

Supplemental Table 1. Major classes of lipids of human meibum detectable in RP-UPLC/MS experiments in positive and negative ion modes.

| Saturated wax esters | Theoretical m/z, (M + H)⁺ | Mono-unsaturated wax esters | Theoretical m/z, (M + H)⁺ |
|---|---|--|---|
| C ₃₆ H ₇₂ O ₂ | 537.56 | C ₃₆ H ₇₀ O ₂ | 535.55 |
| C ₃₇ H ₇₄ O ₂ | 551.58 | C ₃₇ H ₇₂ O ₂ | 549.56 |
| C ₃₈ H ₇₆ O ₂ | 565.59 | C ₃₈ H ₇₄ O ₂ | 563.58 |
| C ₃₉ H ₇₈ O ₂ | 579.61 | C ₃₉ H ₇₆ O ₂ | 577.59 |
| C ₄₀ H ₈₀ O ₂ | 593.62 | C ₄₀ H ₇₈ O ₂ | 591.61 |
| C ₄₁ H ₈₂ O ₂ | 607.64 | C ₄₁ H ₈₀ O ₂ | 605.62 |
| C ₄₂ H ₈₄ O ₂ | 621.65 | C ₄₂ H ₈₂ O ₂ | 619.64 |
| C ₄₃ H ₈₆ O ₂ | 635.67 | C ₄₃ H ₈₄ O ₂ | 633.65 |
| C ₄₄ H ₈₈ O ₂ | 649.69 | C ₄₄ H ₈₆ O ₂ | 647.66 |
| C ₄₅ H ₉₀ O ₂ | 663.70 | C ₄₅ H ₈₈ O ₂ | 661.69 |
| C ₄₆ H ₉₂ O ₂ | 677.72 | C ₄₆ H ₉₀ O ₂ | 675.70 |
| C ₄₇ H ₉₄ O ₂ | 691.73 | C ₄₇ H ₉₂ O ₂ | 689.72 |
| C ₄₈ H ₉₆ O ₂ | 705.5 | C ₄₈ H ₉₄ O ₂ | 703.73 |
| C ₄₉ H ₉₈ O ₂ | 719.76 | C ₄₉ H ₉₆ O ₂ | 717.75 |
| C ₅₀ H ₁₀₀ O ₂ | 733.78 | C ₅₀ H ₉₈ O ₂ | 731.76 |
| Saturated cholesteryl esters | Theoretical m/z, (M – 369 + H)⁺ | Mono-unsaturated cholesteryl esters | Theoretical m/z, (M + H)⁺ |
| C _{14:0} -CE | 597.56 | C _{14:1} -CE | 595.55 |
| C _{15:0} -CE | 611.58 | C _{15:1} -CE | 609.56 |
| C _{16:0} -CE | 625.59 | C _{16:1} -CE | 623.58 |
| C _{17:0} -CE | 639.61 | C _{17:1} -CE | 637.59 |
| C _{18:0} -CE | 653.62 | C _{18:1} -CE | 651.61 |
| C _{19:0} -CE | 667.64 | C _{19:1} -CE | 665.62 |
| C _{20:0} -CE | 681.65 | C _{20:1} -CE | 679.64 |
| C _{21:0} -CE | 695.67 | C _{21:1} -CE | 693.65 |
| C _{22:0} -CE | 709.69 | C _{22:1} -CE | 707.67 |
| C _{23:0} -CE | 723.70 | C _{23:1} -CE | 721.69 |
| C _{24:0} -CE | 737.72 | C _{24:1} -CE | 735.70 |
| C _{25:0} -CE | 751.73 | C _{25:1} -CE | 749.72 |
| C _{26:0} -CE | 765.75 | C _{26:1} -CE | 763.73 |
| C _{27:0} -CE | 779.76 | C _{27:1} -CE | 777.75 |
| C _{28:0} -CE | 793.78 | C _{28:1} -CE | 791.76 |
| C _{29:0} -CE | 807.80 | C _{29:1} -CE | 805.78 |
| C _{30:0} -CE | 821.81 | C _{30:1} -CE | 819.79 |
| C _{31:0} -CE | 835.83 | C _{31:1} -CE | 833.81 |
| C _{32:0} -CE | 849.84 | C _{32:1} -CE | 847.83 |
| C _{33:0} -CE | 863.86 | C _{33:1} -CE | 861.84 |
| C _{34:0} -CE | 877.87 | C _{34:1} -CE | 875.86 |
| C _{35:0} -CE | 891.89 | C _{35:1} -CE | 889.87 |

| Mono-unsaturated ChI-OAHFA | Theoretical m/z, (M + H)⁺ | Diunsaturated ChI-OAHFA, | Theoretical m/z, (M + H)⁺ |
|---|---|---|---|
| C ₆₅ H ₁₁₆ O ₄ | 961.89 | C ₆₅ H ₁₁₄ O ₄ | 959.88 |
| C ₆₆ H ₁₁₈ O ₄ | 975.91 | C ₆₆ H ₁₁₆ O ₄ | 973.89 |
| C ₆₇ H ₁₂₀ O ₄ | 989.93 | C ₆₇ H ₁₁₈ O ₄ | 987.91 |
| C ₆₈ H ₁₂₂ O ₄ | 1003.94 | C ₆₈ H ₁₂₀ O ₄ | 1001.93 |
| C ₆₉ H ₁₂₄ O ₄ | 1017.96 | C ₆₉ H ₁₂₂ O ₄ | 1015.94 |
| C ₇₀ H ₁₂₆ O ₄ | 1031.97 | C ₇₀ H ₁₂₄ O ₄ | 1029.96 |
| C ₇₁ H ₁₂₈ O ₄ | 1045.99 | C ₇₁ H ₁₂₆ O ₄ | 1043.97 |
| C ₇₂ H ₁₃₀ O ₄ | 1060.00 | C ₇₂ H ₁₂₈ O ₄ | 1057.99 |
| C ₇₃ H ₁₃₂ O ₄ | 1074.02 | C ₇₃ H ₁₃₀ O ₄ | 1072.00 |
| C ₇₄ H ₁₃₄ O ₄ | 1088.03 | C ₇₄ H ₁₃₂ O ₄ | 1086.02 |
| C ₇₅ H ₁₃₆ O ₄ | 1102.05 | C ₇₅ H ₁₃₄ O ₄ | 1100.03 |
| C ₇₆ H ₁₃₈ O ₄ | 1116.07 | C ₇₆ H ₁₃₆ O ₄ | 1114.05 |
| C ₇₇ H ₁₄₀ O ₄ | 1130.08 | C ₇₇ H ₁₃₈ O ₄ | 1128.07 |
| C ₇₈ H ₁₄₂ O ₄ | 1144.10 | C ₇₈ H ₁₄₀ O ₄ | 1142.08 |
| C ₇₉ H ₁₄₄ O ₄ | 1158.11 | C ₇₉ H ₁₄₂ O ₄ | 1156.10 |
| C ₈₀ H ₁₄₆ O ₄ | 1172.13 | C ₈₀ H ₁₄₄ O ₄ | 1170.11 |
| | | | |
| Triacylglycerols | Theoretical m/z, (M + H)⁺ | Triacylglycerols | Theoretical m/z, (M + H)⁺ |
| C ₅₁ H ₉₃ O ₆ | 801.697 | C ₅₅ H ₁₀₁ O ₆ | 857.759 |
| C ₅₁ H ₉₅ O ₆ | 803.708 | C ₅₅ H ₁₀₃ O ₆ | 859.772 |
| C ₅₁ H ₉₇ O ₆ | 805.727 | C ₅₇ H ₁₀₁ O ₆ | 881.759 |
| C ₅₃ H ₉₅ O ₆ | 827.712 | C ₅₇ H ₁₀₃ O ₆ | 883.775 |
| C ₅₃ H ₉₇ O ₆ | 829.725 | C ₅₇ H ₁₀₅ O ₆ | 885.791 |
| C ₅₃ H ₉₉ O ₆ | 831.744 | C ₅₉ H ₁₀₇ O ₆ | 911.806 |
| C ₅₅ H ₉₇ O ₆ | 853.728 | C ₆₀ H ₁₀₇ O ₆ | 923.806 |
| C ₅₅ H ₉₉ O ₆ | 855.744 | | |
| | | | |
| OAHFA | Theoretical m/z, (M - H)⁻ | OAHFA | Theoretical m/z, (M - H)⁻ |
| C ₄₈ H ₈₉ O ₄ | 729.677 | C ₅₀ H ₉₃ O ₄ | 757.707 |
| C ₅₂ H ₉₇ O ₄ | 785.739 | | |
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