**Table S4.** Mass transitions (MRM) and instrumental parameters of LC-ESI-MS/MS method.

| Compound | Ionization Mode | Precursor ion | Q1 | | | | | Q2 | | | | RT (min) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Product ion | DP | EP | CE | CXP | Product ion | DP | EP | CE | CXP | |
| **Fatty acids** | | | | | | | | | | | | | |
| Arachidic acid | $[M+HCOO]^-$ | 357.4 | 311.4 | -5 | -10 | -12 | -21 | 45.1 | -5 | -10 | -40 | -5 | 14.5 |
| Behenic acid | $[M+HCOO]^-$ | 385.4 | 339.4 | -60 | -11 | -15 | -10 | 321.4 | -60 | -11 | -47 | -16 | 16.0 |
| Docosahexaenoic acid | $[M-H]^-$ | 373.3 | 327.3 | -60 | -10 | -10 | -21 | 283.4 | -60 | -10 | -20 | -20 | 8.8 |
| Erucic acid | $[M+HCOO]^-$ | 383.2 | 337.3 | -95 | -10 | -12 | -23 | 45.0 | -95 | -10 | -44 | -5 | 14.6 |
| Gondoic acid | $[M-H]^-$ | 309.4 | 291.5 | -167 | -11 | -32.9 | -19 | 155.0 | -167 | -11 | -37 | -10 | 12.7 |
| Lignoceric acid | $[M+HCOO]^-$ | 413.2 | 367.3 | -65 | -10 | -12 | -23 | 45.0 | -65 | -10 | -42 | -5 | 18.6 |
| Linoleic acid | $[M+HCOO]^-$ | 325.2 | 279.2 | -60 | -12 | -10 | -21 | 261.0 | -60 | -12 | -35 | -23 | 9.0 |
| Linolenic acid | $[M+HCOO]^-$ | 323.3 | 277.2 | -65 | -6 | -8 | -17 | 259.3 | -65 | -6 | -27 | -17 | 8.2 |
| Margaric acid | $[M+HCOO]^-$ | 315.4 | 269.3 | -45 | -13 | -10 | -17 | 45.0 | -10 | -10 | -32 | -5 | 11.0 |
| Miristoleic acid | $[M+HCOO]^-$ | 271.3 | 225.3 | -45 | -11 | -20 | -17 | 45.0 | -30 | -10 | -26 | -7 | 6.6 |
| Myristic acid | $[M+HCOO]^-$ | 273.2 | 227.2 | -5 | -10 | -18 | -15 | 45.0 | -5 | -10 | -26 | -7 | 8.4 |
| Oleanolic acid | $[M+NH_4]^+$ | 474.3 | 439.4 | 146 | 10 | 15 | 32 | 191.2 | 146 | 10 | 27 | 12 | 7.8 |
| Oleic acid | $[M+HCOO]^-$ | 327.2 | 281.2 | -50 | -10 | -14 | -17 | 45.1 | -50 | -10 | -34 | -5 | 10.8 |
| Palmitic acid | $[M-H]^-$ | 255.1 | 237.3 | -170 | -10 | -30 | -17 | 44.9 | -55 | -10 | -38 | -5 | 10.4 |
| Palmitoleic acid | $[M+HCOO]^-$ | 299.3 | 253.3 | -55 | -10 | -18 | -15 | 44.7 | -55 | -10 | -34 | -7 | 8.5 |
| Stearic acid | $[M+HCOO]^-$ | 329.3 | 283.3 | -60 | -12 | -9 | -22 | 265.5 | -60 | -12 | -41 | -16 | 12.7 |
| **Carnitines** | | | | | | | | | | | | | |
| Palmitoyl-L-carnitine hydrochloride | $[M+H]^+$ | 400.3 | 341.0 | 173 | 10 | 24 | 14 | 239.0 | 173 | 10 | 28 | 14 | 6.2 |
| Oleoyl-L-carnitine hydrochloride | $[M+H]^+$ | 426.3 | 367.0 | 120 | 11 | 26 | 17 | 265.0 | 120 | 11 | 30 | 13 | 6.5 |
| **Esters** | | | | | | | | | | | | | |
| Ethyl linoleate | $[M+H+H_2O]$ | 326.3 | 263.2 | 26 | 10 | 12 | 20 | 95.0 | 26 | 10 | 35 | 8 | 12.6 |
| Ethyl oleate | $[M+H+H_2O]$ | 328.3 | 311.3 | 61 | 10 | 13 | 22 | 265.2 | 211 | 10 | 13 | 22 | 14.0 |

| Compound | Ionization Mode | Precursor ion | Q1 | | | | | Q2 | | | | | RT (min) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Product ion | DP | EP | CE | CXP | Product ion | DP | EP | CE | CXP | |
| Ethyl stearate | $[M+H]^+$ | 313.3 | 285.3 | 211 | 10 | 19 | 16 | 71.1 | 211 | 10 | 25 | 8 | 15.9 |
| Methyl linoleate | $[M+H+H_2O]$ | 312.3 | 295.3 | 26 | 10 | 11 | 20 | 263.2 | 26 | 10 | 13 | 14 | 11.5 |
| Methyl oleate | $[M+H+H_2O]$ | 314.3 | 297.4 | 41 | 10 | 11 | 18 | 149.0 | 116 | 10 | 25 | 14 | 13.0 |
| Methyl palmitate | $[M+H+H_2O]$ | 288.5 | 271.2 | 71 | 10 | 11 | 24 | 71.2 | 151 | 10 | 27 | 8 | 12.7 |
| Methyl stearate | $[M+H+H_2O]$ | 316.3 | 299.3 | 86 | 10 | 13 | 24 | 71.2 | 86 | 10 | 31 | 8 | 14.8 |
| **Glicerophospholipids** | | | | | | | | | | | | | |
| 1.2-dioleoyl-sn-glycero-3-phospho-rac-(1-glycerol)sodium salt | $[M-Na+NH_4]^+$ | 792.5 | 603.6 | 50 | 6 | 35 | 15 | 339.3 | 50 | 6 | 45 | 14 | 16.3 |
| 1.2-dioleoyl-sn-glycero-3-phosphocholine | $[M+H]^+$ | 786.6 | 184.0 | 116 | 3 | 27 | 14 | 125.0 | 116 | 3 | 134 | 14 | 18.0 |
| 1-palmitoyl-sn-glycero-3-phosphocholine | $[M+H]^+$ | 496.4 | 478.4 | 100 | 14 | 27 | 14 | 184.0 | 100 | 14 | 35 | 14 | 6.5 |
| **Glicerolipidis** | | | | | | | | | | | | | |
| 1-linoleoyl-rac-glycerol | $[M+H]^+$ | 355.3 | 337.0 | 300 | 3 | 15 | 16 | 263.0 | 300 | 3 | 13 | 21 | 7.6 |
| 1-oleoyl-rac-glycerol | $[M+H]^+$ | 357.3 | 265.2 | 250 | 10 | 15 | 13 | 283.2 | 250 | 10 | 13 | 17 | 9.2 |
| Glyceryl tripalmitoleate | $[M+NH_4]^+$ | 818.7 | 547.0 | 300 | 4 | 28 | 27 | 237.3 | 300 | 4 | 53 | 12 | 23.7 |
| 1-monopalmitoleoyl-rac-glycerol | $[M+H]^+$ | 329.3 | 219.3 | 104 | 7 | 17.5 | 17 | 121.2 | 104 | 7 | 29 | 9 | 7.1 |
| **Sfingolipid** | | | | | | | | | | | | | |
| Ceramide | $[M+H]^+$ | 566.6 | 548.6 | 100 | 8 | 18 | 14 | 264.0 | 100 | 8 | 41 | 14 | 19.8 |

| Compound | Ionization Mode | Precursor ion | Q1 | | | | | Q2 | | | | | RT (min) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Product ion | DP | EP | CE | CXP | Product ion | DP | EP | CE | CXP | |
| **Sterols** | | | | | | | | | | | | | |
| Brassicasterolo | $[M+H]^+$ | 416.4 | 381.3 | 16 | 10 | 13 | 20 | 125.1 | 16 | 10 | 21 | 10 | 15.4 |
| Cholesterol | $[M+H]^+$ | 369.5 | 147.0 | 140 | 8 | 25 | 35 | 135.0 | 140 | 8 | 35 | 23 | 16.1 |
| Desmosterolo | $[M+NH_4]^+$ | 402.4 | 367.2 | 146 | 10 | 13 | 20 | | | | | | 14.1 |
| Ergosterolo | $[M+H]^+$ | 397.3 | 69.3 | 6 | 10 | 33 | 14 | 379.4 | 6 | 10 | 17 | 22 | 14.9 |
| Lupeol | $[M+H]^+$ | 444.4 | 427.4 | 35 | 5 | 17 | 14 | 409.4 | 35 | 5 | 17 | 14 | 15.4 |
| Uvaol | $[M+NH_4]^+$ | 460.4 | 443.4 | 100 | 10 | 11 | 22 | 191.4 | 100 | 10 | 21 | 10 | 7.6 |

DP- declustering potential; EP- entrance potential; CE- collision energy; CXP- collision cell exit potential; RT- retention time. DP, EP, CE, and CXP are expressed in volts.