 | Styrene aromatic | GSC |
| 50 | 2,3-Dihydro-benzofuran, | 496-16-2 | C8H8O | 120.2 |  |  |
| 51 | Benzyl alcohol | 100-51-6 | C7H8O | 108.1 | Floral rose phenolic balsamic | (Guo and Ho et al., 2021) |
| 52 | Decanal | 112-31-2 | C10H20O | 156.3 | Sweet aldehydic waxy orange peel citrus floral | GSC |
| 53 | D-Limonene | 138-86-3 | C10H16 | 136.2 | Citrus herbal terpene camphor | (Guo and Ho et al., 2021) |
| 54 | Heptanal | 111-71-7 | C7H14O | 114.2 | Fresh, aldehydic, fatty, green, herbal wine-lee ozone | (Xi and Zhang et al., 2024) |
| 55 | 3,3,5-Trimethyl-heptane, | 7154-80-5 | C10H22 | 142.3 |  |  |
| 56 | Hexanal | 66-25-1 | C6H12O | 100.2 | Fresh, green, fatty, aldehydic, grass, leafy, fruity | (Guo and Ho et al., 2021) |
| 57 | 2,3,4-Trimethyl-hexane | 921-47-1 | C9H20 | 128.7 |  |  |
| 58 | 2,4-Dimethyl-hexane, | 589-43-5 | C8H18 | 114.2 |  |  |
| 59 | [Hexyl caproate](https://pubchem.ncbi.nlm.nih.gov/compound/22873) | 6378-65-0 | C12H24O2 | 200.3 | Herbal, fresh, cut, grass, vegetable, fruity | GSC |
| 60 | 1-Methyl-indan | 767-58-8 | C10H12 | 132.2 |  |  |
| 61 | Isophorone | 78-59-1 | C9H14O | 138.2 | Cooling, woody, sweet, green, camphor, fruity, musty, cedarwood, tobacco, leather | GSC |
| 62 | Naphthalene | 91-20-3 | C10H8 | 128.2 | Pungent, dry, tarry | GSC |
| 63 | Nonanal | 124-19-6 | C9H18O | 142.2 | Waxy, aldehydic, rose, fresh, orris, orange, peel, fatty, peely | (Guo and Ho et al., 2021) |
| 64 | n-Tridecan-1-ol | 112-70-9 | C13H28O | 200.4 | Musty | (Guo and Ho et al., 2021) |
| 65 | Octanal | 124-13-0 | C8H16O | 128.2 | Aldehydic, waxy, citrus, orange, peel, green, herbal, fresh, fatty | (Xi and Zhang et al., 2024) |
| 66 | Phenylethanol | 60-12-8 | C8H10O | 122.2 | Floral, rose, dried rose, flower, rose, water | (Ledauphin and Guichard et al., 2003) |

Aroma description was obtained from literatures and GSC database (Good Scents Company, www.thegoodscentscompany.com/).

**Table S3 Identification of volatile compounds in CWO and RWO by GC-IMS**

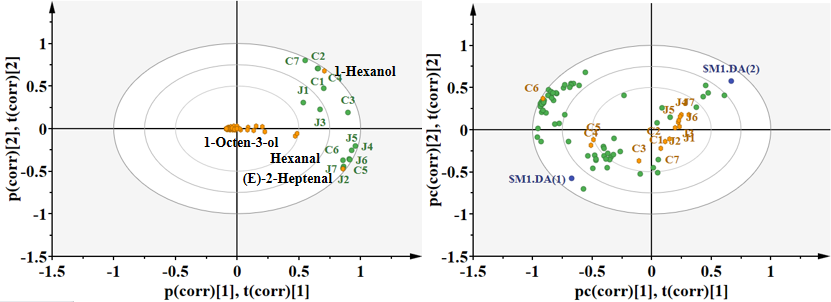
|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NO. | Compound | CAS | Formula | MW | RI | Rt [sec] | Dt [a.u.] | Odor descriptions | References |
| 1 | Benzaldehyde | 100-52-7 | C7H6O | 106.1 | 1543.6 | 1309.844 | 1.14797 | Strong, sharp, sweet, bitter, almond, cherry | GSC |
| 2 | Acetic acid-M | 64-19-7 | C2H4O2 | 60.1 | 1496.3 | 1189.017 | 1.05301 | Sharp, pungent, sour, vinegar | (Schreiner and Bauer et al., 2018) |
| 3 | Acetic acid-P | 64-19-7 | C2H4O2 | 60.1 | 1495 | 1185.865 | 1.15219 |  |  |
| 4 | nonanal | 124-19-6 | C9H18O | 142.2 | 1403.7 | 983.746 | 1.47265 | Waxy, aldehydic, rose, fresh, orris, orange, peel, fatty, peely | (Guo and Ho et al., 2021) |
| 5 | 1-Hexanol-M | 111-27-3 | C6H14O | 102.2 | 1367.3 | 913.153 | 1.32663 | Ethereal, fusel, oil, fruity, alcoholic, sweet, green | (Guo and Ho et al., 2021) |
| 6 | 1-Hexanol-D | 111-27-3 | C6H14O | 102.2 | 1366.9 | 912.44 | 1.64272 |  |  |
| 7 | (E)-2-heptenal-M | 18829-55-5 | C7H12O | 112.2 | 1330.8 | 847.551 | 1.25361 | Pungent, green, vegetable, fresh, fatty | (Xi and Zhang et al., 2024) |
| 8 | (E)-2-heptenal-D | 18829-55-5 | C7H12O | 112.2 | 1330.4 | 846.838 | 1.66765 |  |  |
| 9 | 2,5-dimethylpyrazine-D | 123-32-0 | C6H8N2 | 108.1 | 1330.4 | 846.838 | 1.49936 | Cocoa, roasted, nuts, roast, beef, woody, grass, medical | (Guo and Ho et al., 2021) |
| 10 | 1-Octen-3-one | 4312-99-6 | C8H14O | 126.2 | 1311.1 | 814.038 | 1.27231 | Herbal, mushroom, earthy, musty, dirty | GSC |
| 11 | 3-hydroxy-2-butanone-M | 513-86-0 | C4H8O2 | 88.1 | 1297.7 | 791.933 | 1.06129 | Sweet, buttery, creamy, dairy, milky, fatty | (Chang and Wang et al., 2021) |
| 12 | 3-hydroxy-2-butanone-D | 513-86-0 | C4H8O2 | 88.1 | 1295.9 | 789.081 | 1.3293 |  |  |
| 13 | 1-hydroxypropan-2-one-P | 116-09-6 | C3H6O2 | 74.1 | 1295.9 | 789.081 | 1.23581 | Pungent, sweet, caramellic, ethereal | GSC |
| 14 | 1-Pentanol-M | 71-41-0 | C5H12O | 88.1 | 1262 | 737.027 | 1.25361 | Fusel, oil, sweet, balsam | GSC |
| 15 | 1-Pentanol-D | 71-41-0 | C5H12O | 88.1 | 1262.9 | 738.453 | 1.51094 |  |  |
| 16 | (E)-2-hexenal | 6728-26-3 | C6H10O | 98.1 | 1233.2 | 695.67 | 1.1806 | Green, banana, aldehydic, fatty, cheesy | (Guo and Ho et al., 2021) |
| 17 | 3-Methyl-2-butenal | 107-86-8 | C5H8O | 84.1 | 1215.5 | 671.426 | 1.09334 | Sweet, fruity, pungent, brown, nutty, almond, cherry | GSC |
| 18 | Cyclopentanone-M | 120-92-3 | C5H8O | 84.1 | 1197.2 | 647.182 | 1.10314 | Minty | GSC |
| 19 | Cyclopentanone-D | 120-92-3 | C5H8O | 84.1 | 1198.3 | 648.608 | 1.33375 |  |  |
| 20 | 2-Methyl-1-butanol | 137-32-6 | C5H12O | 88.1 | 1219.5 | 676.836 | 1.23382 | Ethereal, fusel, alcoholic, fatty, greasy, winey, whiskey, leathery cocoa | GSC |
| 21 | 3-Methyl-1-butanol-M | 123-51-3 | C5H12O | 88.1 | 1221.3 | 679.293 | 1.24699 | Fusel, oil, alcoholic, whiskey, fruity, banana | (Guo and Ho et al., 2021) |
| 22 | 3-Methyl-1-butanol-D | 123-51-3 | C5H12O | 88.1 | 1219.1 | 676.222 | 1.49004 |  |  |
| 23 | limonene | 138-86-3 | C10H16 | 136.2 | 1191.1 | 638.455 | 1.22425 |  | (Guo and Ho et al., 2021) |
| 24 | Heptan-2-one | 110-43-0 | C7H14O | 114.2 | 1193.8 | 642.753 | 1.25957 | Fruity, spicy, sweet, herbal, coconut, woody | GSC |
| 25 | Pentyl acetate | 628-63-7 | C7H14O2 | 130.2 | 1172.6 | 602.857 | 1.30871 | Ethereal, fruity, banana, pear, banana, apple | GSC |
| 26 | 2-Methyl-2-pentenal | 623-36-9 | C6H10O | 98.1 | 1174.2 | 605.845 | 1.16104 | Aldehydic, green, cortex, fruity, alliaceous, ripe, cherry, earthy | GSC |
| 27 | Heptanal-P | 111-71-7 | C7H14O | 114.2 | 1166.2 | 590.904 | 1.34217 | Fresh, aldehydic, fatty, green, herbal, wine-lee, ozone | (Xi and Zhang et al., 2024) |
| 28 | Butanol | 71-36-3 | C4H10O | 74.1 | 1155.2 | 571.183 | 1.17995 | Fusel, oil, sweet, balsam, whiskey | (Li and Shi et al., 2023) |
| 29 | (E)-2-pentenal-M | 1576-87-0 | C5H8O | 84.1 | 1146.7 | 556.243 | 1.10502 | Pungent, green, fruity, apple, orange, tomato | (Xi and Zhang et al., 2024) |
| 30 | (E)-2-pentenal-D | 1576-87-0 | C5H8O | 84.1 | 1146 | 555.048 | 1.36036 |  |  |
| 31 | isoamyl acetate | 123-92-2 | C7H14O2 | 130.2 | 1136.5 | 538.912 | 1.30507 | Sweet, fruity, banana, solvent | GSC |
| 32 | 2-methyl-1-propanol-M | 78-83-1 | C4H10O | 74.1 | 1103.9 | 486.92 | 1.17049 | Ethereal, winey, cortex | GSC |
| 33 | 2-methyl-1-propanol-D | 78-83-1 | C4H10O | 74.1 | 1103.5 | 486.322 | 1.36545 |  |  |
| 34 | 2-methyl-1-propanol-P | 78-83-1 | C4H10O | 74.1 | 1124.5 | 519.191 | 1.36327 |  |  |
| 35 | 1-Penten-3-ol | 616-25-1 | C5H10O | 86.1 | 1114.4 | 503.055 | 1.34945 | Ethereal, horseradish, green, radish, chrysanthemum, vegetable, tropical, fruity | (Xi and Zhang et al., 2024) |
| 36 | Hexanal-M | 66-25-1 | C6H12O | 100.2 | 1100.3 | 481.541 | 1.25997 | Fresh, green, fatty, aldehydic, grass, leafy, fruity, sweaty | (Guo and Ho et al., 2021) |
| 37 | Hexanal-P | 66-25-1 | C6H12O | 100.2 | 1098.7 | 479.151 | 1.56114 |  |  |
| 38 | butyl acetate | 123-86-4 | C6H12O2 | 116.2 | 1088.4 | 465.562 | 1.2366 | Ethereal, solvent, fruity, banana | GSC |
| 39 | 2-Methyl butanoic acid ethyl ester | 7452-79-1 | C7H14O2 | 130.2 | 1075.6 | 449.396 | 1.22983 | Sharp, sweet, green, apple, fruity | GSC |
| 40 | ethyl butyrate | 105-54-4 | C6H12O2 | 116.2 | 1061.3 | 431.955 | 1.20045 | Fruity, juicy, fruit, pineapple, cognac | GSC |
| 41 | Propan-1-ol-M | 71-23-8 | C3H8O | 60.1 | 1051.5 | 420.469 | 1.11006 | Alcoholic, fermented, fusel, musty | GSC |
| 42 | Propan-1-ol-D | 71-23-8 | C3H8O | 60.1 | 1051.1 | 420.043 | 1.25544 |  |  |
| 43 | 1-penten-3-one-M | 1629-58-9 | C5H8O | 84.1 | 1039.9 | 407.281 | 1.07767 | Pungent, peppery, mustard, garlic, onion | GSC |
| 44 | 1-penten-3-one-D | 1629-58-9 | C5H8O | 84.1 | 1038.4 | 405.579 | 1.30741 |  |  |
| 45 | Butan-2-ol | 78-92-2 | C4H10O | 74.1 | 1036.1 | 403.027 | 1.14847 | Sweet, apricot | GSC |
| 46 | 2-butanol | 78-92-2 | C4H10O | 74.1 | 1033.8 | 400.474 | 1.32097 |  |  |
| 47 | 4-methyl-2-pentanone | 108-10-1 | C6H12O | 100.2 | 1026.8 | 392.817 | 1.1786 | Sharp, solvent, green, herbal, fruity, dairy, spice | GSC |
| 48 | Thiophene | 110-02-1 | C4H4S | 84.1 | 1027.2 | 393.242 | 1.09047 | Alliaceous, garlic | GSC |
| 49 | α-Pinene-M | 80-56-8 | C10H16 | 136.2 | 1007 | 371.972 | 1.21853 | Fresh, camphor, sweet, pine, earthy, woody | (Schreiner and Bauer et al., 2018) |
| 50 | α-Pinene-D | 80-56-8 | C10H16 | 136.2 | 1002 | 366.867 | 1.29084 |  |  |
| 51 | pentanal | 110-62-3 | C5H10O | 86.1 | 1002.8 | 367.718 | 1.42115 | Fermented, bready, fruity, nutty, berry | (Xi and Zhang et al., 2024) |
| 52 | isobutyl acetate | 110-19-0 | C6H12O2 | 116.2 | 1028 | 394.093 | 1.60947 | Sweet, fruity, ethereal, banana, tropical | (Xi and Zhang et al., 2024) |
| 53 | Ethanol | 64-17-5 | C2H6O | 46.1 | 951.5 | 331.558 | 1.13039 | Strong, alcoholic, ethereal, medical | (Xi and Zhang et al., 2024) |
| 54 | Butan-2-one-M | 78-93-3 | C4H8O | 72.1 | 917.9 | 310.629 | 1.05743 | Acetone-like, ethereal, fruity, camphor |  |
| 55 | Butan-2-one-D | 78-93-3 | C4H8O | 72.1 | 916 | 309.47 | 1.2454 |  |  |
| 56 | 3-Methyl butanal | 590-86-3 | C5H10O | 86.1 | 932 | 319.208 | 1.3981 | Ethereal, aldehydic, chocolate, peach, fatty | (Xi and Zhang et al., 2024) |
| 57 | 2-methylbutanal | 96-17-3 | C5H10O | 86.1 | 898.3 | 299.036 | 1.16074 | Musty, cocoa, phenolic, coffee, nutty, malty, fermented, fatty, alcoholic | (Xi and Zhang et al., 2024) |
| 58 | Diethyl acetal | 105-57-7 | C6H14O2 | 118.2 | 897.1 | 298.34 | 1.04382 | Ether, green, nut, earthy, sweet, vegetable | GSC |
| 59 | ethyl acetate-M | 141-78-6 | C4H8O2 | 88.1 | 898.5 | 299.162 | 1.09552 | Ethereal, fruity, sweet, weedy, green | (Tan and Wang et al., 2022) |
| 60 | ethyl acetate-D | 141-78-6 | C4H8O2 | 88.1 | 899.1 | 299.487 | 1.33661 |  |  |
| 61 | Butyraldehyde-M | 123-72-8 | C4H8O | 72.1 | 892.6 | 295.75 | 1.11192 | Pungent, cocoa, musty, green, malty, bready | (Tan and Wang et al., 2022) |
| 62 | Butyraldehyde-P | 123-72-8 | C4H8O | 72.1 | 893.2 | 296.075 | 1.28044 |  |  |
| 63 | Tetrahydrofuran-M | 109-99-9 | C4H8O | 72.1 | 884.3 | 291.037 | 1.06072 |  |  |
| 64 | Tetrahydrofuran-D | 109-99-9 | C4H8O | 72.1 | 882.3 | 289.9 | 1.22824 |  |  |
| 65 | Methyl acetate-M | 79-20-9 | C3H6O2 | 74.1 | 853.5 | 274.138 | 1.0289 | Ether, sweet, fruity | GSC |
| 66 | Propan-2-one | 67-64-1 | C3H6O | 58.1 | 845.1 | 269.75 | 1.11441 | Solvent, ethereal, apple, pear | GSC |
| 67 | 2-Methylpropanal | 78-84-2 | C4H8O | 72.1 | 840.5 | 267.312 | 1.28044 | Fresh, aldehydic, floral, green | GSC |
| 68 | Propanal | 123-38-6 | C3H6O | 58.1 | 825.5 | 259.675 | 1.14175 | Earthy, alcohol, wine, whiskey, cocoa, nutty | GSC |
| 69 | dimethyl sulfide | 75-18-3 | C2H6S | 62.1 | 746.5 | 222.787 | 1.14473 | Sulfury, onion, sweet, corn, vegetable, cabbage, tomato, green, radish | GSC |
| 70 | diacetyl | 431-03-8 | C4H6O2 | 86.1 | 998.2 | 362.997 | 1.17485 | Strong, butter, sweet, creamy, pungent, caramel | GSC |
| 71 | methyl 2-methylbutanoate | 868-57-5 | C6H12O2 | 116.2 | 1002.4 | 367.285 | 1.18806 | Ethereal, estery, fruity, tutti, frutti, green, apple, lily of the valley, powdery, fatty | GSC |

Monomers, dimers, and trimers of compound formed in the IMS drift tube were represented by M, D, and P, respectively. RI, retention index. Rt, retention time. Dt, relative migration time.Aroma description was obtained from literatures and GSC database (Good Scents Company, www.thegoodscentscompany.com/).

**Table S4** **Relative content of volatile compounds in CWO and RWO by GC-MS**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | C1 | C2 | C3 | C4 | C5 | C6 | C7 | J1 | J2 | J3 | J4 | J5 | J6 | J7 |
| 1 | α-Farnesene | － | 15.99±  2.22 | － | － | － | 183.26±  24.04 | － | － | 16.95±  1.87 | － | － | － | 15.95±  0.67 | － |
| 2 | α-Pinene | 48.98±  7.24 | 32.29±  3.75 | 206.34±  38.36 | 184.50±  13.78 | 316.78±  44.80 | 405.15±  46.2 | 51.42±  8.60 | 34.40±  3.96 | 23.28±  6.71 | 28.34±  5.97 | 37.11±  1.28 | 26.20±  1.72 | 26.95±  3.39 | 36.80±  5.00 |
| 3 | β-Bisabolene | 146.49±  8.06 | 56.53±  2.85 | 97.70±  6.95 | 945.52±  49.80 | 425.34±  47.70 | － | 46.60±  6.38 | 113.33±  29.90 | 52.99±  6.69 | 31.06±  0.76 | 237.23±  18.85 | 262.52±  11.84 | 61.67±  6.75 | 22.41±  1.48 |
| 4 | 3-Methylbutyl acetate | 181.65±  10.90 | 23.72±  6.00 | － | 594.27±  70.90 | 104.06±  16.60 | － | 34.69±  1.83 | 141.62±  12.63 | 10.16±  2.93 | 26.15±  1.99 | 27.22±  1.58 | 49.93±  2.41 | 19.05±  1.03 | － |
| 5 | 2-Hexyl-1-decanol | 20.47±  4.13 | － | 62.83±  8.53 | 144.08±  5.80 | － | 397.01±  31.07 | － | 22.19±  1.71 | 34.15±  2.26 | 48.29±  4.26 | 41.10±  1.89 | 37.51±  3.02 | 89.31±  3.26 | 28.97±  1.82 |
| 6 | 1-Heptanol | － | － | － | － | 105.33±  6.14 | － | － | － | － | － | 146.05±  8.84 | 92.35±  5.79 | － | 47.87±  1.82 |
| 7 | 1-Hexanol | 5412.15±256.70 | 10510.59±534.58 | 10943.23±1220.30 | 11627.13±148.54 | 12812.47±572.70 | 6299.89±  114.94 | 13070.43±1015.84 | 750.75±  21.95 | 307.04±  89.06 | 1202.12±17.35 | 3079.42±83.82 | 2164.74±72.85 | 845.12±  55.65 | 414.80±  28.47 |
| 8 | 2-Ethyl-hexanol | 63.41±  6.78 | 40.47±  2.64 | － | － | － | － | － | 76.22±  4.43 | － | 114.78±  6.36 | 101.48±  3.75 | － | 184.62±  11.71 | 502.61±  24.17 |
| 9 | 1-Octanol | － | 60.20±  14.65 | － | － | － | － | － | 142.52±  10.22 | － | － | 217.51±  7.38 | － | 144.12±  7.70 | 197.06±  20.65 |
| 10 | 2-Butyl-1-octanol | － | － | － | 420.00±  98.30 | 161.57±  74.00 | － | 50.56±  5.14 | － | － | － | 86.56±  7.38 | － | － | － |
| 11 | 1-Octen-3-ol | － | 604.22±  59.60 | 2479.99±  60.03 | 7197.31±  88.36 | 20057.81±331.60 | 11225.37±436.60 | － | 1085.84±48.41 | 906.40±  80.29 | 1596.19±14.21 | 2978.25±71.29 | 1814.53±154.24 | 1377.91±70.83 | 2303.91±41.31 |
| 12 | 1-Octen-3-one | 41.06±  7.00 | 77.75±  4.15 | － | 5784.46±  346.47 | 4099.84±  466.82 | 3751.18±  288.80 | 30.57±  2.74 | 145.87±  28.88 | 211.10±  27.44 | 935.21±  77.58 | 1340.46±89.26 | 1186.38±63.05 | － | 255.02±  37.55 |
| 13 | 1-Pentanol | 267.85±  5.64 | － | 361.58±  14.98 | 1858.48±  94.73 | － | － | － | － | － | 201.42±  18.19 | － | 147.40±  9.43 | 167.23±  5.99 | － |
| 14 | 1-Tetradecanol | － | 28.66±  1.21 | 60.80±  3.61 | 96.70±  6.55 | 151.15±  3.04 | － | － | － | 23.17±  1.31 | － | － | 26.87±  4.17 | 32.12±  1.51 | － |
| 15 | 1-Undecanol | － | 15.28±  1.64 | － | － | 112.15±  3.43 | 1261.64±  36.36 | 44.30±  3.62 | － | － | － | － | － | 87.71±  7.43 | 17.36±  3.88 |
| 16 | 2,3-Heptanedione | 245.26±  46.83 | 85.29±  8.51 | 57.30±  8.72 | 267.45±  14.46 | 125.73±  6.37 | 762.37±  14.72 | 38.64±  4.77 | 59.12±  7.09 | 15.01±  2.78 | 44.54±  7.55 | 53.99±  4.19 | 32.40±  1.05 | 59.41±  3.93 | － |
| 17 | (E,E)-2,4-Decadienal | 49.87±  1.87 | 198.26±  41.58 | 143.30±  14.61 | 169.99±  8.62 | 390.03±  23.83 | 1025.61±  48.63 | 62.65±  3.27 | 40.14±  8.26 | 179.22±  7.52 | 40.17±  2.34 | 58.60±  6.51 | 61.45±  7.68 | 138.49±  5.76 | 60.41±  1.20 |
| 18 | 2,4-Dimethyl-1-heptene | 21.83±  1.29 | － | 35.79±  6.17 | 279.03±  9.42 | － | － | － | 25.72±  4.87 | － | － | － | － | － | － |
| 19 | (E,E)-2,4-Heptadienal | 95.67±  16.18 | 114.66±  4.52 | 1053.66±  21.71 | 1653.48±  125.73 | 2683.45±  62.83 | 4001.27±  168.80 | 181.88±  8.57 | 717.45±  18.97 | 794.72±  18.15 | 694.63±  35.53 | 723.17±  42.556 | 381.91±  15.66 | 651.09±  27.15 | 668.00±  27.31 |
| 20 | (E,E)-2,4-Nonadienal | 126.11±  30.62 | 138.12±  18.42 | － | 798.03±  105.20 | 658.15±  85.52 | 1768.38±  167.10 | 104.72±  6.27 | 157.19±  3.43 | 258.88±  50.62 | 192.45±  17.77 | 198.44±  5.43 | 236.84±  14.23 | 443.32±  22.95 | 147.27±  5.11 |
| 21 | 2,6,6-Trimethyl-2-cyclohexene-1,4-dione | 131.83±  14.57 | 142.06±  21.71 | 272.40±  40.79 | 545.04±  43.43 | 282.56±  21.20 | 761.09±  33.47 | 118.66±  4.18 | 156.49±  8.24 | 136.72±  6.26 | 152.47±  24.20 | 144.55±  12.71 | 139.65±  16.41 | 110.86±  7.50 | 185.13±  13.36 |
| 22 | (E)-2-Decenal | － | 36.63±  5.99 | 183.84±  5.27 | 321.85±  28.00 | 547.80±  47.08 | 936.47±  25.3 | 18.75±  1.08 | 59.77±  6.34 | 97.03±  3.43 | 66.36±  13.50 | 132.97±  15.59 | 142.63±  23.55 | 82.88±  13.23 | 63.96±  13.21 |
| 23 | 2-Heptanone | 91.13±  3.72 | 76.06±  5.87 | 378.31±  24.98 | 298.83±  15.76 | 822.93±  9.35 | 2154.07±  61.89 | 177.82±  6.82 | 121.98±  8.75 | 123.79±  3.89 | 209.53±  18.71 | 212.89±  18.72 | 153.05±  6.12 | 195.21±  18.53 | 203.76±  5.28 |
| 24 | (E)-2-Hepten-1-ol | － | － | － | － | 333.07±  12.01 | － | － | － | 20.77±  1.77 | － | － | － | 35.19±  5.90 | 49.64±  5.04 |
| 25 | (E)-2-Heptenal | 683.96±  46.73 | 1046.40±  61.62 | 9845.62±  44.91 | － | 44976.15±316.48 | 34241.42±933.71 | － | － | 1986.02±236.51 | － | 6233.89±81.92 | 5252.09±56.64 | 3276.94±70.76 | 3673.98±49.61 |
| 26 | (E)-2-Hexenal | － | － | － | － | － | － | － | － | － | － | 58.33±  5.63 | 38.66±  2.49 | 41.96±  2.66 | 62.00±  2.92 |
| 27 | 2-Nonanone | 15.42±  0.67 | 27.84±  1.21 | 189.00±  13.78 | 282.92±  16.23 | 715.85±  44.91 | － | 37.13±  3.16 | 12.50±  1.72 | － | 88.11±  4.59 | 71.29±  13.37 | 59.87±  6.84 | 43.95±  5.94 | 30.93±  5.70 |
| 28 | 2-Octanone | 32.98±  6.51 | － | 424.88±  78.30 | － | － | － | 61.00±  8.62 | 60.79±  6.66 | － | 59.22±  4.41 | － | － | 55.33±  6.27 | 64.87±  7.91 |
| 29 | (E)-2-Octen-1-ol | － | 87.05±  4.69 | 347.73±  32.41 | 1567.12±  220.33 | 3687.46±  120.33 | － | 88.50±  17.30 | 150.20±  16.67 | 179.24±  6.59 | 485.70±  21.60 | 685.38±  17.05 | 655.63±  54.89 | 395.81±  18.16 | 406.42±  13.84 |
| 30 | (E)-2-Octenal | 43.90±  6.72 | 51.17±  1.66 | 610.25±  39.73 | 1025.34±  47.54 | 1192.71±  79.33 | 2444.31±  67.03 | 62.61±  5.73 | 91.77±  6.33 | 91.46±  14.56 | 382.27±  15.96 | 367.63±  12.12 | 356.74±  17.68 | 214.40±  16.33 | 140.35±  9.70 |
| 31 | 1-Ethoxy-4,4-dimethyl-2-pentene | － | 13.74±  4.21 | － | 58.71±  12.23 | － | 182.35±  16.52 | － | 16.36±  2.35 | － | － | － | － | － | － |
| 32 | (E)-3-Methyl-2-undecene | － | － | － | 140.81±  8.81 | 183.49±  8.46 | － | 21.54±  4.08 | － | － | － | － | － | 31.66±  3.33 | － |
| 33 | 3,5-Octadien-2-one | 116.04±  17.04 | 102.75±  2.17 | － | 632.71±  23.19 | － | － | － | 234.76±  34.35 | 245.99±  32.69 | － | 372.43±  18.71 | 373.85±  48.50 | 248.83±  14.87 | 302.90±  18.21 |
| 34 | 2-Methyl-3-heptanone | － | － | 578.15±  57.50 | － | － | － | － | － | 77.55±  9.25 | － | 263.49±  17.85 | － | － | 80.95±  3.89 |
| 35 | 2,5-Dimethyl-3-hexanone | 308.02±  42.17 | 130.15±  29.10 | － | 1794.29±  63.00 | 1143.20±  30.93 | 2886.25±  72.40 | 112.79±  5.73 | 223.53±  6.32 | － | 169.34±  25.52 | － | 188.89±  10.02 | 252.05±  16.03 | － |
| 36 | 3-Octen-2-one | － | 39.97±  1.47 | 109.97±  14.30 | 471.91±  49.81 | 149.96±  3.49 | － | － | 111.67±  7.70 | 146.14±  23.87 | 118.59±  1.49 | 167.75±  14.41 | 216.53±  15.62 | 285.41±  13.59 | 353.41±  26.60 |
| 37 | 2,7-Dimethyl-4,5-octanediol | 65.88±  7.03 | 279.80±  28.17 | 605.91±  30.19 | 5939.91±  139.34 | 3085.17±  39.49 | 5738.89±  403.70 | 189.03±  16.20 | 431.27±  26.90 | 165.37±  16.11 | 1291.98±85.67 | 1416.63±21.01 | 991.39±  64.43 | 852.90±  27.28 | 171.07±  13.50 |
| 38 | 4-Ethylcyclohexanol | － | － | － | 797.24±  54.27 | － | 2522.59±  60.63 | 224.64±  40.30 | － | － | － | 183.03±  1.64 | － | － | － |
| 39 | (E)-6,10-Dimethylundeca-5,9-dien-2-one | － | 20.12±  3.30 | － | － | － | 220.70±  16.45 | 22.01±  2.90 | － | 23.09±  2.76 | － | 18.74±  1.27 | － | 23.37±  1.87 | － |
| 40 | 6-Methyl-5-hepten-2-one, | － | 198.13±  10.52 | 565.30±  69.69 | 1899.28±  49.64 | 2644.92±  87.49 | － | 322.73±  14.53 | 264.03±  16.58 | 181.03±  32.66 | 245.98±  8.53 | 458.15±  20.20 | 290.79±  12.48 | 415.42±  31.74 | 405.11±  26.24 |
| 41 | Acetophenone | 22.81±  2.02 | 25.63±  4.85 | 48.63±  1.48 | 108.87±  7.64 | 256.61±  53.14 | 846.48±  39.67 | 44.90±  9.18 | 23.17±  3.13 | 24.34±  3.25 | 28.25±  4.63 | 34.32±  2.48 | 26.86±  5.57 | 46.17±  2.22 | 36.74±  1.23 |
| 42 | Anisole | － | 85.68±  5.40 | － | 240.76±  29.87 | － | － | － | － | 48.20±  11.00 | － | 43.91±  4.65 | 36.96±  6.07 | － | － |
| 43 | Benzaldehyde | 431.17±  6.03 | 310.02±  15.56 | － | 6928.57±  413.40 | 10805.48±623.56 | 11562.12±536.72 | 397.34±  12.65 | － | 459.66±  34.93 | 1201.98±101.80 | 1582.24±100.10 | 1423.23±74.50 | 1047.81±132.73 | 603.96±  8.88 |
| 44 | 1,3-Bis(1,1-dimethylethyl)-benzene | 72.47±  4.60 | 58.65±  6.65 | － | 249.64±  17.30 | 366.77±  18.63 | 175.66±  5.91 | － | 194.49±  6.09 | 258.01±  51.75 | 189.57±  11.75 | 174.42±  14.75 | 191.30±  16.88 | 243.82±  8.54 | 160.68±  14.36 |
| 45 | 1-Ethenyl-4-ethyl-benzene | － | － | 217.77±  8.43 | － | － | － | － | 13.82±  1.62 | 9.19±  0.86 | 84.66±  5.10 | － | － | 10.14±  0.83 | － |
| 46 | 1-Ethyl-2-methyl-benzene | 18.40±  0.77 | 21.54±  5.20 | 111.00±  5.92 | 555.24±  33.50 | － | 279.38±  18.70 | 78.60±  7.76 | － | － | － | － | 19.44±  2.97 | － | 26.67±  2.10 |
| 47 | 1-Ethyl-3-methyl-benzene | － | 20.48±  4.96 | 164.23±  6.31 | 422.79±  41.99 | － | － | － | 21.01±  6.79 | 19.26±  4.45 | 62.82±  4.71 | － | － | － | － |
| 48 | Benzeneacetaldehyde | 151.02±  8.56 | 293.77±  15.98 | 1555.68±  75.25 | 3845.18±  88.25 | 3408.89±  195.60 | 3733.89±  168.27 | 255.55±  17.55 | 29.33±  3.91 | 29.99±  5.80 | 142.02±  11.79 | 163.44±  14.48 | 150.96±  8.60 | 69.57±  6.06 | 33.66±  1.70 |
| 49 | Benzofuran | － | 161.47±  5.64 | － | 1424.66±  28.87 | － | － | － | － | 110.80±  16.21 | － | － | 83.44±  3.49 | － | － |
| 50 | 2,3-Dihydro-benzofuran, | － | － | 439.45±  36.30 | 100.03±  12.04 | － | － | － | － | － | 120.91±  8.35 | － | 39.17±  3.67 | 27.21±  1.48 | － |
| 51 | Benzyl alcohol | 37.47±  7.91 | － | － | － | － | － | － | 82.52±  5.84 | － | 226.24±  3.31 | 67.56±  7.20 | 157.43±  7.00 | － | － |
| 52 | Decanal | 58.21±  6.75 | 66.94±  7.23 | 205.39±  8.59 | 259.81±  18.20 | 418.58±  16.99 | 959.59±  36.52 | 115.30±  6.31 | 46.96±  7.81 | 46.39±  4.74 | 72.41±  4.30 | 67.89±  2.85 | 57.10±  6.55 | 88.79±  12.23 | 69.15±  5.46 |
| 53 | D-Limonene | 359.02±  15.52 | 327.67±  14.64 | 1096.62±  70.99 | 1287.80±  64.60 | 2028.83±  126.51 | 8789.24±  187.31 | 625.89±  38.45 | 328.13±  15.22 | 297.26±  27.90 | 422.64±  45.13 | 309.51±  17.45 | 300.06±  39.47 | 700.41±  23.91 | 707.34±  35.70 |
| 54 | Heptanal | 57.99±  4.47 | 41.52±  7.41 | 98.54±  9.07 | 180.12±  16.88 | 470.11±  8.75 | 996.56±  6.20 | 82.92±  5.64 | 68.84±  12.58 | 53.83±  12.20 | 64.24±  6.28 | 100.59±  27.55 | 55.66±  15.57 | 82.17±  8.92 | 77.28±  5.34 |
| 55 | 3,3,5-Trimethyl-heptane, | 131.61±  17.24 | 70.41±  14.26 | － | 320.16±  55.82 | 789.63±  62.69 | － | － | 101.49±  9.45 | － | 102.35±  8.37 | 154.73±  3.53 | 116.11±  8.19 | － | － |
| 56 | Hexanal | 1154.44±77.27 | 2850.55±  58.50 | 3007.35±  222.00 | 6758.98±  417.60 | 15565.54±1371.46 | 30263.53±874.63 | 1640.93±  77.24 | － | 900.56±  47.70 | 1455.12±58.12 | 2194.65±88.31 | 1434.59±152.0 | 1915.68±22.69 | 1820.39±31.85 |
| 57 | 2,3,4-Trimethyl-hexane | － | － | 271.80±  34.00 | － | 717.82±  29.68 | － | 37.14±  4.20 | － | － | － | － | － | － | 212.45±  15.39 |
| 58 | 2,4-Dimethyl-hexane, | 206.97±  16.43 | 105.34±  8.70 | 323.99±  22.58 | 1000.18±  68.84 | 1415.35±  70.00 | 3384.08±  93.26 | 579.63±  17.61 | － | － | － | 294.09±  7.83 | 108.37±  6.92 | 133.61±  17.63 | 112.07±  6.12 |
| 59 | [Hexyl caproate](https://pubchem.ncbi.nlm.nih.gov/compound/22873) | 8.57±  0.50 | 13.89±  1.36 | － | － | － | 133.51±  4.71 | － | － | － | － | － | － | 15.20±  2.57 | － |
| 60 | 1-Methyl-indan | － | 13.94±  0.73 | － | － | － | 202.38±  12.57 | 16.39±  0.65 | － | － | 79.37±  2.68 | － | － | － | － |
| 61 | Isophorone | 55.70±  4.51 | 66.35±  7.93 | 101.32±  16.77 | 178.40±  12.23 | 144.10±  13.78 | 157.32±  6.01 | 35.35±  6.10 | 48.44±  7.79 | 58.83±  4.58 | 62.09±  4.02 | 38.65±  5.60 | 45.25±  7.11 | 44.57±  1.49 | 42.85±  6.87 |
| 62 | Naphthalene | 14.58±  0.79 | 71.53±  4.33 | 81.36±  4.94 | 143.25±  16.00 | 65.34±  9.48 | 526.58±  72.59 | 25.03±  3.82 | 14.39±  0.57 | － | 33.08±  3.21 | 38.06±  2.60 | － | 54.62±  7.54 | － |
| 63 | Nonanal | 830.66±  69.94 | 789.23±  49.60 | 2004.28±  61.51 | 2714.42±  67.44 | 4277.70±  44.13 | 10367.64±356.44 | 1406.01±  157.36 | 586.76±  27.89 | 521.83±  39.88 | 795.72±  67.38 | 761.65±  39.5 | 745.49±  58.00 | 854.75±  41.72 | 916.10±  63.13 |
| 64 | n-Tridecan-1-ol | 10.23±  0.94 | － | － | － | － | 234.70±  9.87 | 28.94±  1.68 | － | － | 18.97±  2.40 | － | － | － | － |
| 65 | Octanal | 127.60±  8.95 | － | － | － | － | 1984.66±  51.26 | 178.10±  14.08 | 219.67±  16.39 | 199.00±  12.24 | 290.89±  14.84 | 411.20±  22.99 | 217.00±  18.44 | 168.30±  14.91 | 238.31±  17.63 |
| 66 | Phenylethanol | 213.49±  8.42 | 178.61±  13.61 | － | － | － | － | － | 195.95±  15.20 | 210.47±  7.11 | 709.42±  24.02 | 312.44±  43.93 | 298.98±  8.57 | 439.14±  14.75 | 171.47±  15.00 |

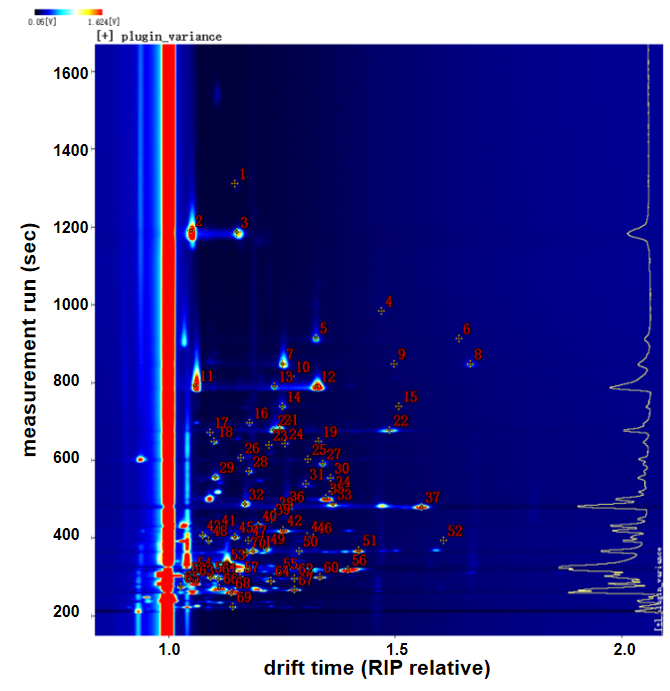
GC-MS results were reported as the mean±standard deviation (SD). “─”Not detected.



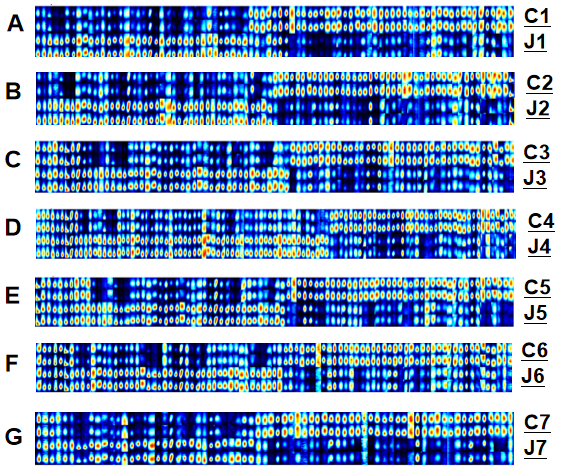
**A**

**B**

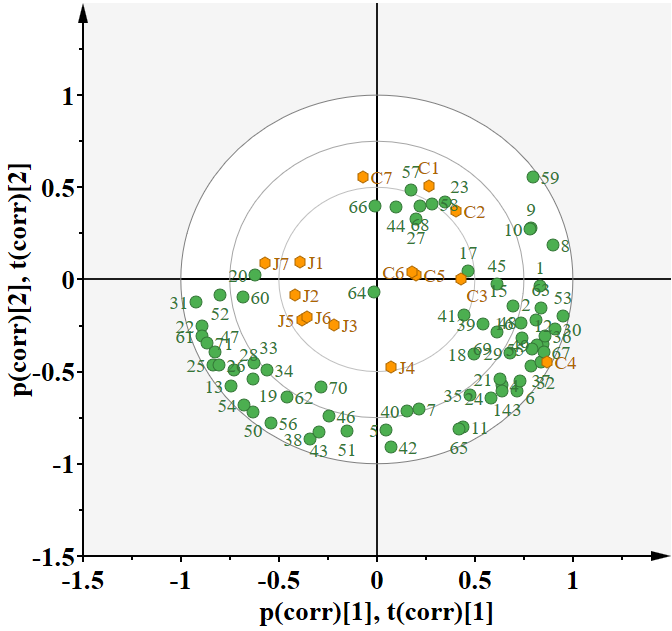
**Fig. S1 PCA bi-plot (A) and PLS-DA bi-plot (B) based on volatile components analyzed by GC-MS of CWO and RWO**



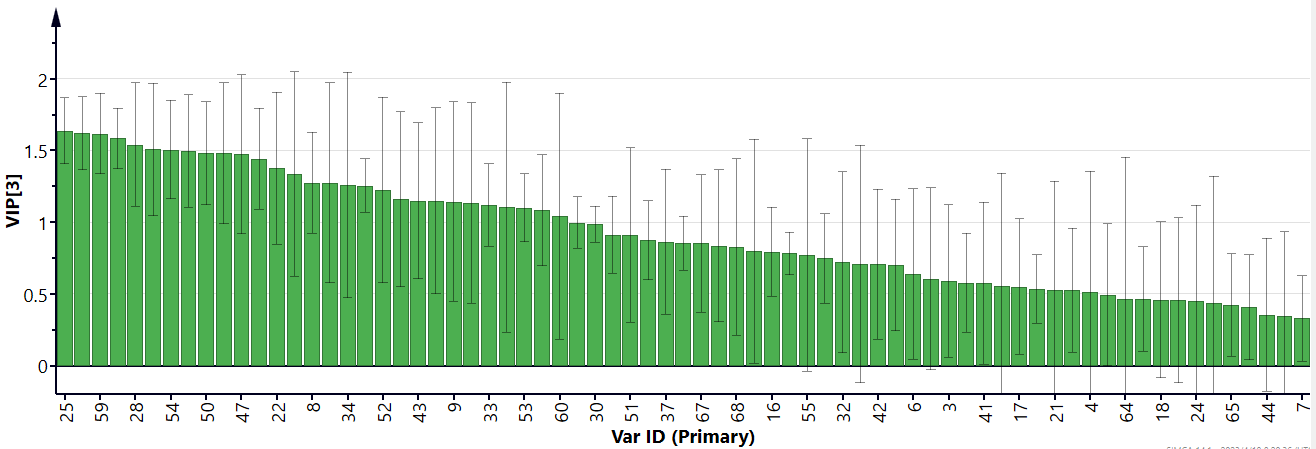
**Fig. S2. Detailed GC-IMS spectrum of walnut oil**



**Fig. S3. Representative fingerprints of CWO and RWO samples as analyzed by Gallery Plot.The compounds in this figure are listed in Table S5, from left to right.**



**Fig. S4. PCA bi-plot based on volatile components analyzed by GC-IMS of CWO and RWO**



**Fig. S5. VIP scores of volatile components in PLS-DA**

**Table S5 Volatile compounds analyzed by Gallery plot shown in Fig. S3**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | A | B | C | D | E | F | G |
| 1 | Acetic acid-M | Acetic acid-M | (E)-2-Heptenal-M | Nonanal | Ethanol | Diacetyl | Hexanal |
| 2 | Acetic acid-P | Acetic acid-P | (E)-2-Heptenal-D | Benzaldehyde | (E)-2-Heptenal-M | Butanol | Nonanal |
| 3 | 3-Hydroxy-2-butanone-M | 1-Hexanol-M | 1-Octen-3-one | (E)-2-Heptenal-M | 1-Hexanol-M | Ethyl butyrate | Butanol |
| 4 | 1-Hydroxypropan-2-one | 2,5-Dimethyl pyrazine | α-Pinene-M | 1-Octen-3-one | Butanol | Hexanal-M | 1-Hexanol-M |
| 5 | 3-Hydroxy-2-butanone-D | 3-Hydroxy-2-butanone-M | Butanol | (E)-2-heptenal-D | 1-Octen-3-one | Hexanal-P | Acetic acid-M |
| 6 | 1-Pentanol | 1-Hydroxypropan-2-one | Ethonal | Hexanal | (E)-2-heptenal-D | Ethanol | Acetic acid-P |
| 7 | 1-Penten-3-ol | 3-Hydroxy-2-butanone-D | Hexanal | Ethanol | Hexanal | Cyclopentanone | 3-Hydroxy-2-butanone-M |
| 8 | 3-Methyl-1-butanol-M | 3-Methyl-1-butanol-M | 3-Methyl butanal | 3-Methyl butanal | α-Pinene-D | Acetic acid-M | 3-Hydroxy-2-butanone-D |
| 9 | 3-Methyl-1-butanol-D | 3-Methyl-1-butanol-D | 2-Methyl propanal | Butan-2-one-D | 1-Penten-3-one-D | Acetic acid-P | 1-Pentanol |
| 10 | 2-Methyl-1-propanol-D | 1-Pentanol | Acetic acid-M | Acetic acid-M | Benzaldehyde | 1-Penten-3-ol | 3-Methyl-1-butanol-M |
| 11 | 2-Methyl-1-propanol-M | Cyclopentanone | Acetic acid-P | Acetic acid-P | Acetic acid-M | 3-Methyl-1-butanol-M | 3-Methyl-1-butanol-D |
| 12 | 1-Hexanol-M | Cyclopentanone | Area 3 | 1-Hexanol-M | Acetic acid-P | 3-Methyl-1-butanol-D | 1-Penten-3-ol |
| 13 | Propan-1-ol-M | Limonene | 1-Hexanol-M | 1-Hexanol-D | Area 3 | 2-Methyl-1-propanol-M | 2-Methyl-1-propanol-M |
| 14 | Propan-1-ol-D | 1-Penten-3-ol | 3-Hydroxy-2-butanone-M | 2,5-Dimethyl pyrazine | 2,5-Dimethyl pyrazine | 2-Methyl-1-propanol-D | 2-Methyl-1-propanol-D |
| 15 | Butan-2-ol | Heptanal | 1-Hydroxypropan-2-one | 3-Hydroxy-2-butanone-M | 3-Hydroxy-2-butanone-M | Propan-1-ol-M | Propan-1-ol-M |
| 16 | 2-Methyl-1-butanol | 2-Methyl propanal | 3-Hydroxy-2-butanone-D | 1-Hydroxypropan-2-one | 3-Hydroxy-2-butanone-D | Propan-1-ol-D | Propan-1-ol-D |
| 17 | isobutyl acetate | 3-Methyl butanal | Area 14 | 3-Hydroxy-2-butanone-D | 1-Hydroxypropan-2-one | Butan-2-ol | Butan-2-ol |
| 18 | α-Pinene-M | 2-Methyl-1-propanol-M | 1-Pentanol | 1-Penten-3-one-D | Area 14 | 1-Pentanol | 2-Methyl-1-butanol |
| 19 | Heptanal | 2-Methyl-1-propanol-D | 3-Methyl-2-butenal | 1-Pentanol | 1-Pentanol | 1-Hexanol-M | 2-Methyl propanal |
| 20 | 3-Methyl butanal | Propan-1-ol-M | 3-Methyl-1-butanol-M | 3-Methyl-2-butenal | 3-Methyl-2-butenal | 2-Butanol | heptanal |
| 21 | 2-Methyl propanal | Propan-1-ol-D | 3-Methyl-1-butanol-D | 3-Methyl-1-butanol-M | 3-Methyl-1-butanol-M | 3-Hydroxy-2-butanone-M | 3-Methyl butanal |
| 22 | Isoamyl acetate | Butan-2-ol | Cyclopentanone | 3-Methyl-1-butanol-D | 3-Methyl-1-butanol-D | 1-Hydroxypropan-2-one | ethyl acetate-M |
| 23 | Ethyl acetate-M | 2-Butanol | 1-Penten-3-ol | Cyclopentanone | 1-Penten-3-ol | 3-Hydroxy-2-butanone-D | ethyl acetate-D |
| 24 | Ethyl acetate-D | 2-Methyl-1-butanol | Propan-1-ol-M | 2-Methyl-2-pentenal | Propan-1-ol-M | α-Pinene-D | Methyl acetate |
| 25 | Methyl acetate | α-Pinene-M | Propan-1-ol-D | 2-Methyl propanal | Propan-1-ol-D | Heptanal | Butyl acetate |
| 26 | Butyl acetate | Ethyl acetate-D | 2-Methyl-1-propanol-M | Limonene | Butan-2-ol | 2-Methyl propanal | Area 3 |
| 27 | Tetrahydrofuran-M | Ethyl acetate-M | 2-Methyl-1-propanol-D | Heptanal | 2-butanol | 3-Methyl butanal | Area 43 |
| 28 | Tetrahydrofuran-D | Butyl acetate | Butan-2-ol | Butanol | 2-Methyl-1-propanol-M | Butan-2-one-D | Area 48 |
| 29 | Area 3 | Methyl acetate | 2-Butanol | Isoamyl acetate | 2-Methyl-1-propanol-D | Ethyl acetate-D | Area 101 |
| 30 | Area 69 | Tetrahydrofuran-M | Pentan-1-ol | 1-Penten-3-ol | 2-Methyl-1-butanol | Ethyl acetate-M | Area 102 |
| 31 | Area 33 | Tetrahydrofuran-D | Ethyl butyrate | 2-Methyl-1-propanol-D | Heptanal | Methyl acetate | Area 111 |
| 32 | Area 43 | Area 3 | Ethyl acetate-M | 2-Methyl-1-propanol-M | 2-Methyl propanal | Butyl acetate | Area 116 |
| 33 | Area 48 | Area 23 | Ethyl acetate-D | Ethyl butyrate | 3-Methyl butanal | Dimethyl sufide | Area 120 |
| 34 | Area 73 | Area 48 | Butyl acetate | Butan-2-ol | Ethyl butyrate | Area 14 | Cyclopentanone |
| 35 | Area 101 | Area 55 | Methyl acetate | Propan-1-ol-D | Ethyl acetate-M | Area 48 | Pentyl acetate |
| 36 | Area 111 | Area 56 | Tetrahydrofuran-D | 2-Methyl-1-butanol | Ethyl acetate-D | Area 56 | Isobutanol |
| 37 | Heptan-2-one | Area 73 | Tetrahydrofuran-M | 2-Butanol | Methyl acetate | Area 69 | Ethyl butyrate |
| 38 | Cyclopentanone | Area 83 | Area 56 | Pentan-1-ol | Butyl acetate | Area 77 | Thiophene |
| 39 | Pentyl acetate | Area 108 | Area 48 | Thiophene | Thiophene | Area 83 | 4-Methyl-2-pentanone |
| 40 | Diacetyl | Area 101 | Area 101 | Ethyl acetate-M | Area 48 | Area 84 | α-Pinene-D |
| 41 | Butanol | Area 111 | Area 102 | Ethyl acetate-D | Area 56 | Area 101 | 1-Octen-3-one |
| 42 | Propanal | Area 117 | Area 111 | Methyl acetate | Area 84 | Area 102 | Heptan-2-one |
| 43 | Hexanal | Pentyl acetate | Area 118 | Butyl acetate | Area 101 | Area 111 | 1-Penten-3-one-M |
| 44 | 2-Methyl butanal | Isobutanol | Area 124 | Area 3 | Area 111 | Area 114 | 1-Penten-3-one-D |
| 45 | (E)-2-Hexenal | 2-Methyl butanoic acid ethyl ester | 2-Methyl butanoic acid ethyl ester | Area 14 | Area 120 | Area 121 | Propan-2-one |
| 46 | (E)-2-Heptenal-M | Ethyl butyrate | Cyclopentanone | Area 18 | (E)-2-Hexenal | (E)-2-Heptenal-D | Butan-2-one-M |
| 47 | (E)-2-Pentenal-M | Heptan-2-one | Pentyl acetate | Area 23 | 2-Methyl butanal | (E)-2-Heptenal-M | Butan-2-one-D |
| 48 | (E)-2-Pentenal-D | 1-Penten-3-one-M | Thiophene | Area 27 | Pentanal | (E)-2-hexenal | Butyraldehyde-M |
| 49 | Pentanal | 1-Penten-3-one-D | 4-Methyl-2-pentanone | Area 37 | Propanal | Pentyl acetate | Butyraldehyde-D |
| 50 | Isobutanol | Propan-2-one | Methyl 2-methyl butanoate | Area 48 | Hexanal | (E)-2-Pentenal-M | 3-Methyl-2-butenal |
| 51 | 2-Methyl butanoic acid ethyl ester | Butan-2-one-D | Benzaldehyde | Area 55 | (E)-2-Pentenal-M | (E)-2-Pentenal-D | Pentanal |
| 52 | Methyl 2-methyl butanoate | Butan-2-one-M | Butyraldehyde-M | Area 56 | (E)-2-Pentenal-D | 2-Methyl butanal | (E)-2-Heptenal-M |
| 53 | Ethyl butyrate | Thiophene | Butyraldehyde-D | Area 73 | Heptan-2-one | Pentanal | (E)-2-Heptenal-D |
| 54 | 1-Penten-3-one-M | Hexanal | (E)-2-Pentenal-M | Area 75 | Butan-2-one-M | Nonanal | (E)-2-Hexenal |
| 55 | 1-Penten-3-one-D | (E)-2-Hexenal | (E)-2-Pentenal-D | Area 85 | Butan-2-one-D | Propanal | (E)-2-Pentenal-M |
| 56 | Thiophene | (E)-2-Heptenal-M | (E)-2-Hexenal | Area 111 | Propan-2-one | Butyraldehyde-M | (E)-2-Pentenal-D |
| 57 | 4-Methyl-2-pentanone | (E)-2-Heptenal-D | Heptanal | Area 101 | Cyclopentanone | Butyraldehyde-D | 2-Methyl butanal |
| 58 | α-Pinene-M | (E)-2-Pentenal-M | Hexanal | Area 118 | Pentyl acetate | Benzaldehyde | Propanal |
| 59 | Diethyl acetal | (E)-2-Pentenal-D | Pentanal | Area 120 | Diethyl acetal | Isobutanol | Diethyl acetal |
| 60 | Butan-2-one-D | Propanal | Propanal | Area 122 | Isobutanol | 2-Methyl butanoic acid ethyl ester | 2-Methyl butanoic acid ethyl ester |
| 61 | Butan-2-one-M | Pentanal | Isobutanol | Area 130 | 2-Methyl butanoic acid ethyl ester | 1-Octen-3-one | Methyl 2-methyl butanoate |
| 62 | Butyraldehyde-M | Diacetyl | 2-Methyl butanal | Area 131 | Methyl 2-methyl butanoate | Heptan-2-one | Area 6 |
| 63 | Butyraldehyde-DA | Diethyl acetal | Heptan-2-one | Pentyl acetate | 4-Methyl-2-pentanone | 1-Penten-3-one-M | Area 16 |
| 64 | Area 6 | Butyraldehyde-M | 1-Penten-3-one-M | Isobutanol | Butyraldehyde-M | 1-Penten-3-one-D | Area 29 |
| 65 | Area 16 | Butyraldehyde-D | Butan-2-one-M | 4-Methyl-2-pentanone | Butyraldehyde-D | Propan-2-one | Area 41 |
| 66 | Area 29 | 2-Methyl butanal | Butan-2-one-D | Cyclopentanone | Diacetyl | Thiophene | Area 51 |
| 67 | Area 51 | Methyl 2-methyl butanoate | Propan-2-one | Heptan-2-one | Area 6 | 4-Methyl-2-pentanone | Area 71 |
| 68 | Area 63 | Area 6 | Diethyl acetal | Butan-2-one-M | Area 16 | Diethyl acetal | Area 97 |
| 69 | Area 65 | Area 16 | Diacetyl | Propan-2-one | Area 29 | Methyl 2-methyl butanoate | Area 99 |
| 70 | Area 71 | Area 29 | Area 16 | Diethyl acetal | Area 41 | Area 16 | Area 105 |
| 71 | Area 74 | Area 41 | Area 29 | Butyraldehyde-M | Area 63 | Area 29 | Area 123 |
| 72 | Area 41 | Area 71 | Area 41 | Butyraldehyde-D | Area 69 | Area 41 | Area 125 |
| 73 | Area 76 | Area 74 | Area 69 | (E)-2-Pentenal-M | Area 71 | Area 63 |  |
| 74 | Area 105 | Area 76 | Area 71 | (E)-2-Pentenal-D | Area 76 | Area 71 |  |
| 75 | Area 80 | Area 77 | Area 76 | (E)-2-Hexenal | Area 77 | Area 76 |  |
| 76 | Area 81 | Area 80 | Area 77 | Hexanal | Area 80 | Area 80 |  |
| 77 | Area 97 | Area 96 | Area 81 | Pentanal | Area 81 | Area 81 |  |
| 78 | Area 99 | Area 97 | Area 97 | Propanal | Area 96 | Area 96 |  |
| 79 | Area 107 | Area 99 | Area 99 | Diacetyl | Area 97 | Area 97 |  |
| 80 | Area 118 | Area 100 | Area 113 | Methyl 2-methyl butanoate | Area 99 | Area 99 |  |
| 81 | Area 123 | Area 105 | Area 117 | α-Pinene-D | Area 100 | Area 105 |  |
| 82 |  | Area 107 | Area 133 | 2-Methyl butanoic acid ethyl ester | Area 105 | Area 113 |  |
| 83 |  | Area 118 | Area 134 | Area 6 | Area 113 | Area 116 |  |
| 84 |  | Area 123 |  | Area 16 | Area 123 | Area 120 |  |
| 85 |  | Ethanol |  | Area 41 | Area 133 | Area 123 |  |

**References**

Chang, Y., Wang, S., Chen, H., Zhang, N., & Sun, J. (2021). Characterization of the key aroma compounds in pork broth by sensory‐directed flavor analysis. *Journal of Food Science*, 86(11), 4932-4945.

Guo, X., Ho, C. T., Wan, X., Zhu, H., Liu, Q., & Wen, Z. (2021). Changes of volatile compounds and odor profiles in Wuyi rock tea during processing. *Food Chemistry*, 341, 128230.

Ledauphin, J., Guichard, H., Saint-Clair, J. F., Picoche, B., & Barillier, D. (2003). Chemical and sensorial aroma characterization of freshly distilled calvados. 2. Identification of volatile compounds and key odorants. *Journal of Agricultural and Food Chemistry*, 51(2), 433-442.

Li, R., Shi, J., Li, C., Ren, X., Tao, Y., Ma, F., & Liu, C. (2023). Characterization of the key odorant compounds in ‘Qinguan’apples (*Malus× domestica*). *LWT*, 184, 115052.

Schreiner, L., Bauer, P., & Buettner, A. (2018). Resolving the smell of wood-identification of odour-active compounds in Scots pine (*Pinus sylvestris L.*). *Scientific Reports*, 8(1), 8294.

Tan, F., Wang, P., Zhan, P., & Tian, H. (2022). Characterization of key aroma compounds in flat peach juice based on gas chromatography-mass spectrometry-olfactometry (GC-MS-O), odor activity value (OAV), aroma recombination, and omission experiments. *Food Chemistry*, 366, 130604.

Xi, B. N., Zhang, J. J., Xu, X., Li, C., Shu, Y., Zhang, Y., & Shen, Y. (2024). Characterization and metabolism pathway of volatile compounds in walnut oil obtained from various ripening stages via HS-GC-IMS and HS-SPME-GC–MS. *Food Chemistry*, 435, 137547.