# Supporting Information – S1 Table

# Exploring the *Saccharomyces cerevisiae* metabolomics biodiversity: indigenous versus commercial strains

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**S1 Table**. Volatile metabolites identified by HS-SPME/GC×GC-ToFMS in four *S. cerevisiae* strains under study: BT2453 and BT2652 corresponding to strains isolated from wine, and CSc1 and CSc2, corresponding to commercial yeast strains.

| Nº | $^1t_R$ [a] (s) | $^2t_R$ [a] (s) | Compound | Formula | CAS | RI $_{Calc}$ [c] | RI $_{Lit}$ [d] | BT2453 | BT2652 | CSc1 | CSc2 | Ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Peak Area[b] (x10$^6$) and RSD (%) | | | | |
| | | | **Acetals** | | | | | | | | | |
| 1 | 145 | 0.432 | 1,1-Diethoxyethane | $C_6H_{14}O_2$ | 105-57-7 | 711 | 690 | 1.33 (20) | 1.64 (11) | 1.00 (17) | 1.30 (35) | [1] |
| 2 | 145 | 0.456 | 2,4,5-Trimethyl-1,3-dioxolane | $C_6H_{12}O_2$ | 3299-32-9 | 711 | 690 | 2.26 (35) | 3.04 (9) | 1.31 (3) | 1.66 (25) | [1] |
| 3 | 290 | 0.728 | 2,2,3-Trimethyloxetane | $C_6H_{12}O$ | 23120-43-6 | 917 | - | 0.22 (18) | - | - | - | |
| | | | **Subtotal (GC Peak Area)** | | | | | **3.81** | **4.68** | **2.31** | **2.96** | |
| | | | **Subtotal (%)** | | | | | **0.36** | **0.64** | **0.33** | **0.39** | |
| | | | **Acids** | | | | | | | | | |
| 4 | 100 | 3.336 | Acetic acid | $C_2H_4O_2$ | 64-19-7 | 636 | 600 | 63.93 (32) | 63.10 (22) | 40.84 (8) | 1.50 (6) | [2] |
| 5 | 135 | 4.344 | Propanoic acid | $C_3H_6O_2$ | 79-09-4 | 699 | 700 | 1.17 (13) | 0.90 (17) | - | 0.31 (6) | [3] |
| 6 | 170 | 3.904 | 2-Methylpropanoic acid | $C_4H_8O_2$ | 79-31-2 | 768 | 775 | 12.28 (11) | 8.43 (15) | 4.49 (15) | 5.93 (8) | [4] |
| 7 | 190 | 4.640 | Butanoic acid | $C_4H_8O_2$ | 107-92-6 | 805 | 821 | 8.17 (4) | 4.02 (8) | 2.86 (8) | 4.09 (18) | [5] |
| 8 | 235 | 4.056 | Isovaleric acid | $C_5H_{10}O_2$ | 503-74-2 | 858 | 864 | 11.36 (18) | 7.59 (7) | 4.08 (11) | 5.93 (12) | [6] |
| 9 | 245 | 3.776 | 2-Methylbutanoic acid | $C_5H_{10}O_2$ | 116-53-0 | 869 | 873 | 6.27 (26) | 5.33 (6) | 2.50 (15) | 2.82 (12) | [5] |
| 10 | 365 | 3.648 | Hexanoic acid | $C_6H_{12}O_2$ | 142-62-1 | 999 | 1019 | 37.94 (13) | 9.07 (8) | 18.35 (13) | 19.46 (19) | [5] |
| 11 | 545 | 2.616 | Octanoic acid | $C_8H_{16}O_2$ | 124-07-2 | 1197 | 1182 | 214.92 (6) | 141.41 (20) | 131.62 (12) | 141.76 (17) | [7] |
| 12 | 615 | 2.448 | Nonanoic acid | $C_9H_{18}O_2$ | 112-05-0 | 1279 | 1280 | 9.36 (161) | 0.39 (49) | - | - | [8] |
| 13 | 695 | 2.616 | Dec-9-enoic acid | $C_{10}H_{18}O_2$ | 14436-32-9 | 1378 | 1389 | 13.91 (12) | 12.03 (65) | - | - | [9] |
| 14 | 700 | 2.184 | Decanoic acid | $C_{10}H_{20}O_2$ | 334-48-5 | 1378 | 1380 | 97.46 (17) | 50.06 (8) | 63.33 (18) | 73.65 (14) | [10] |
| | | | **Subtotal (GC Peak Area)** | | | | | **476.78** | **302.34** | **268.07** | **255.45** | |
| | | | **Subtotal (%)** | | | | | **45.47** | **41.48** | **38.51** | **33.44** | |
| | | | **Alcohols** | | | | | | | | | |
| | | | ***Aliphatics*** | | | | | | | | | |
| 15 | 85 | 0.648 | 1-Propanol | $C_3H_8O$ | 71-23-8 | 591 | 574 | 3.29 (12) | 3.45 (9) | 2.41 (16) | 2.51 (12) | [11] |
| 16 | 100 | 0.712 | 2-Methyl-1-propanol | $C_4H_{10}O$ | 78-83-1 | 621 | 615 | 11.88 (25) | 8.84 (10) | 15.61 (11) | 12.41 (11) | [12] |
| 17 | 105 | 0.568 | 2-Methyl-2-butanol | $C_5H_{12}O$ | 75-85-4 | 631 | 622 | 1.87 (67) | 2.36 (13) | 1.49 (25) | 1.38 (50) | [12] |
| 18 | 115 | 0.784 | 1-Butanol | $C_4H_{10}O$ | 71-36-3 | 652 | 646 | 1.18 (24) | 1.38 (19) | 0.91 (24) | 0.74 (11) | [13] |
| 19 | 130 | 0.696 | 2-Pentanol | $C_5H_{12}O$ | 6032-29-7 | 681 | 685 | - | 0.04 (19) | - | - (13) | [14] |
| 20 | 145 | 0.640 | 2-Methyl-2-pentanol | $C_6H_{14}O$ | 590-36-3 | 721 | 698 | 0.47 (82) | 0.36 (13) | 0.26 (16) | 0.35 (8) | [12] |
| 21 | 150 | 0.944 | 3-Methyl-1-butanol | $C_5H_{12}O$ | 123-51-3 | 722 | 706 | 35.55 (20) | 32.61 (16) | 33.68 (23) | 38.32 (22) | [12] |
| 22 | 155 | 0.864 | 2-Methyl-1-butanol | $C_5H_{12}O$ | 137-32-6 | 732 | 739 | - | - | 16.93 (5) | 16.58 (7) | [2] |
| 23 | 165 | 0.720 | 4-Methyl-2-pentanol | $C_6H_{14}O$ | 108-11-2 | 751 | 758 | 0.08 (15) | 0.06 (14) | 0.08 (19) | 0.09 (15) | [3] |
| 24 | 175 | 0.912 | 1-Pentanol | $C_5H_{12}O$ | 71-41-0 | 772 | 776 | 0.40 (10) | - | - | - | [15] |
| 25 | 180 | 1.184 | 3-Methyl-2-buten-1-ol | $C_5H_{10}O$ | 556-82-1 | 782 | 778 | 0.17 (35) | - | - | - | [8] |
| 26 | 185 | 0.632 | 2,4-Dimethyl-2-pentanol | $C_7H_{16}O$ | 625-06-9 | 791 | - | 0.12 (33) | 0.16 (24) | 0.12 (2) | 0.11 (26) | |
| 27 | 220 | 0.672 | 2-Methyl-2-hexanol | $C_7H_{16}O$ | 625-23-0 | 836 | - | 0.10 (24) | 0.09 (18) | 0.08 (21) | 0.08 (22) | |
| 28 | 225 | 0.904 | 2-Methyl-1-pentanol | $C_6H_{14}O$ | 105-30-6 | 842 | 843 | 0.56 (7) | - | 0.28 (3) | 0.29 (3) | [16] |

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 29 | 260 | 0.944 | 1-Hexanol | $C_6H_{14}O$ | 111-27-3 | 883 | 874 | 0.10 | (5) | 0.08 | (58) | - | | - | | [17] |
| 30 | 280 | 0.792 | 2-Heptanol | $C_7H_{16}O$ | 543-49-7 | 906 | 904 | 0.07 | (25) | - | | 0.10 | (10) | 0.09 | (9) | [11] |
| 31 | 305 | 0.664 | 4-Methyl-4-heptanol | $C_8H_{18}O$ | 598-01-6 | 932 | - | 0.53 | (29) | 0.45 | (11) | 0.45 | (22) | 0.48 | (9) | |
| 32 | 305 | 0.680 | 2-Methyl-2-heptanol | $C_8H_{18}O$ | 625-25-2 | 932 | - | 0.63 | (31) | 0.44 | (12) | 0.46 | (20) | 0.45 | (18) | |
| 33 | 330 | 0.768 | 4-Methyl-2-heptanol | $C_8H_{18}O$ | 56298-90-9 | 959 | 950 | 4.54 | (22) | 3.91 | (19) | 3.15 | (6) | 3.42 | (5) | [18] |
| 34 | 345 | 0.960 | 1-Heptanol | $C_7H_{16}O$ | 111-70-6 | 975 | 974 | 3.00 | (42) | 3.71 | (9) | 0.45 | (8) | 0.74 | (13) | [15] |
| 35 | 350 | 0.656 | 2,3-Dimethyl-2-hexanol | $C_8H_{18}O$ | 19550-03-9 | 980 | - | 6.23 | (16) | 5.68 | (16) | 6.21 | (6) | 6.31 | (6) | |
| 36 | 355 | 0.624 | 3-Ethyl-2-methyl-3-pentanol | $C_8H_{18}O$ | 597-05-7 | 985 | - | 0.66 | (20) | 0.54 | (16) | 0.59 | (13) | 0.62 | (7) | |
| 37 | 360 | 0.760 | 2-Methyl-2-octen-4-ol | $C_9H_{18}O$ | - | 990 | - | 0.36 | (22) | - | | 0.57 | (10) | 0.29 | (19) | |
| 38 | 380 | 0.728 | $C_8$ Alcohol (*m/z* 45, 57, 69) | $C_8H_{18}O$ | - | 1011 | - | 0.76 | (10) | 0.78 | (15) | 0.63 | (17) | 0.66 | (10) | |
| 39 | 395 | 0.656 | 4-Methyl-4-octanol | $C_9H_{20}O$ | 23418-37-3 | 1027 | - | 0.57 | (25) | 0.43 | (20) | 0.50 | (8) | 0.54 | (4) | |
| 40 | 395 | 0.688 | 4,5-Dimethyl-3-heptanol | $C_9H_{20}O$ | - | 1027 | - | - | | - | | 0.33 | (49) | 0.43 | (7) | |
| 41 | 400 | 0.624 | 2-Methyl-2-octanol | $C_9H_{20}O$ | 628-44-4 | 1032 | 1033 | 0.77 | (11) | 0.83 | (15) | 0.63 | (11) | 0.65 | (20) | [19] |
| 42 | 400 | 0.872 | 2-Ethyl-1-hexanol | $C_8H_{18}O$ | 104-76-7 | 1033 | 1038 | 8.29 | (20) | 6.23 | (19) | 5.52 | (12) | 6.05 | (2) | [17] |
| 43 | 430 | 1.800 | 2,5-Dimethyl-2,5-hexanediol | $C_8H_{18}O_2$ | 110-03-2 | 1065 | - | 0.66 | (32) | 0.11 | (59) | - | | 0.40 | (16) | |
| 44 | 435 | 0.744 | $C_8$ Alcohol (*m/z* 45, 55, 70) | $C_8H_{18}O$ | - | 1069 | - | 0.56 | (25) | - | | - | | - | | |
| 45 | 445 | 0.888 | 1-Octanol | $C_8H_{18}O$ | 111-87-5 | 1075 | 1079 | 0.87 | (18) | 1.11 | (15) | 1.54 | (13) | 1.63 | (34) | [17] |
| 46 | 450 | 0.632 | 2,4-Dimethyl-3-hexanol | $C_8H_{18}O$ | 13432-25-2 | 1085 | - | 0.28 | (40) | 0.22 | (5) | 0.25 | (5) | 0.17 | (5) | |
| 47 | 455 | 0.840 | 2,4-Dimethyl-1-heptanol | $C_9H_{20}O$ | - | 1090 | - | - | | - | | 4.61 | (25) | 1.89 | (14) | |
| 48 | 460 | 0.896 | 2,3,4-Trimethyl-5-hexen-3-ol | $C_9H_{18}O$ | 28638-29-1 | 1090 | - | 1.54 | (35) | 0.83 | (12) | 5.36 | (22) | 0.76 | (40) | |
| 49 | 465 | 0.768 | 2-Nonanol | $C_9H_{20}O$ | 628-99-9 | 1101 | 1098 | 0.22 | (9) | - | | 0.17 | (6) | 0.20 | (14) | [8] |
| 50 | 465 | 1.008 | 2-Nonen-1-ol | $C_9H_{18}O$ | 31502-14-4 | 1101 | 1074 | 1.43 | (22) | - | | - | | - | | [20] |
| 51 | 480 | 0.640 | 4-Ethyl-4-heptanol | $C_9H_{20}O$ | 597-90-0 | 1118 | - | | | 0.21 | (17) | - | | - | | |
| 52 | 485 | 0.648 | 4-Methyl-4-nonanol | $C_{10}H_{22}O$ | 23418-38-4 | 1124 | - | 1.98 | (19) | 1.28 | (15) | 1.02 | (10) | 1.17 | (7) | |
| 53 | 495 | 0.616 | $C_{10}$ Alcohol (*m/z* 41, 55,59) | $C_{10}H_{22}O$ | - | 1136 | - | - | | - | | - | | 0.70 | (20) | |
| 54 | 525 | 0.616 | 3,4-Diethyl-3-hexanol | $C_{10}H_{22}O$ | 19398-78-8 | 1171 | - | 7.02 | (8) | 6.79 | (15) | 6.10 | (12) | 5.53 | (19) | |
| 55 | 530 | 0.720 | $C_{10}$ Alcohol (*m/z* 45, 55, 70) | $C_{10}H_{22}O$ | - | 1177 | - | - | | 0.14 | (27) | 1.47 | (16) | 3.95 | (11) | |
| 56 | 545 | 0.832 | 1-Nonanol | $C_9H_{20}O$ | 143-08-8 | 1195 | 1179 | 5.04 | (61) | 3.01 | (21) | 3.17 | (26) | 3.95 | (12) | [17] |
| 57 | 555 | 0.680 | 2-Decanol | $C_{10}H_{22}O$ | 1120-06-5 | 1207 | 1209 | 3.16 | (14) | 2.32 | (12) | 1.14 | (26) | 1.25 | (38) | [21] |
| 58 | 565 | 0.616 | 3-Decanol | $C_{10}H_{22}O$ | 1565-81-7 | 1218 | 1197 | 6.12 | (21) | 4.93 | (32) | 5.30 | (17) | - | | [8] |
| 59 | 620 | 0.832 | 1-Decanol | $C_{10}H_{22}O$ | 112-30-1 | 1283 | 1281 | 1.96 | (16) | 2.84 | (22) | 3.10 | (15) | 3.08 | (23) | [17] |
| 60 | 650 | 0.440 | 2-Butyl-1-octanol | $C_{12}H_{26}O$ | 3913-02-8 | 1319 | - | 0.41 | (21) | - | | - | | - | | |
| | | | ***Aromatics*** | | | | | | | | | | | | | |
| 61 | 450 | 1.600 | 2-Phenylisopropanol | $C_9H_{12}O$ | 617-94-7 | 1086 | 1080 | - | | - | | - | | 0.12 | (13) | [22] |
| 62 | 480 | 2.272 | 2-Phenylethanol | $C_8H_{10}O$ | 60-12-8 | 1121 | 1110 | 78.54 | (20) | 30.40 | (19) | 45.23 | (10) | 58.52 | (2) | [8] |
| | | | **Cyclic** | | | | | | | | | | | | | |
| 63 | 365 | 0.688 | 1-Cyclopentyl-1-propanol | $C_8H_{16}O$ | - | 995 | - | - | | - | | - | | 0.19 | (8) | |
| | | | **Subtotal (GC Peak Area)** | | | | | **191.93** | | **126.64** | | **165.07** | | **177.18** | | |
| | | | **Subtotal (%)** | | | | | **18.30** | | **17.37** | | **23.71** | | **23.19** | | |
| | | | **Aldehydes** | | | | | | | | | | | | | |
| | | | ***Aliphatics*** | | | | | | | | | | | | | |
| 64 | 85 | 0.408 | Butanal | $C_4H_8O$ | 123-72-8 | 591 | 614 | 1.38 | (85) | - | | 1.78 | (20) | 2.17 | (18) | [20] |
| 65 | 110 | 0.464 | 3-Methyl-butanal | $C_5H_{10}O$ | 590-86-3 | 641 | 649 | 6.65 | (33) | 6.52 | (29) | 5.68 | (27) | 7.44 | (19) | [11] |
| 66 | 115 | 0.456 | 2-Methyl-butanal | $C_5H_{10}O$ | 96-17-3 | 651 | 646 | 3.92 | (46) | 3.17 | (34) | 4.04 | (12) | 4.37 | (5) | [23] |
| 67 | 425 | 0.736 | 2-Octenal | $C_8H_{14}O$ | 2548-87-0 | 1059 | 1056 | - | | 2.60 | (4) | 0.81 | (83) | 0.70 | (9) | [15] |

| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 68 | 605 | 0.728 | 2-Decenal | $C_{10}H_{18}O$ | 3913-81-3 | 1266 | 1261 | 1.60 | (12) | - | | - | | - | | [8] |
| | | | ***Aromatics*** | | | | | | | | | | | | | |
| 69 | 335 | 1.288 | Benzaldehyde | $C_7H_6O$ | 100-52-7 | 965 | 964 | 9.91 | (62) | 1.65 | (19) | 3.45 | (15) | 7.20 | (20) | [20] |
| 70 | 410 | 1.344 | 2-Phenylacetaldehyde | $C_8H_8O$ | 122-78-1 | 1044 | 1043 | 11.25 | (51) | 3.22 | (10) | 5.28 | (4) | 7.61 | (12) | [8] |
| 71 | 410 | 1.528 | 2-Hydroxy benzaldehyde | $C_7H_6O_2$ | 90-02-8 | 1044 | 1041 | 0.08 | (53) | - | | - | | - | | [8] |
| 72 | 565 | 1.208 | 3,5-Dimethyl-benzaldehyde | $C_9H_{10}O$ | 5779-95-3 | 1219 | - | 6.55 | (15) | - | | 1.27 | (16) | - | | |
| 73 | 615 | 1.312 | 2-Phenyl-2-butenal | $C_{10}H_{10}O$ | 4411-89-6 | 1278 | 1273 | 0.17 | (37) | - | | - | | - | | [24] |
| | | | **Subtotal (GC Peak Area)** | | | | | **41.50** | | **17.16** | | **22.32** | | **29.49** | | |
| | | | **Subtotal (%)** | | | | | **3.96** | | **2.35** | | **3.21** | | **3.86** | | |
| | | | **Ketones** | | | | | | | | | | | | | |
| | | | ***Aliphatics*** | | | | | | | | | | | | | |
| 74 | 90 | 0.552 | 2,3-Butanedione | $C_4H_6O_2$ | 431-03-8 | 601 | 592 | - | | - | | - | | 0.29 | (12) | [2] |
| 75 | 95 | 0.448 | 2-Butanone | $C_4H_8O$ | 78-93-3 | 611 | 601 | - | | - | | 0.50 | (3) | 0.56 | (13) | [20] |
| 76 | 125 | 0.504 | 2-Pentanone | $C_5H_{10}O$ | 107-87-9 | 671 | 686 | 1.04 | (44) | 0.95 | (22) | 0.97 | (12) | 1.04 | (14) | [25] |
| 77 | 125 | 0.624 | 2,3-Pentanedione | $C_5H_8O_2$ | 600-14-6 | 671 | 693 | - | | 0.14 | (54) | 0.33 | (45) | 0.31 | (15) | [3] |
| 78 | 140 | 1.232 | 3-Hydroxy-2-butanone | $C_4H_8O_2$ | 513-86-0 | 702 | 733 | 5.43 | (77) | 3.34 | (72) | 5.24 | (46) | 5.29 | (17) | [15] |
| 79 | 150 | 0.512 | 4-Methyl-2-pentanone | $C_6H_{12}O$ | 180-10-1 | 721 | 736 | 1.50 | (25) | 1.36 | (20) | 1.27 | (14) | 1.26 | (11) | [3] |
| 80 | 185 | 0.576 | 2-Hexanone | $C_6H_{12}O$ | 591-78-6 | 791 | 787 | 0.39 | (26) | - | | 0.38 | (8) | 0.37 | (12) | [11] |
| 81 | 190 | 0.648 | 4-Methyl-3-penten-2-one | $C_6H_{10}O$ | 141-79-7 | 801 | 801 | 0.82 | (63) | - | | 0.37 | (9) | 0.37 | (12) | [12] |
| 82 | 195 | 1.216 | 3-Hydroxy-2-pentanone | $C_5H_{10}O_2$ | 3142-66-3 | 807 | 803 | 0.13 | (45) | 0.49 | (15) | 0.11 | (17) | 0.14 | (23) | [26] |
| 83 | 220 | 0.616 | 2,3-Heptanedione | $C_7H_{12}O_2$ | 96-04-8 | 836 | - | - | | 0.07 | (15) | - | | 0.07 | (15) | |
| 84 | 230 | 0.568 | 4-Methyl-2-hexanone | $C_7H_{14}O$ | 105-42-0 | 848 | 846 | 0.31 | (48) | 0.26 | (16) | 0.29 | (8) | 0.29 | (10) | [27] |
| 85 | 230 | 1.120 | 4-Hydroxy-4-methyl-2-pentanone | $C_6H_{12}O_2$ | 123-42-2 | 848 | 840 | 0.25 | (135) | - | | - | | - | | [28] |
| 86 | 240 | 0.584 | 5-Methyl-2-hexanone | $C_7H_{14}O$ | 110-12-3 | 860 | 857 | 0.68 | (30) | 0.55 | (16) | - | | - | | [29] |
| 87 | 270 | 0.600 | 2-Heptanone | $C_7H_{14}O$ | 110-43-0 | 895 | 895 | 3.07 | (37) | 2.46 | (52) | 4.70 | (20) | 4.92 | (10) | [15] |
| 88 | 280 | 0.552 | 3,4-Dimethyl-2-hexanone | $C_8H_{16}O$ | 19550-10-8 | 906 | - | 0.24 | (31) | 0.18 | (36) | 0.20 | (14) | 0.20 | (17) | |
| 89 | 305 | 0.560 | 6-Methyl-2-heptanone | $C_8H_{16}O$ | 928-68-7 | 932 | 958 | - | | 7.84 | (19) | 9.17 | (7) | 9.36 | (9) | [15] |
| 90 | 305 | 1.368 | 2,5-Hexanedione | $C_6H_{10}O_2$ | 110-13-4 | 933 | 933 | 0.65 | (29) | 0.29 | (18) | 0.26 | (18) | 0.26 | (10) | [10] |
| 91 | 315 | 0.584 | 4-Methyl-2-heptanone | $C_8H_{16}O$ | 6137-06-0 | 943 | 936 | 15.10 | (15) | 15.40 | (9) | 15.00 | (9) | 15.60 | (10) | [27] |
| 92 | 320 | 1.040 | 2,5-Dimethyl-3-hexanone | $C_8H_{16}O$ | 1888-57-9 | 948 | - | - | | 0.22 | (70) | - | | - | | |
| 93 | 330 | 0.472 | 2,3-Octanedione | $C_8H_{14}O_2$ | 585-25-1 | 958 | 980 | - | | 0.13 | (12) | 0.10 | (18) | 0.11 | (13) | [3] |
| 94 | 330 | 0.624 | 4-Methyl-3-hepten-2-one (isomer) | $C_8H_{14}O$ | 22319-25-1 | 959 | - | 0.28 | (23) | 0.20 | (24) | - | | - | | |
| 95 | 345 | 0.568 | 4-Octanone | $C_8H_{16}O$ | 589-63-9 | 974 | 974 | 0.24 | (19) | 0.16 | (14) | 0.16 | (20) | - | | [3] |
| 96 | 350 | 0.520 | 2,4-Dimethyl-3-heptanone | $C_9H_{18}O$ | 18641-71-9 | 979 | - | - | | - | | 0.19 | (25) | 0.32 | (8) | |
| 97 | 355 | 0.544 | $C_9$ Ketone (*m/z* 43, 57, 86) | $C_9H_{18}O$ | - | 985 | - | 0.49 | (32) | 0.48 | (20) | 0.48 | (10) | 0.65 | (32) | |
| 98 | 360 | 0.584 | $C_9$ Ketone (*m/z* 57, 72, 99) | $C_9H_{18}O$ | - | 990 | - | 7.15 | (18) | 7.25 | (3) | 9.92 | (13) | 7.49 | (6) | |
| 99 | 360 | 0.664 | 4-Methyl-3-hepten-2-one (isomer) | $C_8H_{14}O$ | 22319-25-1 | 990 | - | 0.70 | (17) | - | | 0.54 | (15) | 0.66 | (12) | |
| 100 | 395 | 0.568 | $C_9$ Ketone (*m/z* 43, 71) | $C_9H_{18}O$ | 6137-15-1 | 1027 | - | - | | - | | - | | 0.10 | (8) | |
| 101 | 400 | 0.608 | 2-Methyl-2-octen-4-one | $C_9H_{16}O$ | - | 1032 | - | 0.28 | (13) | 0.26 | (8) | 0.23 | (3) | 0.24 | (2) | |
| 102 | 405 | 0.592 | $C_9$ Ketone (*m/z* 43, 58, 85) | $C_9H_{18}O$ | - | 1038 | - | 1.49 | (26) | 1.28 | (16) | 1.27 | (9) | 1.26 | (20) | |
| 103 | 410 | 0.704 | 3,3,6-Trimethylhepta-1,5-dien-4-one | $C_{10}H_{16}O$ | 546-49-6 | 1043 | 1062 | 0.54 | (30) | 0.37 | (6) | 0.39 | (19) | 0.40 | (15) | [8] |
| 104 | 430 | 0.696 | 5-Nonen-2-one | $C_9H_{16}O$ | 27039-84-5 | 1064 | - | 0.87 | (30) | 0.70 | (15) | 0.46 | (1) | 0.63 | (19) | |
| 105 | 440 | 0.576 | 5-Nonanone | $C_9H_{18}O$ | 502-56-7 | 1074 | 1073 | 0.60 | (34) | 0.34 | (36) | 0.51 | (19) | - | | [3] |
| 106 | 450 | 0.584 | 3,5-Dimethyl-2-octanone | $C_{10}H_{20}O$ | 19781-14-7 | 1085 | - | 0.12 | (24) | 0.10 | (8) | 0.08 | (14) | 0.10 | (11) | |
| 107 | 455 | 0.624 | 2-Nonanone | $C_9H_{18}O$ | 821-55-6 | 1090 | 1093 | 3.94 | (35) | 3.03 | (21) | 4.54 | (14) | 6.19 | (1) | [20] |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 108 | 475 | 0.752 | 2,6-Dimethyl-2,5-heptadien-4-one | $C_9H_{14}O$ | 504-20-1 | 1113 | - | 7.55 | (13) | 6.39 | (7) | 5.68 | (11) | 6.08 | (10) | |
| 109 | 480 | 0.560 | 4-Decanone | $C_{10}H_{20}O$ | 624-16-8 | 1118 | - | 0.67 | (12) | 0.59 | (17) | 0.64 | (12) | 0.57 | (2) | |
| 110 | 540 | 0.608 | 3-Decanone | $C_{10}H_{20}O$ | 928-80-3 | 1189 | 1186 | 2.32 | (34) | 0.10 | (13) | 0.12 | (29) | 0.12 | (20) | [8] |
| 111 | 580 | 0.640 | 2-Methyl-2-nonen-4-one | $C_{10}H_{18}O$ | 2903-23-3 | 1236 | 1215 | - | | - | | 0.43 | (20) | 0.43 | (20) | [30] |
| 112 | 630 | 0.640 | 2-Undecanone | $C_{11}H_{22}O$ | 112-12-9 | 1295 | 1291 | 1.20 | (16) | - | | - | | - | | [17] |
| | | | ***Aromatics*** | | | | | | | | | | | | | |
| 113 | 430 | 1.288 | 1-Phenylethanone | $C_8H_8O$ | 98-86-2 | 1065 | 1067 | 2.64 | (12) | 0.57 | (11) | - | | - | | [15] |
| 114 | 490 | 1.248 | 1-Phenylpropan-2-one | $C_9H_{10}O$ | 103-79-7 | 1131 | 1124 | 0.15 | (1) | - | | - | | - | | [31] |
| 115 | 495 | 0.968 | 1-(2-Methylphenyl)ethanone | $C_9H_{10}O$ | 577-16-2 | 1136 | 1139 | 0.09 | (21) | - | | - | | - | | [32] |
| 116 | 540 | 1.192 | 1-(4-Methylphenyl)ethanone | $C_9H_{10}O$ | 122-00-9 | 1190 | 1182 | 0.08 | (25) | 0.06 | (20) | - | | - | | [8] |
| 117 | 575 | 1.112 | 1-Phenyl-2-butanone | $C_{10}H_{12}O$ | 1007-32-5 | 1231 | - | 0.10 | (6) | 0.05 | (4) | - | | - | | |
| 118 | 625 | 1.352 | 4-Phenyl-3-buten-2-one | $C_{10}H_{10}O$ | 1896-62-4 | 1290 | 1330 | 0.10 | (41) | - | | - | | - | | [33] |
| 119 | 650 | 1.208 | 1-(3,4-Dimethyphenyl)-ethanone | $C_{10}H_{12}O$ | 03637-01-2 | 1320 | - | 0.20 | (21) | 0.11 | (30) | - | | - | | |
| | | | ***Cyclic*** | | | | | | | | | | | | | |
| 120 | 270 | 0.808 | Cyclohexanone | $C_6H_{10}O$ | 108-94-1 | 895 | 895 | 0.41 | (21) | 0.31 | (12) | 0.40 | (17) | 0.36 | (8) | [10] |
| | | | **Subtotal (GC Peak Area)** | | | | | **61.79** | | **56.01** | | **64.93** | | **66.07** | | |
| | | | **Subtotal (%)** | | | | | **5.89** | | **7.68** | | **9.33** | | **8.65** | | |
| | | | **Terpenic compounds** | | | | | | | | | | | | | |
| 121 | 365 | 0.504 | β-Myrcene | $C_{10}H_{16}$ | 123-35-3 | 995 | 986 | 0.50 | (9) | 0.27 | (15) | 0.20 | (14) | 0.24 | (17) | [34] |
| 122 | 385 | 0.504 | α-Terpinene | $C_{10}H_{16}$ | 99-86-5 | 1016 | 1021 | 0.68 | (147) | - | | - | | - | | [35] |
| 123 | 400 | 0.504 | Limonene | $C_{10}H_{16}$ | 138-86-3 | 1032 | 1027 | 0.22 | (29) | 0.91 | (14) | 0.38 | (14) | 0.46 | (6) | [35] |
| 124 | 415 | 0.528 | β-Ocimene | $C_{10}H_{16}$ | 13877-91-3 | 1048 | 1042 | 0.39 | (40) | 0.25 | (16) | 0.13 | (23) | 0.18 | (11) | [35] |
| 125 | 415 | 0.712 | Dihydromyrcenol | $C_{10}H_{20}O$ | 53219-21-9 | 1048 | 1076 | - | | 0.09 | (37) | - | | 0.15 | (13) | [36] |
| 126 | 425 | 0.520 | γ-Terpinene | $C_{10}H_{16}$ | 99-85-4 | 1058 | 1061 | 0.54 | (145) | - | | - | | - | | [35] |
| 127 | 440 | 0.648 | 6,10-Dihydromyrcenol | $C_{10}H_{22}O$ | 18479-58-8 | 1074 | 1072 | 0.87 | (14) | 0.11 | (18) | 0.10 | (4) | 0.11 | (15) | [37] |
| 128 | 455 | 0.528 | α-Terpinolene | $C_{10}H_{16}$ | 586-62-9 | 1090 | 1093 | 1.31 | (155) | 0.11 | (17) | - | | - | | [35] |
| 129 | 465 | 0.816 | Linalool | $C_{10}H_{18}O$ | 78-70-6 | 1101 | 1107 | 21.43 | (25) | 6.26 | (6) | 3.59 | (12) | 4.24 | (4) | [35] |
| 130 | 545 | 0.920 | α-Terpineol | $C_{10}H_{18}O$ | 98-55-5 | 1195 | 1206 | 2.19 | (3) | 1.70 | (16) | 0.67 | (14) | 0.88 | (14) | [38] |
| 131 | 585 | 1.016 | Nerol | $C_{10}H_{18}O$ | 106-25-2 | 1237 | 1242 | 0.55 | (26) | 0.48 | (6) | - | | 0.50 | (16) | [35] |
| 132 | 590 | 1.024 | Isogeraniol | $C_{10}H_{18}O$ | 5944-20-7 | 1248 | 1248 | 2.44 | (87) | - | | - | | - | | [39] |
| 133 | 605 | 1.048 | Geraniol | $C_{10}H_{18}O$ | 106-24-1 | 1266 | 1265 | 4.00 | (6) | 1.26 | (19) | 0.65 | (17) | 0.94 | (10) | [36] |
| 134 | 610 | 0.848 | Citral | $C_{10}H_{16}O$ | 5392-40-5 | 1272 | 1240 | 0.26 | (17) | 0.22 | (17) | - | | - | | [40] |
| 135 | 700 | 0.704 | Geranyl acetate | $C_{12}H_{20}O_2$ | 105-87-3 | 1382 | 1382 | 0.25 | (22) | - | | - | | - | | [41] |
| 136 | 760 | 0.568 | β-Farnesene | $C_{15}H_{24}$ | 28973-97-9 | 1461 | 1465 | 0.48 | (56) | 0.47 | (21) | 0.36 | (18) | 0.43 | (19) | [38] |
| 137 | 795 | 0.608 | α-Farnesene | $C_{15}H_{24}$ | 502-61-4 | 1508 | 1505 | 0.46 | (8) | - | | - | | 0.20 | (16) | [42] |
| 138 | 835 | 0.840 | Nerolidol | $C_{15}H_{26}O$ | 40716-66-3 | 1566 | 1568 | 3.44 | (22) | 2.35 | (7) | 1.30 | (18) | 1.60 | (11) | [43] |
| | | | **Subtotal (GC Peak Area)** | | | | | **40.02** | | **14.47** | | **7.40** | | **9.93** | | |
| | | | **Subtotal (%)** | | | | | **3.82** | | **1.99** | | **1.06** | | **1.30** | | |
| | | | **Esters** | | | | | | | | | | | | | |
| | | | ***Aliphatics*** | | | | | | | | | | | | | |
| 139 | 75 | 0.648 | Propyl formate | $C_4H_8O_2$ | 110-74-7 | 571 | - | - | | - | | 2.59 | (9) | 2.29 | (3) | |
| 140 | 100 | 0.456 | Ethyl acetate | $C_4H_8O_2$ | 141-78-6 | 621 | 608 | 12.72 | (14) | 16.11 | (34) | 13.43 | (16) | 12.03 | (2) | [44] |
| 141 | 135 | 0.472 | Ethyl propanoate | $C_5H_{10}O_2$ | 105-37-3 | 691 | 714 | 1.46 | (28) | 1.36 | (19) | 0.84 | (10) | 0.91 | (4) | [8] |
| 142 | 140 | 0.488 | Propyl acetate | $C_5H_{10}O_2$ | 109-60-4 | 701 | 712 | - | | - | | 0.16 | (32) | 0.15 | (7) | [10] |
| 143 | 165 | 0.464 | Ethyl isobutyrate | $C_6H_{12}O_2$ | 97-62-1 | 751 | 747 | 0.32 | (70) | 0.19 | (24) | 0.12 | (14) | 0.13 | (16) | [45] |

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 144 | 175 | 0.496 | Isobutyl acetate | $C_6H_{12}O_2$ | 110-19-0 | 771 | 770 | - | | 0.47 | (45) | 0.88 | (20) | 0.81 | (9) | [14] |
| 145 | 185 | 0.560 | Isopentyl formate | $C_6H_{12}O_2$ | 110-45-2 | 791 | 792 | 0.28 | (24) | 0.24 | (17) | 0.20 | (8) | 0.24 | (15) | [46] |
| 146 | 195 | 0.520 | Ethyl butyrate | $C_6H_{12}O_2$ | 105-54-4 | 806 | 800 | 3.69 | (20) | 3.19 | (28) | 2.46 | (14) | 2.24 | (8) | [8] |
| 147 | 200 | 0.472 | 1,1-Dimethylpropyl acetate | $C_7H_{14}O_2$ | 625-16-1 | 812 | - | - | | 0.38 | (20) | 0.39 | (6) | 0.29 | (29) | |
| 148 | 205 | 1.152 | Ethyl 2-hydroxypropanoate | $C_5H_{10}O_3$ | 97-64-3 | 819 | - | 0.04 | (18) | - | | - | | - | | |
| 149 | 230 | 0.624 | Ethyl 2-butenoate | $C_6H_{10}O_2$ | 10544-63-5 | 848 | 863 | 0.09 | (29) | 0.06 | (20) | - | | 0.06 | (9) | [47] |
| 150 | 235 | 0.496 | Ethyl 2-methylbutanoate | $C_7H_{14}O_2$ | 7452-79-1 | 854 | 846 | - | | 0.14 | (25) | - | | - | | [48] |
| 151 | 255 | 0.552 | 2/3-Methylbutyl acetate | $C_7$-$H_{14}O_2$ | 624-41-9 / 123-92-2 | 877 | 880 | 12.89 | (5) | 12.80 | (50) | 13.10 | (18) | 12.86 | (10) | [10] |
| 152 | 280 | 0.536 | Ethyl pentanoate | $C_7H_{14}O_2$ | 539-82-2 | 906 | 898 | 0.06 | (21) | - | | - | | - | | [8] |
| 153 | 290 | 0.520 | 2-Hexyl acetate | $C_8H_{16}O_2$ | 142-92-7 | 916 | 1008 | - | | - | | 0.11 | (13) | 0.11 | (37) | [8] |
| 154 | 325 | 1.112 | Methyl 2-hydroxy-4-methylpentanoate | $C_7H_{14}O_3$ | 40348-72-9 | 954 | - | - | | - | | - | | 0.30 | (7) | |
| 155 | 340 | 0.536 | Pentyl propionate | $C_8H_{16}O_2$ | 624-54-4 | 969 | 972 | 0.38 | (17) | 0.18 | (37) | - | | 0.41 | (33) | [8] |
| 156 | 345 | 0.664 | Methyl 2,4-dimethyl-3-oxopentanoate | $C_8H_{14}O_3$ | - | 974 | - | 4.93 | (19) | 6.67 | (10) | 5.92 | (6) | 6.66 | (10) | |
| 157 | 345 | 2.640 | 1,3-Propanodiol diacetate | $C_7H_{12}O_4$ | 628-66-0 | 976 | - | 0.51 | (18) | 1.02 | (21) | - | | - | | |
| 158 | 365 | 0.544 | Butyl butanoate | $C_8H_{16}O_2$ | 109-21-7 | 995 | 993 | 0.09 | (28) | 0.07 | (17) | - | | - | | [8] |
| 159 | 370 | 0.552 | Ethyl hexanoate | $C_8H_{16}O_2$ | 123-66-0 | 1001 | 996 | 14.00 | (3) | 15.61 | (10) | 14.90 | (5) | 13.04 | (3) | [8] |
| 160 | 400 | 0.720 | Butyl pivalate | $C_9H_{18}O_2$ | 5129-37-3 | 1032 | - | - | | - | | 0.08 | (32) | - | | |
| 161 | 425 | 0.528 | 3-Methylbutyl butyrate | $C_9H_{18}O_2$ | 106-27-4 | 1059 | 1060 | - | | 0.06 | (47) | - | | 0.04 | (22) | [8] |
| 162 | 440 | 0.920 | Octyl formate | $C_9H_{18}O_2$ | 112-32-3 | 1075 | 1060 | - | | - | | 1.54 | (13) | 1.23 | (18) | [8] |
| 163 | 460 | 0.560 | Ethyl heptanoate | $C_9H_{18}O_2$ | 106-30-9 | 1095 | 1095 | 0.63 | (19) | 0.61 | (9) | 0.39 | (20) | 0.37 | (27) | [8] |
| 164 | 475 | 0.584 | Heptyl acetate | $C_9H_{18}O_2$ | 112-06-1 | 1113 | 1113 | - | | 0.17 | (41) | - | | - | | [8] |
| 165 | 510 | 0.536 | Isobutyl hexanoate | $C_{10}H_{20}O_2$ | 105-79-3 | 1154 | - | 0.10 | (31) | 0.07 | (2) | - | | 0.06 | (28) | |
| 166 | 540 | 0.616 | Ethyl 7-octenoate | $C_{10}H_{18}O_2$ | 35194-38-8 | 1189 | 1186 | 0.59 | (18) | 0.54 | (15) | - | | - | | [49] |
| 167 | 545 | 0.640 | Ethyl octanoate | $C_{10}H_{20}O_2$ | 106-32-1 | 1201 | 1195 | 54.29 | (26) | 66.64 | (25) | 5.18 | (18) | 61.62 | (28) | [8] |
| 168 | 595 | 0.552 | 3-Methylbutyl hexanoate | $C_{11}H_{22}O_2$ | 2198-61-0 | 1254 | 1250 | 0.97 | (4) | 0.59 | (11) | 0.61 | (12) | 0.62 | (9) | [10] |
| 169 | 605 | 0.944 | $C_{11}$ Ester (*m/z* 42, 43, 113) | $C_{11}H_{22}O_2$ | - | 1266 | - | 0.28 | (14) | - | | - | | - | | |
| 170 | 630 | 0.560 | Propyl octanoate | $C_{11}H_{22}O_2$ | 624-13-5 | 1295 | 1290 | 2.29 | (34) | 2.26 | (4) | - | | - | | [3] |
| 171 | 630 | 0.576 | Ethyl nonanoate | $C_{11}H_{22}O_2$ | 123-29-5 | 1295 | 1294 | 2.51 | (13) | 3.64 | (20) | 3.22 | (17) | 2.63 | (20) | [10] |
| 172 | 675 | 0.552 | Butyl octanoate | $C_{12}H_{24}O_2$ | 589-75-3 | 1351 | 1387 | 0.60 | (26) | 0.31 | (31) | 0.28 | (26) | 0.30 | (20) | [50] |
| 173 | 690 | 0.848 | Butoxyethanol acetate | $C_{10}H_{20}O_4$ | 124-17-4 | 1364 | 1366 | 0.21 | (2) | - | | - | | - | | [51] |
| 174 | 700 | 0.832 | 2-Methyl, 3-hydroxy-2,4,4-trimethylpentyl propanoate | $C_{12}H_{24}O_3$ | - | 1382 | 1387 | 0.64 | (11) | - | | - | | 0.32 | (19) | [52] |
| 175 | 705 | 0.632 | Ethyl dec-9-enoate | $C_{12}H_{22}O_2$ | 67233-91-4 | 1388 | 1387 | - | | - | | 14.81 | (7) | - | | [49] |
| 176 | 710 | 0.592 | Ethyl decanoate | $C_{12}H_{24}O_2$ | 110-38-3 | 1395 | 1394 | 34.69 | (15) | 13.17 | (24) | 43.47 | (20) | 67.08 | (14) | [8] |
| 177 | 720 | 0.608 | Decyl acetate | $C_{12}H_{24}O_2$ | 112-17-4 | 1408 | 1408 | 0.32 | (12) | - | | - | | - | | [53] |
| 178 | 750 | 0.576 | 3-Methylbutyl octanoate | $C_{13}H_{26}O_2$ | 2035-99-6 | 1447 | 1444 | 3.41 | (16) | 2.11 | (39) | 1.93 | (25) | 2.00 | (19) | [44] |
| 179 | 780 | 0.608 | Propyl decanoate | $C_{13}H_{26}O_2$ | 30673-60-0 | 1488 | 1493 | 0.59 | (15) | - | | - | | 0.15 | (27) | [46] |
| 180 | 820 | 0.616 | 2-Methylpropyl decanoate | $C_{14}H_{28}O_2$ | 30673-38-2 | 1544 | 1545 | 0.29 | (34) | - | | - | | - | | [54] |
| 181 | 855 | 0.624 | Ethyl dodecanoate | $C_{14}H_{28}O_2$ | 106-33-2 | 1594 | 1595 | 7.99 | (29) | 3.88 | (30) | 2.69 | (11) | 3.81 | (41) | [8] |
| 182 | 865 | 0.704 | Dodecyl acetate | $C_{14}H_{28}O_2$ | 112-66-3 | 1608 | 1609 | 0.56 | (26) | - | | - | | - | | [55] |
| 183 | 890 | 0.688 | 3-Methylbutyl decanoate | $C_{15}H_{30}O_2$ | - | 1641 | 1647 | - | | 0.59 | (6) | 0.72 | (25) | 0.81 | (22) | [56] |
| | | | ***Aromatics*** | | | | | | | | | | | | | |
| 184 | 460 | 1.056 | Methyl benzoate | $C_8H_8O_2$ | 93-58-3 | 1096 | 1091 | 4.19 | (9) | 2.49 | (2) | 2.36 | (11) | 2.74 | (16) | [8] |
| 185 | 520 | 1.112 | Benzyl acetate | $C_9H_{10}O_2$ | 140-11-4 | 1166 | 1163 | 0.25 | (23) | - | | - | | - | | [8] |
| 186 | 525 | 0.944 | Ethyl benzoate | $C_9H_{10}O_2$ | 93-89-0 | 1172 | 1170 | 0.12 | (2) | 0.08 | (20) | - | | - | | [8] |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 187 | 590 | 1.000 | Ethylphenyl acetate | $C_{10}H_{12}O_2$ | 101-97-3 | 1248 | 1244 | 0.25 | (18) | - | | 0.07 | (18) | 0.12 | (45) [10] |
| 188 | 600 | 1.040 | 2-Phenylethyl acetate | $C_{10}H_{12}O_2$ | 103-45-7 | 1260 | 1256 | 4.34 | (3) | 1.43 | (15) | 2.37 | (32) | 3.11 | (40) [8] |
| 189 | 675 | 0.960 | Ethyl 3-phenylpropanoate | $C_{11}H_{14}O_2$ | 2021-28-5 | 1351 | 1353 | 0.06 | (16) | - | | - | | - | [57] |
| 190 | 675 | 1.056 | Methyl 3,4-dimethylbenzoate | $C_{10}H_{12}O_2$ | 38404-42-1 | 1351 | 1353 | 0.37 | (14) | 0.24 | (19) | 0.16 | (8) | 0.19 | (6) [8] |
| 191 | 680 | 0.952 | 2-Phenylethyl propionate | $C_{11}H_{14}O_2$ | 122-70-3 | 1357 | 1350 | 0.05 | (41) | - | | - | | - | [8] |
| 192 | 745 | 0.936 | 2-Phenylethyl butanonate | $C_{12}H_{16}O_2$ | 103-52-6 | 1441 | 1439 | 0.06 | (7) | - | | - | | - | [8] |
| | | | **Subtotal (GC Peak Area)** | | | | | **172.09** | | **157.38** | | **134.98** | | **199.75** | |
| | | | **Subtotal (%)** | | | | | **16.41** | | **21.59** | | **19.39** | | **26.14** | |
| | | | **Ethers** | | | | | | | | | | | | |
| 193 | 100 | 0.376 | 2-Ethoxy-2-methylpropane | $C_6H_{14}O$ | 637-92-3 | 621 | 620 | 2.06 | (5) | 2.17 | (12) | 3.17 | (32) | 2.89 | (44) [58] |
| 194 | 120 | 0.392 | 2-Methoxy-2-methylbutane | $C_6H_{14}O$ | 994-05-8 | 661 | 642 | 0.21 | (9) | 0.38 | (11) | 0.34 | (38) | 0.32 | (50) [12] |
| 195 | 135 | 0.392 | 2-Methyl-2-(1-methylethoxy)propane | $C_7H_{16}O$ | 17348-59-3 | 691 | - | 0.24 | (57) | 0.31 | (44) | 0.28 | (35) | 0.26 | (49) |
| 196 | 305 | 0.480 | 1-Butoxypent-2-ene | $C_9H_{18}O$ | - | 932 | - | 0.17 | (9) | - | | - | | - | |
| 197 | 345 | 0.464 | 1-(1-Ethoxyethoxy)pentane | $C_9H_{20}O_2$ | 13442-89-2 | 974 | 977 | 0.25 | (46) | 0.23 | (38) | 0.15 | (21) | 0.19 | (24) [1] |
| 198 | 470 | 0.536 | 2,5-Dimethoxy-2,5-dimethylhexane | $C_{10}H_{22}O_2$ | 53273-13-5 | 1107 | - | 0.06 | (19) | 0.07 | (65) | - | | 0.03 | (10) |
| | | | **Subtotal (GC Peak Area)** | | | | | **2.99** | | **3.15** | | **3.94** | | **3.70** | |
| | | | **Subtotal (%)** | | | | | **0.28** | | **0.43** | | **0.57** | | **0.48** | |
| | | | **Furan-type compounds** | | | | | | | | | | | | |
| 199 | 165 | 0.408 | Tetrahydro-2,2,5,5-tetramethylfuran | $C_8H_{16}O$ | 15045-43-9 | 751 | - | 3.16 | (39) | 3.39 | (19) | 3.64 | (11) | 3.58 | (33) |
| 200 | 170 | 0.752 | 2-Vinylfuran | $C_6H_6O$ | 1487-18-9 | 762 | 761 | 0.05 | (11) | - | | - | | - | [24] |
| 201 | 200 | 0.920 | Dihydro-2-methyl-3-furanone | $C_5H_8O_2$ | 3188-00-9 | 813 | 804 | 0.15 | (48) | - | | - | | - | [10] |
| 202 | 290 | 1.472 | 1-(2-Furanyl)-ethanone | $C_6H_6O_2$ | 1192-62-7 | 917 | 917 | 0.17 | (50) | - | | - | | - | [59] |
| 203 | 370 | 0.712 | (5-Methyl-2-furyl)methanethiol | $C_6H_8OS$ | 59303-05-8 | 1001 | 995 | 0.97 | (37) | - | | - | | - | [60] |
| 204 | 465 | 0.464 | 2,2,4,4-Tetramethyltetrahydrofuran | $C_8H_{16}O$ | 3358-28-9 | 1101 | - | 0.22 | (52) | 0.20 | (40) | 0.21 | (22) | 0.15 | (20) |
| 205 | 575 | 1.256 | 3-Phenylfuran | $C_{10}H_8O$ | 13679-41-9 | 1231 | 1228 | 0.26 | (8) | 0.14 | (16) | 0.07 | (34) | 0.06 | (39) [29] |
| 206 | 580 | 0.632 | 2,2,3,3,4,4-Hexamethyltetrahydrofuran | $C_{10}H_{20}O$ | - | 1236 | - | 0.82 | (4) | - | | - | | - | |
| 207 | 600 | 1.360 | 5-Butyldihydrofuran-2-one | $C_8H_{14}O_2$ | 104-50-7 | 1260 | 1260 | 0.08 | (27) | - | | - | | - | [10] |
| 208 | 655 | 0.784 | 2,2,4-Trimethyl-5-(2,2-dimethylpropyl)-3-furanone | $C_{12}H_{20}O_2$ | - | 1326 | - | 1.20 | (13) | - | | 0.66 | (15) | 0.76 | (12) |
| | | | **Subtotal (GC Peak Area)** | | | | | **7.08** | | **3.72** | | **4.57** | | **4.56** | |
| | | | **Subtotal (%)** | | | | | **0.68** | | **0.51** | | **0.66** | | **0.60** | |
| | | | **Hydrocarbons** | | | | | | | | | | | | |
| | | | ***Aliphatics*** | | | | | | | | | | | | |
| 209 | 170 | 0.384 | 2,3-Dimethylhexane | $C_8H_{18}$ | 584-94-1 | 761 | 758 | - | | 0.37 | (10) | - | | - | [27] |
| 210 | 225 | 0.408 | 2,4-Dimethyl-1-heptene | $C_9H_{18}$ | 19549-87-2 | 842 | 836 | 1.14 | (98) | 1.16 | (11) | 0.35 | (15) | 0.44 | (20) [20] |
| 211 | 245 | 0.384 | 4-Methyloctane | $C_9H_{20}$ | 2216-34-4 | 865 | 864 | - | | 0.65 | (68) | - | | - | [61] |
| 212 | 280 | 0.400 | Nonane | $C_9H_{20}$ | 111-84-2 | 906 | 900 | - | | 0.06 | (19) | 0.19 | (8) | 0.15 | (18) [20] |
| 213 | 335 | 0.408 | 2-Methylnonane | $C_{10}H_{22}$ | 871-83-0 | 964 | 969 | - | | 0.29 | (15) | 0.21 | (8) | 0.14 | (12) [20] |
| 214 | 370 | 0.400 | Decane | $C_{10}H_{22}$ | 124-18-5 | 1000 | 1000 | - | | 0.16 | (20) | 0.27 | (36) | 0.22 | (9) [62] |
| 215 | 405 | 0.432 | 3-Undecene | $C_{11}H_{22}$ | 821-97-6 | 1037 | - | 0.16 | (15) | - | | 0.14 | (6) | 0.16 | (15) |
| 216 | 445 | 0.424 | 7-Methyl-2-decene | $C_{11}H_{22}$ | 74630-23-2 | 1079 | - | 0.37 | (35) | 0.88 | (1) | 0.31 | (51) | 0.23 | (15) |
| 217 | 455 | 0.480 | $C_{11}$ Hydrocarbon (*m/z* 41,67, 109) | $C_{11}H_{22}$ | - | 1090 | - | - | | - | | 0.14 | (35) | 0.21 | (16) |
| 218 | 465 | 0.424 | Undecane | $C_{11}H_{24}$ | 1120-21-4 | 1101 | 1101 | - | | - | | 0.90 | (13) | - | [17] |
| 219 | 520 | 0.424 | 2-Methylundecane | $C_{12}H_{26}$ | 7045-71-8 | 1165 | 1165 | 0.10 | (7) | - | | 0.15 | (18) | 0.11 | (10) [27] |
| 220 | 555 | 0.432 | Dodecane | $C_{12}H_{26}$ | 112-40-3 | 1206 | 1201 | 0.80 | (25) | 0.80 | (44) | 0.97 | (13) | 0.71 | (4) [17] |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 221 | 620 | 0.424 | Tridecane | $C_{13}H_{28}$ | 629-50-5 | 1301 | 1301 | 0.43 (8) | 0.32 (3) | 0.39 (15) | 0.35 (11) | [15] |
| 222 | 790 | 0.480 | Pentadecane | $C_{15}H_{32}$ | 629-62-9 | 1501 | 1500 | 0.39 (18) | 0.43 (10) | 0.40 (36) | 0.37 (11) | [62] |
| 223 | 860 | 0.512 | Hexadecane | $C_{16}H_{34}$ | 544-76-3 | 1601 | 1600 | - | 0.41 (5) | - | 0.42 (5) | [62] |
| | | | ***Aromatics*** | | | | | | | | | |
| 224 | 250 | 0.576 | 1,3-Dimethylbenzene | $C_8H_{10}$ | 108-38-3 | 871 | 874 | 1.21 (8) | - | 1.25 (9) | 1.15 (16) | [3] |
| 225 | 270 | 0.616 | 1,2-Dimethylbenzene | $C_8H_{10}$ | 95-47-6 | 895 | 908 | 1.42 (6) | 1.55 (17) | 1.37 (12) | 1.23 (12) | [63] |
| 226 | 270 | 0.728 | Ethenylbenzene | $C_8H_8$ | 100-42-5 | 895 | 891 | 1.72 (20) | 1.41 (31) | - | - | [10] |
| 227 | 390 | 0.656 | 1,2,3-Trimethylbenzene | $C_9H_{12}$ | 526-73-8 | 1021 | 1022 | 1.06 (9) | 1.17 (23) | 1.21 (15) | 1.05 (11) | [64] |
| 228 | 450 | 0.616 | 1-Ethyl-2,3-dimethylbenzene | $C_{10}H_{14}$ | 933-98-2 | 1085 | 1094 | - | 0.04 (32) | - | - | [27] |
| 229 | 455 | 0.704 | 1-Methyl-4-(1-methylethenyl)-benzene | $C_{10}H_{12}$ | 1195-32-0 | 1090 | 1090 | - | - | 0.08 (13) | - | [65] |
| 230 | 540 | 1.104 | Naphthalene | $C_{10}H_8$ | 91-20-3 | 1190 | 1179 | 0.52 (16) | 0.52 (17) | 0.55 [8] | 0.86 (58) | [8] |
| 231 | 600 | 0.520 | 1,3-bis(1,1-Dimethylethyl)benzene | $C_{14}H_{22}$ | 1014-60-4 | 1259 | - | 5.00 (10) | 5.41 (9) | 4.90 (10) | 4.06 (10) | |
| 232 | 700 | 1.136 | Biphenyl | $C_{12}H_{10}$ | 92-52-4 | 1383 | 1385 | 0.26 (12) | 0.21 (19) | 0.15 (14) | 0.15 (18) | [16] |
| | | | ***Cyclics*** | | | | | | | | | |
| 233 | 495 | 0.904 | 1,2-Dimethyl-1-pentyl-cyclopropane | $C_{10}H_{20}$ | 62238-04-4 | 1136 | - | - | - | 6.18 (5) | - | |
| 234 | 500 | 0.864 | 1-Methylpentyl cyclopropane | $C_9H_{18}$ | 6976-28-9 | 1142 | - | 20.63 (26) | 20.57 (3) | - | - | |
| 235 | 640 | 0.448 | 1-Butyl-2-propyl-cyclopentane | $C_{12}H_{24}$ | 62199-50-2 | 1307 | - | - | - | - | 0.08 (14) | |
| | | | **Subtotal (GC Peak Area)** | | | | | **35.22** | **36.42** | **20.10** | **12.08** | |
| | | | **Subtotal (%)** | | | | | **3.36** | **5.00** | **2.89** | **1.58** | |
| | | | **Pyrans** | | | | | | | | | |
| 236 | 275 | 0.488 | 2,2,4,6-Tetramethyl-2H-pyran | $C_9H_{14}O$ | - | 901 | - | - | 0.21 (11) | - | - | |
| 237 | 295 | 0.512 | 2,2,6-Trimethyl-4-methylene-2H-pyran | $C_9H_{14}O$ | - | 922 | - | 0.14 (17) | 0.15 (3) | - | - | |
| 238 | 340 | 0.864 | 2,5-Dimethyl-2-hydroxymethyltetrahydropyran | $C_8H_{16}O_2$ | - | 969 | - | 1.13 (13) | 1.21 (5) | 1.01 (15) | 1.09 (5) | |
| | | | **Subtotal (GC Peak Area)** | | | | | **1.27** | **1.56** | **1.01** | **1.09** | |
| | | | **Subtotal (%)** | | | | | **0.12** | **0.21** | **0.14** | **0.14** | |
| | | | **Pyrazines** | | | | | | | | | |
| 239 | 295 | 0.824 | Ethylpyrazine | $C_6H_8N_2$ | 13925-00-3 | 922 | 920 | 0.10 (32) | - | - | - | [8] |
| 240 | 295 | 0.856 | 2,3-Dimethylpyrazine | $C_6H_8N_2$ | 5910-89-4 | 922 | 920 | 0.08 (28) | - | - | - | [25] |
| 241 | 370 | 0.776 | 2-Ethyl-5-methylpyrazine | $C_7H_{10}N_2$ | 13360-64-0 | 1001 | 1000 | 1.05 (29) | 0.13 (64) | - | 0.11 (46) | [8] |
| 242 | 375 | 0.784 | Trimethylpyrazine | $C_7H_{10}N_2$ | 14667-55-1 | 1006 | 999 | 0.66 (17) | 0.10 (38) | 0.16 (16) | 0.16 (31) | [29] |
| 243 | 390 | 0.952 | 2-Ethenyl-5-methylpyrazine | $C_7H_8N_2$ | 13925-08-1 | 1022 | 1022 | 0.49 (9) | - | - | - | [8] |
| 244 | 420 | 0.704 | 2-Methyl-3-isopropylpyrazine | $C_8H_{12}N_2$ | 15986-81-9 | 1053 | 1056 | 0.35 (20) | 0.09 (27) | - | 0.08 (36) | [66] |
| 245 | 445 | 0.712 | 3-Ethyl-2,5-dimethylpyrazine | $C_8H_{12}N_2$ | 13360-65-1 | 1080 | 1079 | 1.33 (36) | - | - | - | [67] |
| 246 | 515 | 0.672 | 3,5-Diethyl-2-methylpyrazine | $C_9H_{14}N_2$ | 18138-05-1 | 1160 | 1160 | 0.25 (5) | - | - | - | [68] |
| 247 | 555 | 0.648 | 2,5-dimethyl-3-(2-methylpropyl)pyrazine | $C_{10}H_{16}N_2$ | 32736-94-0 | 1207 | 1207 | 0.08 (30) | - | - | - | [69] [70] |
| 248 | 600 | 0.688 | 2-Butyl-3,5-dimethylpyrazine | $C_{10}H_{16}N_2$ | 50888-63-6 | 1260 | 1254 | 0.14 (16) | - | - | - | [71] |
| | | | **Subtotal (GC Peak Area)** | | | | | **4.51** | **0.32** | **0.16** | **0.36** | |
| | | | **Subtotal (%)** | | | | | **0.43** | **0.04** | **0.02** | **0.05** | |
| | | | **S-compounds** | | | | | | | | | |
| 249 | 155 | 0.600 | Methyldisulfide | $C_2H_6S_2$ | 624-92-0 | 731 | 738 | 0.17 (28) | 0.09 (25) | - | 0.07 (11) | [72] |
| 250 | 285 | 0.952 | 1,3-Oxathiane | $C_4H_8OS$ | - | 912 | - | 2.59 (18) | 1.27 (14) | 0.74 (16) | 0.80 (14) | |
| 251 | 360 | 1.168 | Dihydro-2-methylthiophen-3(2H)-one | $C_5H_8OS$ | 13679-85-1 | 991 | 994 | 0.87 (80) | 1.19 (25) | 0.46 (20) | 0.53 (13) | [25] |
| 252 | 360 | 2.200 | 3-(Methylthio)propanol | $C_4H_{10}OS$ | 505-10-2 | 987 | 978 | 5.30 (5) | 2.37 (56) | - | - | [2] |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 253 | 385 | 1.536 | 2-Acetylthiazole | $C_5H_5NOS$ | 24295-03-2 | 1017 | 1014 | 0.27 (6) | - | - | - | [8] |
| 254 | 485 | 0.968 | 3-(Methylthio)propyl acetate | $C_6H_{12}O_2S$ | 16630-55-0 | 1125 | 1123 | 0.13 (26) | - | - | - | [40] |
| 255 | 485 | 1.640 | 3-Methyl-2-thiophenecarboxaldehyde | $C_6H_6OS$ | 5834-16-2 | 1126 | 1133 | 0.08 (11) | - | - | - | [25] |
| 256 | 545 | 1.256 | Benzothiofuran | $C_8H_6S$ | 95-15-8 | 1196 | 1172 | 0.09 (18) | - | - | - | [73] |
| 257 | 575 | 1.648 | Benzothiazole | $C_7H_5NS$ | 95-16-9 | 1231 | 1223 | 0.14 (14) | 0.10 (34) | - | - | [20] |
| | | | **Subtotal (GC Peak Area)** | | | | | **9.65** | **5.02** | **1.20** | **1.39** | |
| | | | **Subtotal (%)** | | | | | **0.92** | **0.69** | **0.17** | **0.18** | |
| | | | **Total** | | | | | **1048.64** | **728.89** | **696.06** | **764.00** | |
| | | | **Number of identified compounds** | | | | | **210** | **170** | **156** | **172** | |

[a] Retention times for first ($^1t_R$) and second ($^2t_R$) dimensions in seconds.

[b] Mean of three independent assays (n=3).

[c] Retention Index obtained through the modulated chromatogram.

[d] RI, Retention Index reported in the literature for Equity-5 column or equivalents:


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