**Supplementary Materials**

**Comparative evaluation of triacylglycerols, fatty acids, and volatile organic compounds as markers for authenticating sesame oil**

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Analytical ion chromatograms of identified volatile organic compound compositions in oil samples analyzed in this study. Unique mass was used for calculations for a particular peak.

**Supplementary Table 1.** Triacyglycerol compositions (%) in edible oils selected for multivariate analysis in this study

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Oil sample*a* | LLLn | LLL | PLL | OOL | OOO | POO |
| SSO 1 | nd | 13.06 | 5.14 | 22.56 | 7.25 | 9.15 |
| SSO 2 | nd | 15.29 | 5.77 | 21.48 | 7.66 | 7.67 |
| SSO 3 | nd | 13.44 | 5.18 | 21.64 | 7.12 | 9.41 |
| SSO 4 | nd | 10.22 | 4.54 | 23.40 | 9.85 | 11.74 |
| SSO 5 | nd | 9.96 | 4.80 | 23.56 | 9.90 | 11.27 |
| SSO 6 | nd | 9.64 | 5.02 | 23.75 | 10.96 | 11.31 |
| CO 1 | nd | 18.68 | 12.72 | 16.78 | 5.41 | 4.05 |
| CO 2 | nd | 16.10 | 11.99 | 17.51 | 4.97 | 4.77 |
| CO 3 | nd | 22.95 | 13.93 | 13.73 | 3.39 | 2.67 |
| SSO:CO (95:5) | nd | 11.58 | 5.05 | 23.30 | 8.79 | 9.05 |
| SSO:CO (95:5) | nd | 12.49 | 5.11 | 22.72 | 7.91 | 9.57 |
| SSO:CO (95:5) | nd | 14.22 | 5.67 | 21.34 | 7.05 | 8.99 |
| SSO:CO (95:5) | nd | 9.11 | 4.18 | 26.80 | 9.41 | 10.22 |
| SSO:CO (95:5) | nd | 11.06 | 5.04 | 21.83 | 7.79 | 10.49 |
| SSO:CO (95:5) | nd | 10.60 | 5.06 | 23.28 | 8.96 | 10.89 |
| SSO:CO (90:10) | nd | 12.42 | 5.31 | 22.57 | 8.75 | 8.96 |
| SSO:CO (90:10) | nd | 13.00 | 5.42 | 22.38 | 8.07 | 9.39 |
| SSO:CO (90:10) | nd | 14.63 | 5.97 | 21.01 | 6.78 | 8.15 |
| SSO:CO (90:10) | nd | 10.22 | 4.56 | 24.03 | 8.07 | 9.98 |
| SSO:CO (90:10) | nd | 12.03 | 6.16 | 21.42 | 7.72 | 9.48 |
| SSO:CO (90:10) | nd | 10.77 | 5.77 | 23.42 | 8.02 | 10.47 |
| SSO:CO (80:20) | nd | 12.72 | 6.00 | 22.24 | 8.34 | 8.15 |
| SSO:CO (80:20) | nd | 13.23 | 5.82 | 21.88 | 7.20 | 8.33 |
| SSO:CO (80:20) | nd | 11.75 | 6.20 | 22.95 | 7.77 | 8.05 |
| SSO:CO (80:20) | nd | 10.63 | 4.86 | 25.25 | 7.62 | 9.48 |
| SSO:CO (80:20) | nd | 12.45 | 6.64 | 21.66 | 7.22 | 8.42 |
| SSO:CO (80:20) | nd | 11.76 | 6.20 | 22.98 | 7.67 | 8.06 |
| SBO 1 | 4.50 | 24.18 | 14.71 | 10.13 | 4.01 | 5.07 |
| SBO 2 | 5.29 | 27.30 | 14.49 | 8.97 | 3.27 | 4.20 |
| SBO 3 | 4.21 | 26.40 | 14.69 | 8.76 | 4.74 | 3.81 |
| SSO:SBO (95:5) | nd | 12.71 | 4.58 | 23.27 | 6.44 | 8.87 |
| SSO:SBO (95:5) | 0.10 | 14.70 | 5.75 | 22.73 | 8.55 | 9.43 |
| SSO:SBO (95:5) | nd | 13.33 | 4.88 | 20.83 | 5.09 | 11.95 |
| SSO:SBO (95:5) | 0.10 | 8.74 | 5.28 | 24.43 | 10.29 | 10.99 |
| SSO:SBO (95:5) | 0.05 | 11.43 | 4.43 | 22.55 | 7.10 | 10.23 |
| SSO:SBO (95:5) | nd | 11.10 | 3.84 | 19.11 | 9.46 | 9.95 |
| SSO:SBO (90:10) | nd | 13.17 | 5.01 | 22.29 | 7.16 | 8.82 |
| SSO:SBO (90:10) | 0.19 | 15.52 | 6.66 | 20.66 | 9.47 | 10.56 |
| SSO:SBO (90:10) | nd | 14.16 | 4.62 | 19.81 | 6.58 | 8.60 |
| SSO:SBO (90:10) | 0.17 | 12.58 | 5.47 | 23.13 | 9.58 | 10.75 |
| SSO:SBO (90:10) | 0.01 | 12.04 | 5.23 | 22.69 | 6.29 | 8.75 |
| SSO:SBO (90:10) | nd | 12.03 | 4.44 | 23.01 | 8.81 | 9.79 |
| SSO:SBO (80:20) | nd | 13.76 | 6.02 | 21.83 | 7.05 | 8.31 |
| SSO:SBO (80:20) | 0.41 | 15.78 | 6.88 | 20.65 | 8.01 | 8.86 |
| SSO:SBO (80:20) | 1.05 | 18.67 | 4.36 | 15.78 | 13.58 | 9.79 |
| SSO:SBO (80:20) | 0.39 | 13.75 | 6.22 | 21.87 | 8.73 | 10.16 |
| SSO:SBO (80:20) | 0.36 | 15.52 | 5.52 | 17.41 | 8.95 | 11.65 |
| SSO:SBO (80:20) | 0.45 | 14.07 | 6.69 | 21.69 | 8.14 | 10.05 |

*a* Each sample was analyzed in triplicate.

SSO, sesame oil; CO, corn oil; SBO, soybean oil.

nd: not detected.

**Supplementary Table 2**. Fatty acid compositions (%) in edible oils selected for multivariate analysis in this study

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Oil sample*a* | C16:0 | C18:0 | C18:1(n-7) | C18:2 | C18:3(n-3) | C20:2 | C22:2 |
| SSO 1 | 8.78 | 5.31 | 0.80 | 45.29 | 0.33 | 0.17 | 0.13 |
| SSO 2 | 8.87 | 5.03 | 0.83 | 45.85 | 0.35 | 0.18 | 0.13 |
| SSO 3 | 8.84 | 5.15 | 0.82 | 46.03 | 0.36 | 0.18 | 0.16 |
| SSO 4 | 9.16 | 5.54 | 0.83 | 42.91 | 0.30 | 0.22 | 0.14 |
| SSO 5 | 9.11 | 5.84 | 0.80 | 43.63 | 0.31 | 0.25 | 0.14 |
| SSO 6 | 9.19 | 5.70 | 0.85 | 42.98 | 0.30 | 0.23 | 0.14 |
| CO 1 | 11.24 | 2.04 | 0.67 | 51.13 | 1.09 | 0.41 | 0.21 |
| CO 2 | 11.08 | 1.92 | 0.62 | 53.21 | 1.04 | 0.29 | 0.18 |
| CO 3 | 10.97 | 1.78 | 0.57 | 55.26 | 1.01 | 0.29 | 0.17 |
| SSO:CO (95:5) | 8.90 | 5.18 | 0.87 | 46.24 | 0.30 | 0.16 | 0.12 |
| SSO:CO (95:5) | 9.28 | 5.15 | 0.87 | 44.72 | 0.37 | 0.21 | 0.11 |
| SSO:CO (95:5) | 9.20 | 5.02 | 0.87 | 46.59 | 0.35 | 0.16 | 0.08 |
| SSO:CO (95:5) | 9.52 | 5.51 | 0.90 | 42.45 | 0.33 | 0.25 | 0.12 |
| SSO:CO (95:5) | 9.62 | 5.74 | 0.85 | 43.77 | 0.37 | 0.26 | 0.11 |
| SSO:CO (95:5) | 9.67 | 5.40 | 0.89 | 42.87 | 0.35 | 0.23 | 0.10 |
| SSO:CO (90:10) | 8.93 | 4.99 | 0.81 | 46.30 | 0.39 | 0.17 | 0.16 |
| SSO:CO (90:10) | 9.42 | 4.98 | 0.85 | 45.17 | 0.42 | 0.20 | 0.13 |
| SSO:CO (90:10) | 9.31 | 4.86 | 0.86 | 47.02 | 0.37 | 0.15 | 0.11 |
| SSO:CO (90:10) | 9.65 | 5.28 | 0.91 | 43.00 | 0.38 | 0.26 | 0.11 |
| SSO:CO (90:10) | 10.06 | 4.77 | 0.92 | 44.73 | 0.38 | 0.27 | 0.12 |
| SSO:CO (90:10) | 9.78 | 5.20 | 0.86 | 43.48 | 0.38 | 0.25 | 0.12 |
| SSO:CO (80:20) | 9.29 | 4.68 | 0.78 | 46.72 | 0.47 | 0.21 | 0.15 |
| SSO:CO (80:20) | 9.62 | 4.68 | 0.82 | 45.99 | 0.48 | 0.21 | 0.13 |
| SSO:CO (80:20) | 9.53 | 4.52 | 0.82 | 47.86 | 0.45 | 0.21 | 0.11 |
| SSO:CO (80:20) | 9.88 | 4.94 | 0.87 | 43.82 | 0.46 | 0.26 | 0.11 |
| SSO:CO (80:20) | 10.19 | 4.42 | 0.89 | 45.74 | 0.45 | 0.29 | 0.12 |
| SSO:CO (80:20) | 9.95 | 4.78 | 0.83 | 44.93 | 0.46 | 0.26 | 0.11 |
| SBO 1 | 10.49 | 4.19 | 1.42 | 54.04 | 5.65 | 0.31 | 0.46 |
| SBO 2 | 10.73 | 4.07 | 1.46 | 53.42 | 5.29 | 0.32 | 0.53 |
| SBO 3 | 10.49 | 4.17 | 1.42 | 54.29 | 5.64 | 0.29 | 0.46 |
| SSO:SBO (95:5) | 8.76 | 5.27 | 0.85 | 46.20 | 0.57 | 0.17 | 0.15 |
| SSO:SBO (95:5) | 9.21 | 5.27 | 0.90 | 44.73 | 0.58 | 0.21 | 0.14 |
| SSO:SBO (95:5) | 9.16 | 5.13 | 0.91 | 46.55 | 0.55 | 0.18 | 0.11 |
| SSO:SBO (95:5) | 9.52 | 5.59 | 0.96 | 42.58 | 0.55 | 0.23 | 0.12 |
| SSO:SBO (95:5) | 9.94 | 5.04 | 0.98 | 44.37 | 0.56 | 0.25 | 0.12 |
| SSO:SBO (95:5) | 9.64 | 5.52 | 0.94 | 42.82 | 0.59 | 0.23 | 0.12 |
| SSO:SBO (90:10) | 8.87 | 5.20 | 0.88 | 46.62 | 0.82 | 0.18 | 0.17 |
| SSO:SBO (90:10) | 9.33 | 5.22 | 0.93 | 45.14 | 0.82 | 0.21 | 0.14 |
| SSO:SBO (90:10) | 9.24 | 5.09 | 0.94 | 46.92 | 0.83 | 0.20 | 0.12 |
| SSO:SBO (90:10) | 9.59 | 5.52 | 0.98 | 43.11 | 0.78 | 0.25 | 0.13 |
| SSO:SBO (90:10) | 9.96 | 5.00 | 1.00 | 44.91 | 0.83 | 0.24 | 0.13 |
| SSO:SBO (90:10) | 9.69 | 5.47 | 0.95 | 43.39 | 0.84 | 0.23 | 0.13 |
| SSO:SBO (80:20) | 9.09 | 5.08 | 0.93 | 47.47 | 1.35 | 0.17 | 0.21 |
| SSO:SBO (80:20) | 9.55 | 5.09 | 0.99 | 46.01 | 1.30 | 0.23 | 0.18 |
| SSO:SBO (80:20) | 9.41 | 4.99 | 0.99 | 47.72 | 1.35 | 0.19 | 0.16 |
| SSO:SBO (80:20) | 9.75 | 5.37 | 1.03 | 44.21 | 1.27 | 0.25 | 0.17 |
| SSO:SBO (80:20) | 10.08 | 4.91 | 1.04 | 45.94 | 1.38 | 0.26 | 0.16 |
| SSO:SBO (80:20) | 9.83 | 5.32 | 1.02 | 44.51 | 1.36 | 0.24 | 0.18 |

*a* Each sample was analyzed in triplicate.

SSO, sesame oil; CO, corn oil; SBO, soybean oil.

**Supplementary Table 3**. Volatile organic compound compositions (a.u. $×$ 104) in edible oils selected for multivariate analysis in this study

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Oil sample*a* | Pyridine | Pyrazine | Thiazole | 2-Methyl pyrazine | 2,3-Dimethyl pyrazine | 2-Propenal |
| SSO 1 | 106.24 | 202.88 | 48.55 | 2390.14 | 139.13 | nd |
| SSO 2 | 158.57 | 425.30 | 130.73 | 4157.86 | 178.86 | nd |
| SSO 3 | 126.72 | 408.92 | 100.80 | 3595.92 | 143.30 | nd |
| SSO 4 | 156.87 | 623.52 | 134.50 | 5622.57 | 209.37 | nd |
| SSO 5 | 129.51 | 462.90 | 82.36 | 3173.84 | 147.00 | nd |
| SSO 6 | 94.95 | 462.55 | 74.58 | 2890.77 | 134.98 | nd |
| CO 1 | nd | nd | nd | nd | nd | 45.08 |
| CO 2 | nd | nd | nd | nd | nd | 19.95 |
| CO 3 | nd | nd | nd | nd | nd | 10.44 |
| SSO:CO (95:5) | 89.09 | 176.72 | 40.13 | 2112.51 | 124.66 | 0.73 |
| SSO:CO (95:5) | 150.45 | 407.11 | 120.63 | 4110.03 | 181.63 | 0.47 |
| SSO:CO (95:5) | 118.07 | 399.37 | 94.64 | 3581.27 | 148.04 | 0.55 |
| SSO:CO (95:5) | 82.72 | 420.80 | 66.51 | 2596.37 | 120.27 | 1.04 |
| SSO:CO (95:5) | 138.37 | 574.41 | 119.73 | 5167.81 | 194.58 | 0.71 |
| SSO:CO (95:5) | 118.04 | 444.18 | 76.35 | 3057.43 | 141.31 | 0.65 |
| SSO:CO (90:10) | 94.03 | 186.54 | 42.36 | 2229.88 | 131.58 | 0.78 |
| SSO:CO (90:10) | 158.81 | 429.73 | 127.33 | 4338.36 | 191.72 | 0.49 |
| SSO:CO (90:10) | 124.63 | 421.55 | 99.90 | 3780.23 | 156.26 | 0.58 |
| SSO:CO (90:10) | 87.31 | 444.18 | 70.21 | 2740.61 | 126.96 | 1.10 |
| SSO:CO (90:10) | 146.06 | 606.32 | 126.38 | 5454.92 | 205.39 | 0.75 |
| SSO:CO (90:10) | 124.60 | 468.86 | 80.59 | 3227.29 | 149.16 | 0.69 |
| SSO:CO (80:20) | 105.79 | 209.86 | 47.65 | 2508.61 | 148.03 | 0.87 |
| SSO:CO (80:20) | 178.66 | 483.44 | 143.25 | 4880.66 | 215.68 | 0.55 |
| SSO:CO (80:20) | 140.20 | 474.25 | 112.39 | 4252.76 | 175.80 | 0.66 |
| SSO:CO (80:20) | 98.23 | 499.70 | 78.98 | 3083.19 | 142.83 | 1.24 |
| SSO:CO (80:20) | 164.31 | 682.11 | 142.17 | 6136.78 | 231.07 | 0.84 |
| SSO:CO (80:20) | 140.17 | 527.47 | 90.66 | 3630.70 | 167.81 | 0.77 |
| SBO 1 | nd | nd | nd | nd | nd | 100.18 |
| SBO 2 | nd | nd | nd | nd | nd | 17.43 |
| SBO 3 | nd | nd | nd | nd | nd | 74.17 |
| SSO:SBO (95:5) | 101.49 | 194.43 | 44.07 | 2365.52 | 141.31 | 1.26 |
| SSO:SBO (95:5) | 140.80 | 398.97 | 114.36 | 4142.73 | 183.45 | 0.58 |
| SSO:SBO (95:5) | 115.69 | 376.64 | 86.89 | 3484.10 | 146.37 | 1.42 |
| SSO:SBO (95:5) | 81.17 | 407.52 | 63.58 | 2535.68 | 118.58 | 0.65 |
| SSO:SBO (95:5) | 139.44 | 567.44 | 116.42 | 5206.00 | 197.51 | 1.06 |
| SSO:SBO (95:5) | 109.11 | 411.67 | 69.14 | 2898.39 | 136.54 | 1.39 |
| SSO:SBO (90:10) | 107.13 | 205.23 | 46.52 | 2496.94 | 149.16 | 1.33 |
| SSO:SBO (90:10) | 148.63 | 421.13 | 120.71 | 4372.88 | 193.64 | 0.62 |
| SSO:SBO (90:10) | 122.12 | 397.57 | 91.72 | 3677.66 | 154.51 | 1.50 |
| SSO:SBO (90:10) | 85.68 | 430.16 | 67.11 | 2676.55 | 125.16 | 0.69 |
| SSO:SBO (90:10) | 147.18 | 598.96 | 122.89 | 5495.22 | 208.48 | 1.12 |
| SSO:SBO (90:10) | 115.18 | 434.54 | 72.98 | 3059.41 | 144.13 | 1.46 |
| SSO:SBO (80:20) | 120.52 | 230.89 | 52.33 | 2809.05 | 167.81 | 1.50 |
| SSO:SBO (80:20) | 167.20 | 473.77 | 135.80 | 4919.49 | 217.85 | 0.69 |
| SSO:SBO (80:20) | 137.39 | 447.26 | 103.18 | 4137.37 | 173.82 | 1.68 |
| SSO:SBO (80:20) | 96.39 | 483.92 | 75.50 | 3011.12 | 140.81 | 0.77 |
| SSO:SBO (80:20) | 165.58 | 673.83 | 138.25 | 6182.12 | 234.54 | 1.26 |
| SSO:SBO (80:20) | 129.57 | 488.86 | 82.10 | 3441.83 | 162.14 | 1.65 |

*a* Each sample was analyzed in triplicate.

SSO, sesame oil; CO, corn oil; SBO, soybean oil.

nd, not detected.



**Supplementary Figure 1.** Representative chromatograms of identified triacyglycerol compositions in oil samples analyzed in this study.



**Supplementary Figure 2.** Representative chromatograms of identified fatty acid compositions in oil samples analyzed in this study.



**Supplementary Figure 3.** Analytical ion chromatograms of identified volatile organic compound compositions in oil samples analyzed in this study. Unique mass was used for calculations for a particular peak.