

Nutritional composition and untargeted metabolomics reveal the potential of *Tetraedesmus obliquus*, *Chlorella vulgaris* and *Nannochloropsis oceanica* as valuable nutrient sources for dogs

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Supplementary Information

S1. Processing of raw HPLC-MS data using MZmine

The raw files obtained by HPLC-MS/MS analyses were extracted and converted to mzXML files using the ProteoWizard MSconvert tool [1] and subsequently processed using MZmine 2.53 [2]. Mass detection was performed both in MS¹ level (noise level set at 1×10^5) and MS² level (noise level set at 1×10^4). The ADAP Chromatogram Builder Module [3] was used for the chromatogram builder using MS¹ (10 scans as minimum group size; group intensity threshold 3×10^5 ; minimum highest intensity 3×10^5 ; m/z tolerance of 0.01 m/z or 5 ppm). The chromatograms were deconvoluted using the local minimum feature resolver using the following parameters: chromatographic threshold of 30%, minimum search range 0.05 minutes; minimum relative height of 5%; minimum absolute height 1×10^6 ; minimum ratio of peak top/edge 5; peak duration range 0.1-2 minutes, m/z range for MS² scan pairing (Da): 0.01; RT range for MS² scan pairing (min): 0.1. The chromatograms were deisotoped using the isotopic peaks grouper algorithm with a m/z tolerance of 0.01 m/z or 10 ppm and a retention time (RT) tolerance of 0.5 minutes, considering a maximum charge of 2 and the most intense isotope as the representative. Peak alignment was achieved by join aligner using m/z tolerance of 0.01 m/z or 5 ppm (weight for m/z: 75) and RT tolerance of 0.5 minute (weight for retention time: 25). The final peaks list was filtered keeping only the features with MS² scan and a minimum of 2 peaks per row. The peak list was gap-filled with the peak finder (multithreaded) module (intensity tolerance at 20%, m/z tolerance of 0.01 m/z or 5 ppm, and absolute RT tolerance of 0.5 min). Fragment peaks were searched considering a RT tolerance of 0.5 minutes, m/z tolerance of MS² data of 0.01 m/z or 5 ppm, maximum fragment peak height of 80% and a minimum MS² peak height of 1×10^4 . Adducts with formic acid, sodium, sodium formate, chlorine, and complexes were searched using the following parameters: RT tolerance: 0.5; m/z tolerance: 0.01 m/z or 5 ppm; max relative adduct/complex peak height: 80%. Fragments, adducts, and complexes, were removed from the final peaks' list.

Table S1. List of metabolites by class identified in the methanolic extracts of *Tetraedesmus obliquus*, *Chlorella vulgaris*, and *Nannochloropsis oceanica* by HPLC-MS/MS, with the information of the ion type, calculated m/z, experimental m/z, mass error ($\Delta m/z$), and peak area for each microalgae species.

| Metabolite | Ion | Calculated m/z | Experimental m/z | $\Delta m/z$ (ppm) | <i>Tetraedesmus obliquus</i> | <i>Chlorella vulgaris</i> | <i>Nannochloropsis oceanica</i> |
|--|-----------|----------------|------------------|--------------------|------------------------------|---------------------------|---------------------------------|
| <i>Benzoic acids and derivatives</i> | | | | | | | |
| Benzoic acid | [M-H]- | 121.0295 | 121.0295 | 0.0000 | 8.48E+07 | 1.24E+08 | 4.07E+07 |
| <i>Lipids and lipid-like molecules</i> | | | | | | | |
| <i>Betaine monoacylglycerols</i> | | | | | | | |
| MGTS(16:0) I | [M+HCOO]- | 518.3698 | 518.3698 | 0.0000 | 2.35E+07 | 1.02E+06 | 2.18E+07 |
| MGTS(16:0) II | [M+HCOO]- | 518.3698 | 518.3697 | -0.1929 | 9.59E+07 | 2.92E+06 | 8.36E+07 |
| MGTS(16:4) | [M+HCOO]- | 510.3072 | 510.3071 | -0.1960 | 3.00E+07 | | |
| MGTS(18:3) I | [M+HCOO]- | 540.3542 | 540.3541 | -0.1851 | 3.08E+07 | 2.29E+06 | |
| MGTS(18:3) II | [M+HCOO]- | 540.3542 | 540.3541 | -0.1851 | 5.60E+07 | 3.14E+06 | 5.68E+06 |
| MGTS(18:4) I | [M+HCOO]- | 538.3385 | 538.3415 | 5.5727 | 7.85E+07 | | |
| MGTS(18:4) II | [M+HCOO]- | 538.3385 | 538.3413 | 5.2012 | 2.18E+08 | | |
| MGTS(20:4) | [M+HCOO]- | 566.3698 | 566.3692 | -1.0594 | | 7.52E+06 | 7.01E+07 |
| <i>Betaine diacylglycerols</i> | | | | | | | |
| DGTS(14:0/16:1) | [M+HCOO]- | 726.5526 | 726.5532 | 0.8258 | | | 4.64E+07 |
| DGTS(18:3/18:4) | [M+HCOO]- | 798.5526 | 798.5521 | -0.6261 | 1.46E+08 | | 1.60E+06 |
| <i>Glycerophosphocholines</i> | | | | | | | |
| LPC(16:0) I | [M+HCOO]- | 540.3307 | 540.3307 | 0.0000 | 1.26E+07 | 3.00E+07 | 3.60E+07 |
| LPC(16:0) II | [M+HCOO]- | 540.3307 | 540.3306 | -0.1851 | 5.03E+07 | 1.30E+08 | 1.56E+08 |
| LPC(16:2) I | [M+HCOO]- | 536.2994 | 536.2993 | -0.1865 | 1.67E+07 | 1.83E+08 | 3.38E+06 |
| LPC(16:2) II | [M+HCOO]- | 536.2994 | 536.2993 | -0.1865 | 5.06E+07 | 1.54E+08 | 3.74E+07 |
| LPC(16:3) I | [M+HCOO]- | 534.2837 | 534.2834 | -0.5615 | 3.29E+06 | 4.40E+08 | |
| LPC(18:1) I | [M+HCOO]- | 566.3463 | 566.3462 | -0.1766 | 2.13E+07 | 9.19E+07 | 3.81E+07 |
| LPC(18:1) II | [M+HCOO]- | 566.3463 | 566.3461 | -0.3531 | 9.83E+07 | 1.31E+08 | 1.61E+08 |
| LPC(18:2) I | [M+HCOO]- | 564.3307 | 564.3306 | -0.1772 | 4.42E+07 | 2.70E+08 | 5.05E+07 |
| LPC(18:2) II | [M+HCOO]- | 564.3307 | 564.3306 | -0.1772 | 1.80E+08 | 3.68E+08 | 1.75E+08 |
| LPC(18:3) | [M+HCOO]- | 562.3150 | 562.3149 | -0.1778 | 1.62E+08 | 5.28E+08 | 2.98E+06 |
| LPC(18:4) I | [M+HCOO]- | 560.2994 | 560.2993 | -0.1642 | 4.13E+07 | | |
| LPC(18:4) II | [M+HCOO]- | 560.2994 | 560.2996 | 0.3712 | 1.30E+08 | | |
| <i>sn</i> -glycerol-3-phosphocholine | [M+HCOO]- | 302.1010 | 302.1009 | -0.3310 | 5.20E+07 | 2.47E+08 | |
| <i>Glycerophosphoethanolamines</i> | | | | | | | |
| PE(16:1/16:1) I | [M-H]- | 686.4766 | 686.4767 | 0.1355 | 1.83E+08 | 1.59E+07 | |
| PE(16:1/16:1) II | [M-H]- | 686.4766 | 686.4766 | -0.0102 | 1.18E+08 | 2.92E+07 | |
| Glycerylphosphorylethanolamine | [M-H]- | 214.0486 | 214.0486 | 0.0000 | 1.38E+08 | 7.20E+08 | |
| <i>Glycerophosphoinositols</i> | | | | | | | |
| Glycerophosphoinositol | [M-H]- | 333.0592 | 333.0592 | 0.0047 | 1.66E+08 | 1.47E+09 | |
| <i>Glycosylmonoacylglycerols</i> | | | | | | | |
| DGMG(14:0) I | [M+HCOO]- | 671.3496 | 671.3499 | 0.4469 | 1.06E+07 | 5.66E+06 | 5.64E+07 |
| DGMG(14:0) II | [M+HCOO]- | 671.3496 | 671.3486 | -1.4895 | 1.10E+07 | | 6.97E+07 |
| DGMG(16:0) I | [M+HCOO]- | 699.3809 | 699.3807 | -0.2860 | 2.99E+07 | 7.38E+07 | 1.00E+08 |
| DGMG(16:0) II | [M+HCOO]- | 699.3809 | 699.3810 | 0.1430 | 1.11E+08 | 3.96E+07 | 3.70E+08 |

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|------------------|-----------|----------|----------|---------|----------|----------|
| DGMG(16:3) I | [M+HCOO]- | 693.3339 | 693.3325 | -2.0192 | 4.46E+07 | 2.44E+08 |
| DGMG(16:3) II | [M+HCOO]- | 693.3339 | 693.3337 | -0.2885 | 1.66E+08 | 9.90E+07 |
| DGMG(18:2) I | [M+HCOO]- | 723.3809 | 723.3808 | -0.1382 | 2.59E+07 | 3.21E+07 |
| DGMG(18:2) II | [M+HCOO]- | 723.3809 | 723.3808 | -0.1382 | 4.23E+07 | 4.33E+07 |
| MGMG(13:0) I | [M+HCOO]- | 495.2811 | 495.2802 | -1.8171 | | 6.43E+07 |
| MGMG(13:0) II | [M+HCOO]- | 495.2811 | 495.2808 | -0.6057 | | 1.10E+08 |
| MGMG(14:0) I | [M+HCOO]- | 509.2967 | 509.2964 | -0.5890 | 4.50E+06 | 8.67E+06 |
| MGMG(14:0) II | [M+HCOO]- | 509.2967 | 509.2964 | -0.5890 | 1.90E+07 | 8.88E+06 |
| MGMG(16:0) I | [M+HCOO]- | 537.3280 | 537.3271 | -1.6750 | 8.91E+06 | 2.73E+07 |
| MGMG(16:0) II | [M+HCOO]- | 537.3280 | 537.3278 | -0.3722 | 7.64E+07 | 1.84E+07 |
| MGMG(16:2) I | [M+HCOO]- | 533.2967 | 533.2964 | -0.5625 | 4.26E+07 | 7.63E+08 |
| MGMG(16:2) II | [M+HCOO]- | 533.2967 | 533.2965 | -0.3750 | 1.54E+08 | 4.58E+08 |
| MGMG(16:3) I | [M+HCOO]- | 531.2811 | 531.2807 | -0.7529 | 1.56E+08 | 2.92E+09 |
| MGMG(16:3) II | [M+HCOO]- | 531.2811 | 531.2809 | -0.3764 | 5.42E+08 | 1.39E+09 |
| MGMG(16:3) III | [M+HCOO]- | 531.2811 | 531.2811 | 0.0000 | 9.51E+07 | 9.66E+06 |
| MGMG(16:4) I | [M+HCOO]- | 529.2654 | 529.2643 | -2.0784 | 1.01E+09 | 2.30E+06 |
| MGMG(16:4) II | [M+HCOO]- | 529.2654 | 529.2642 | -2.2673 | 3.86E+09 | 2.30E+06 |
| MGMG(16:4;O) I | [M+HCOO]- | 545.2603 | 545.2590 | -2.3842 | 1.02E+08 | 1.80E+06 |
| MGMG(16:4;O) II | [M+HCOO]- | 545.2603 | 545.2590 | -2.3842 | 3.16E+08 | 1.80E+06 |
| MGMG(16:4;O) III | [M-H]- | 499.2548 | 499.2541 | -1.4021 | 7.95E+07 | |
| MGMG(16:4;O) IV | [M+HCOO]- | 545.2603 | 545.2591 | -2.2008 | 1.41E+08 | |
| MGMG(17:3) I | [M+HCOO]- | 545.2967 | 545.2958 | -1.6505 | 1.46E+07 | 1.60E+07 |
| MGMG(17:3) II | [M+HCOO]- | 545.2967 | 545.2966 | -0.1834 | 8.78E+07 | 2.17E+07 |
| MGMG(18:3) I | [M+HCOO]- | 559.3124 | 559.3121 | -0.5364 | 1.09E+09 | 4.38E+08 |
| MGMG(18:3) II | [M+HCOO]- | 559.3124 | 559.3121 | -0.5364 | 3.09E+09 | 7.27E+08 |
| MGMG(18:3;O) I | [M+HCOO]- | 575.3073 | 575.3069 | -0.6953 | 4.84E+07 | |
| MGMG(18:3;O) II | [M+HCOO]- | 575.3073 | 575.3070 | -0.5215 | 2.87E+08 | 1.22E+07 |
| MGMG(18:3;O) III | [M+HCOO]- | 575.3073 | 575.3069 | -0.6953 | 1.44E+09 | 3.76E+07 |
| MGMG(18:3;O) IV | [M+HCOO]- | 575.3073 | 575.3069 | -0.6953 | 5.44E+07 | |
| MGMG(18:4) I | [M+HCOO]- | 557.2967 | 557.2963 | -0.7178 | 5.65E+07 | |
| MGMG(18:4) II | [M+HCOO]- | 557.2967 | 557.2965 | -0.3589 | 2.81E+08 | |
| MGMG(20:5) I | [M+HCOO]- | 583.3124 | 583.3116 | -1.3715 | 7.80E+06 | 1.18E+07 |
| MGMG(20:5) II | [M+HCOO]- | 583.3124 | 583.3120 | -0.6857 | 1.03E+07 | 1.47E+07 |

Glycosylglycerols

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|--------------------|-----------|----------|----------|--------|----------|----------|
| Galactosylglycerol | [M+HCOO]- | 299.0984 | 299.0990 | 2.0060 | 5.97E+07 | 1.99E+08 |
|--------------------|-----------|----------|----------|--------|----------|----------|

Glycosyldiacylglycerols

| | | | | | | |
|-------------------|-----------|----------|----------|---------|----------|----------|
| DGDG(16:0/4:1) | [M+HCOO]- | 767.4071 | 767.4084 | 1.6940 | | 5.29E+07 |
| MGDG(10:3;O/20:5) | [M+HCOO]- | 747.3961 | 747.3956 | -0.6690 | | 5.99E+07 |
| MGDG(14:0/7:1;O) | [M+HCOO]- | 635.3648 | 635.3670 | 3.4626 | | 7.71E+07 |
| MGDG(16:1/16:3) | [M+HCOO]- | 767.4951 | 767.4951 | 0.0000 | 3.18E+07 | 2.53E+08 |
| MGDG(16:1/4:1) | [M+HCOO]- | 603.3386 | 603.3384 | -0.3315 | 2.20E+07 | 2.83E+06 |
| MGDG(16:2/16:3) I | [M+HCOO]- | 765.4794 | 765.4792 | -0.2613 | 2.38E+07 | 5.84E+08 |
| MGDG(16:3;O/18:3) | [M+HCOO]- | 807.4900 | 807.4898 | -0.2477 | 5.85E+07 | 4.01E+08 |
| MGDG(16:4/11:1;O) | [M+HCOO]- | 711.3961 | 711.3966 | 0.7028 | 7.42E+07 | 1.00E+06 |
| MGDG(16:4/14:3;O) | [M+HCOO]- | 749.4118 | 749.4105 | -1.7347 | 6.52E+07 | 4.51E+07 |

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|-----------------------|-----------|----------|----------|---------|----------|----------|
| MGDG(16:4/17:3) | [M+HCOO]- | 775.4638 | 775.4620 | -2.3212 | 4.59E+07 | |
| MGDG(16:4/9:1;O) | [M+HCOO]- | 683.3648 | 683.3650 | 0.2927 | 7.39E+07 | |
| MGDG(18:2/16:2) | [M+HCOO]- | 795.5264 | 795.5255 | -1.1313 | 8.21E+07 | 3.46E+08 |
| MGDG(18:2/16:3) | [M+HCOO]- | 793.5107 | 793.5092 | -1.8903 | 7.98E+07 | 4.10E+08 |
| MGDG(18:2/16:4) | [M+HCOO]- | 791.4951 | 791.4950 | -0.1263 | 1.86E+08 | 9.39E+08 |
| MGDG(18:3/16:4) | [M+HCOO]- | 789.4794 | 789.4820 | 3.2933 | 9.06E+08 | 5.09E+06 |
| MGDG(18:3/16:4;O) | [M+HCOO]- | 805.4744 | 805.4734 | -1.2415 | 9.83E+08 | 2.21E+07 |
| MGDG(18:3/16:4;O2) I | [M+HCOO]- | 821.4693 | 821.4684 | -1.0956 | 6.26E+08 | 2.49E+07 |
| MGDG(18:3/16:4;O2) II | [M+HCOO]- | 821.4693 | 821.4688 | -0.6087 | 5.93E+07 | 1.90E+06 |
| MGDG(18:3/3:1) | [M+HCOO]- | 613.3229 | 613.3227 | -0.3261 | 1.41E+08 | |
| MGDG(18:3/6:0;O4) I | [M+HCOO]- | 721.3652 | 721.3649 | -0.4159 | 1.39E+08 | 5.08E+07 |
| MGDG(18:3/6:0;O4) II | [M+HCOO]- | 721.3652 | 721.3656 | 0.5545 | 5.06E+08 | 6.79E+07 |
| MGDG(18:3/9:2;O) | [M+HCOO]- | 711.3961 | 711.3962 | 0.1406 | 6.51E+07 | 1.74E+06 |
| MGDG(18:3;O/16:3) | [M+HCOO]- | 807.4900 | 807.4897 | -0.3715 | 4.47E+07 | 4.20E+08 |
| MGDG(18:3;O/16:4) | [M+HCOO]- | 805.4744 | 805.4738 | -0.7449 | 1.07E+09 | |
| MGDG(18:3;O/16:4;O) | [M+HCOO]- | 821.4693 | 821.4687 | -0.7304 | 5.97E+08 | 8.37E+06 |
| MGDG(18:3;O/3:1) | [M+HCOO]- | 629.3179 | 629.3177 | -0.3178 | 6.90E+07 | |
| MGDG(18:3;O2/16:4) | [M+HCOO]- | 821.4693 | 821.4698 | 0.6087 | 1.04E+08 | 7.89E+07 |
| MGDG(20:4/5:1;O2) I | [M-H]- | 653.3542 | 653.3534 | -1.2245 | 5.13E+06 | 1.66E+07 |
| MGDG(20:5/4:1) I | [M+HCOO]- | 651.3386 | 651.3383 | -0.4606 | | 1.38E+08 |
| MGDG(20:5/5:1;O) | [M+HCOO]- | 681.3492 | 681.3490 | -0.2935 | | 2.60E+07 |
| MGDG(20:5/6:0;O2) I | [M+HCOO]- | 713.3754 | 713.3742 | -1.6821 | | 4.36E+07 |
| MGDG(20:5/6:0;O2) II | [M+HCOO]- | 713.3754 | 713.3748 | -0.8411 | | 5.60E+07 |
| MGDG(5:2;O/16:0) | [M-H]- | 605.3542 | 605.3550 | 1.3215 | | 3.95E+07 |
| MGDG(9:1;O2 /16:4) | [M-H]- | 653.3542 | 653.3532 | -1.5306 | 1.47E+08 | |

Hydroxy fatty acids

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|----------------|--------|----------|----------|---------|----------|----------|
| FA 10:0;O | [M-H]- | 187.1339 | 187.1338 | -0.7748 | 2.72E+07 | 2.12E+07 |
| FA 10:1;O2 I | [M-H]- | 201.1132 | 201.1132 | -0.0497 | 4.19E+07 | |
| FA 10:1;O2 II | [M-H]- | 201.1132 | 201.1132 | -0.0497 | 8.56E+07 | 4.75E+07 |
| FA 10:1;O2 III | [M-H]- | 201.1132 | 201.1132 | -0.0497 | | 3.25E+07 |
| FA 13:3;O2 I | [M-H]- | 239.1289 | 239.1287 | -0.6691 | 8.73E+07 | 1.79E+07 |
| FA 15:0;O | [M-H]- | 257.2122 | 257.2122 | 0.0194 | 1.07E+08 | 7.18E+07 |
| FA 18:0;O | [M-H]- | 299.2591 | 299.2589 | -0.8187 | 1.10E+09 | 9.98E+06 |
| FA 18:1;O3 I | [M-H]- | 329.2333 | 329.2334 | 0.3037 | 9.99E+07 | 5.51E+07 |
| FA 18:1;O3 II | [M-H]- | 329.2333 | 329.2334 | 0.3037 | 3.90E+07 | 5.03E+07 |
| FA 18:2;O I | [M-H]- | 295.2278 | 295.2278 | 0.0000 | 7.43E+07 | 2.81E+08 |
| FA 18:2;O II | [M-H]- | 295.2278 | 295.2278 | 0.0000 | 3.32E+08 | 5.54E+08 |
| FA 18:4;O2 I | [M-H]- | 307.1915 | 307.1913 | -0.6511 | 2.63E+07 | 2.48E+07 |
| FA11:0;O | [M-H]- | 201.1496 | 201.1496 | 0.0000 | 1.44E+08 | 1.21E+06 |
| FA16:0;O I | [M-H]- | 271.2278 | 271.2279 | 0.3687 | 1.16E+08 | 3.44E+07 |
| FA16:1;O I | [M-H]- | 269.2122 | 269.2122 | 0.0000 | 4.67E+07 | 1.33E+07 |
| FA16:1;O II | [M-H]- | 269.2122 | 269.2122 | 0.0000 | 3.76E+07 | 2.04E+07 |
| FA16:1;O III | [M-H]- | 269.2122 | 269.2122 | 0.0000 | 9.05E+06 | 1.75E+06 |
| FA16:1;O IV | [M-H]- | 269.2122 | 269.2122 | 0.0000 | 3.12E+07 | 1.40E+07 |
| FA16:3;O I | [M-H]- | 265.1809 | 265.1809 | 0.0189 | 1.77E+06 | 2.57E+07 |

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|--------------------------------------|--------|----------|----------|---------|----------|----------|
| FA16:3;O II | [M-H]- | 265.1809 | 265.1809 | 0.0189 | 1.77E+06 | 1.77E+07 |
| FA16:3;O III | [M-H]- | 265.1809 | 265.1809 | 0.0189 | 2.96E+07 | 4.51E+08 |
| FA16:3;O IV | [M-H]- | 265.1809 | 265.1809 | 0.0189 | 2.69E+06 | 3.24E+07 |
| FA16:4;O I | [M-H]- | 263.1652 | 263.1652 | 0.0000 | 1.98E+07 | |
| FA16:4;O II | [M-H]- | 263.1652 | 263.1652 | 0.0000 | 2.10E+07 | |
| FA16:4;O III | [M-H]- | 263.1652 | 263.1652 | 0.0000 | 1.70E+08 | 1.12E+07 |
| FA16:4;O IV | [M-H]- | 263.1652 | 263.1652 | 0.0000 | 1.50E+08 | 1.32E+07 |
| FA16:4;O V | [M-H]- | 263.1652 | 263.1652 | -0.1710 | 3.59E+07 | 1.12E+07 |
| FA16:4;O VI | [M-H]- | 263.1652 | 263.1652 | -0.1710 | 9.13E+07 | 3.20E+07 |
| FA16:4;O VII | [M-H]- | 263.1652 | 263.1652 | -0.1710 | 1.14E+08 | 4.82E+06 |
| FA18:2;O3 I | [M-H]- | 327.2177 | 327.2175 | -0.5348 | 5.45E+08 | 2.34E+07 |
| FA18:2;O3 II | [M-H]- | 327.2177 | 327.2173 | -1.1460 | 1.77E+08 | 2.41E+07 |
| FA18:3;O I | [M-H]- | 293.2122 | 293.2120 | -0.6821 | 1.75E+09 | 1.32E+09 |
| FA18:3;O II | [M-H]- | 293.2122 | 293.2120 | -0.6821 | 3.53E+07 | 5.27E+07 |
| FA18:3;O III | [M-H]- | 293.2122 | 293.2120 | -0.6821 | 6.79E+07 | 5.24E+07 |
| FA18:4;O I | [M-H]- | 291.1965 | 291.1966 | 0.3434 | 2.83E+07 | |
| FA18:4;O II | [M-H]- | 291.1965 | 291.1966 | 0.3434 | 1.00E+08 | 3.69E+06 |
| (-)-hydroxycitric acid (FA6:2;O6) | [M-H]- | 207.0146 | 207.0165 | 9.1781 | | 8.55E+07 |

Monoacylglycerophosphates

| | | | | | | |
|----------|-----------|----------|----------|--------|----------|--|
| LPA(4:0) | [M+HCOO]- | 287.0537 | 287.0537 | 0.0000 | 7.43E+07 | |
|----------|-----------|----------|----------|--------|----------|--|

Monoacylglycerophosphoethanolamines

| | | | | | | |
|--------------|--------|----------|----------|---------|----------|----------|
| LPE(16:0) I | [M-H]- | 452.2782 | 452.2782 | 0.0000 | 2.81E+07 | 4.43E+07 |
| LPE(16:0) II | [M-H]- | 452.2782 | 452.2781 | -0.2211 | 1.14E+08 | 1.68E+08 |
| LPE(16:1) I | [M-H]- | 450.2626 | 450.2625 | -0.2221 | 2.64E+08 | 3.65E+08 |
| LPE(16:1) II | [M-H]- | 450.2626 | 450.2624 | -0.4442 | 7.62E+08 | 3.25E+08 |
| LPE(16:3) I | [M-H]- | 446.2313 | 446.2331 | 4.0338 | 6.55E+06 | 2.18E+08 |
| LPE(16:3) II | [M-H]- | 446.2313 | 446.2312 | -0.2241 | 3.54E+07 | 1.12E+08 |
| LPE(17:1) | [M-H]- | 464.2782 | 464.2780 | -0.4308 | 2.03E+07 | 9.11E+07 |
| LPE(18:1) I | [M-H]- | 478.2939 | 478.2938 | -0.1924 | 9.37E+06 | 1.58E+08 |
| LPE(18:1) II | [M-H]- | 478.2939 | 478.2938 | -0.1924 | 4.36E+07 | 1.42E+08 |
| LPE(18:2) I | [M-H]- | 476.2782 | 476.2779 | -0.7181 | 1.94E+07 | 4.69E+08 |
| LPE(18:2) II | [M-H]- | 476.2782 | 476.2780 | -0.5081 | 8.66E+07 | 2.97E+08 |
| LPE(18:3) I | [M-H]- | 474.2626 | 474.2624 | -0.4048 | 4.55E+07 | 3.80E+08 |
| LPE(18:3) II | [M-H]- | 474.2626 | 474.2625 | -0.1940 | 1.43E+08 | 2.60E+08 |

Saturated fatty acids

| | | | | | | |
|-------|-----------|----------|----------|---------|----------|----------|
| C14:0 | [M-H]- | 227.2016 | 227.2018 | 0.8803 | 3.05E+06 | |
| C15:0 | [M+HCOO]- | 287.2228 | 287.2228 | 0.0000 | 1.24E+08 | |
| C16:0 | [M-H]- | 255.2329 | 255.2328 | -0.3918 | 7.86E+08 | 9.91E+08 |
| C17:0 | [M-H]- | 269.2486 | 269.2487 | 0.3714 | 5.30E+07 | 2.09E+08 |
| C18:0 | [M-H]- | 283.2642 | 283.2644 | 0.7061 | 1.48E+08 | 2.60E+08 |

Unsaturated fatty acids

| | | | | | | |
|-------|--------|----------|----------|---------|----------|----------|
| C13:3 | [M-H]- | 207.1390 | 207.1389 | -0.4828 | 2.60E+08 | 1.54E+07 |
| C15:4 | [M-H]- | 233.1547 | 233.1545 | -0.7720 | 1.76E+08 | 1.58E+08 |
| C16:1 | [M-H]- | 253.2173 | 253.2172 | -0.3949 | 2.10E+08 | 2.94E+08 |
| C16:2 | [M-H]- | 251.2016 | 251.2014 | -0.7962 | 3.07E+07 | 1.21E+08 |

| | | | | | | | |
|---------|--------|----------|----------|---------|----------|----------|----------|
| C16:3 I | [M-H]- | 249.1860 | 249.1860 | 0.0000 | 3.14E+07 | 2.55E+08 | 3.02E+07 |
| C16:4 | [M-H]- | 247.1703 | 247.1702 | -0.4046 | 2.25E+08 | | |
| C17:1 | [M-H]- | 267.2329 | 267.2328 | -0.4865 | 1.28E+07 | 7.76E+07 | 2.89E+07 |
| C18:1 I | [M-H]- | 281.2486 | 281.2483 | -1.0667 | 1.44E+09 | 1.10E+09 | 7.86E+08 |
| C18:2 I | [M-H]- | 279.2329 | 279.2330 | 0.3581 | 4.07E+08 | 1.39E+09 | 1.61E+08 |
| C18:3 | [M-H]- | 277.2173 | 277.2172 | -0.3607 | 1.22E+09 | 2.07E+09 | 9.28E+07 |
| C18:4 | [M-H]- | 275.2016 | 275.2017 | 0.3634 | 1.43E+08 | 2.69E+07 | 3.58E+07 |
| C20:3 | [M-H]- | 305.2486 | 305.2483 | -0.9828 | 1.32E+07 | 3.76E+07 | 3.75E+07 |
| C20:4 | [M-H]- | 303.2329 | 303.2329 | 0.0000 | 8.16E+07 | 3.37E+08 | 3.84E+08 |
| C20:5 | [M-H]- | 301.2173 | 301.2170 | -0.9960 | 9.25E+07 | 1.44E+08 | 8.35E+08 |
| C22:5 | [M-H]- | 329.2486 | 329.2486 | 0.0000 | 9.92E+07 | 1.24E+08 | 1.74E+06 |
| C22:6 | [M-H]- | 327.2329 | 327.2329 | 0.0000 | 1.87E+07 | 6.33E+07 | 6.10E+06 |

Nucleosides, nucleotides, and analogues

5'-deoxyribonucleosides

| | | | | | | | |
|------------------------|-----------|----------|----------|---------|----------|----------|----------|
| 5'-methylthioadenosine | [M+HCOO]- | 342.0878 | 342.0877 | -0.2923 | 5.67E+07 | 4.52E+07 | 2.08E+06 |
|------------------------|-----------|----------|----------|---------|----------|----------|----------|

Purine nucleosides

| | | | | | | | |
|--|-----------|----------|----------|---------|----------|----------|----------|
| Adenine | [M-H]- | 134.0472 | 134.0474 | 1.4920 | 2.76E+07 | 6.00E+07 | |
| Adenosine I | [M+HCOO]- | 312.0950 | 312.0948 | -0.6408 | 4.19E+06 | 5.01E+07 | |
| Inosine I | [M-H]- | 267.0735 | 267.0733 | -0.7489 | 8.54E+07 | 8.85E+07 | 6.56E+07 |
| Inosine II | [M-H]- | 267.0735 | 267.0734 | -0.3744 | 5.00E+07 | 7.48E+07 | 9.00E+07 |
| Adenosine 2',3'-cyclic phosphate | [M-H]- | 328.0452 | 328.0453 | 0.3048 | 1.92E+07 | 2.04E+08 | |
| Adenosine 5'-monophosphate I | [M-H]- | 346.0558 | 346.0557 | -0.2890 | 8.00E+07 | 2.70E+07 | 1.12E+08 |
| Adenosine 5'-monophosphate II | [M-H]- | 346.0558 | 346.0557 | -0.2890 | 4.68E+08 | 1.71E+09 | 4.09E+06 |
| Adenosine diphosphate ribose | [M-H]- | 558.0644 | 558.0653 | 1.6586 | 4.21E+07 | 2.59E+08 | |
| Guanosine 3',5'-cyclic monophosphate (cGMP) I | [M-H]- | 344.0401 | 344.0400 | -0.2907 | 1.03E+08 | 7.02E+07 | |
| Guanosine 3',5'-cyclic monophosphate (cGMP) II | [M-H]- | 344.0401 | 344.0400 | -0.2907 | 1.79E+07 | 6.01E+08 | |
| Guanosine-5'-monophosphate | [M-H]- | 362.0507 | 362.0505 | -0.5508 | 2.59E+06 | 1.47E+08 | 1.83E+06 |

Pyrimidine nucleosides

| | | | | | | | |
|---|--------|----------|----------|---------|----------|----------|----------|
| Uridine I | [M-H]- | 243.0622 | 243.0622 | 0.0000 | 1.78E+08 | 1.94E+08 | |
| Thymidine-5'-phosphate I | [M-H]- | 321.0493 | 321.0493 | -0.0076 | 6.44E+06 | 5.60E+07 | 2.02E+06 |
| Thymidine-5'-phosphate II | [M-H]- | 321.0493 | 321.0492 | -0.3191 | | 9.46E+07 | |
| Uridine 2',3'-cyclic monophosphate; Cyclic 3',5'-uridine monophosphate I | [M-H]- | 305.0180 | 305.0181 | 0.3278 | 1.06E+08 | 5.68E+07 | |
| Uridine 2',3'-cyclic monophosphate; Cyclic 3',5'-uridine monophosphate II | [M-H]- | 305.0180 | 305.0181 | 0.3203 | 2.42E+07 | 5.46E+08 | |
| Uridine 3'-monophosphate | [M-H]- | 323.0286 | 323.0285 | -0.3096 | 1.16E+07 | 4.74E+08 | |
| Uridine 5'-monophosphate | [M-H]- | 323.0286 | 323.0285 | -0.3096 | 5.64E+08 | 2.57E+08 | 5.31E+07 |

| Ribonucleoside 3'-phosphates | | | | | | |
|---|-----------|----------|----------|---------|----------|----------|
| Adenosine 3'-monophosphate (3'-AMP) I | [M-H]- | 346.0558 | 346.0557 | -0.2890 | 5.00E+06 | 3.90E+08 |
| Guanosine-3'-monophosphate I | [M-H]- | 362.0507 | 362.0506 | -0.2746 | | 2.42E+08 |
| Guanosine-3'-monophosphate II | [M-H]- | 362.0507 | 362.0508 | 0.2778 | | 1.58E+08 |
| Amino acids, peptides, and analogues | | | | | | |
| Asparagine | [M-H]- | 131.0462 | 131.0461 | -0.7631 | 1.79E+08 | 1.94E+08 |
| Aspartic acid | [M-H]- | 132.0302 | 132.0303 | 0.7574 | 1.46E+08 | 1.12E+08 |
| Citrulline | [M-H]- | 174.0884 | 174.0885 | 0.5744 | 6.04E+07 | 3.85E+07 |
| Cysteic acid | [M-H]- | 167.9972 | 167.9967 | -2.9762 | 6.99E+07 | 3.36E+07 |
| Diaminopimelic acid | [M-H]- | 189.0881 | 189.0881 | 0.0000 | 1.72E+06 | 1.03E+07 |
| Glutathione (oxidized) | [M-H]- | 611.1447 | 611.1446 | -0.1636 | 4.99E+07 | |
| Glutathionesulfonic acid I | [M-H]- | 354.0612 | 354.0612 | 0.0000 | 8.54E+08 | 1.83E+07 |
| Homocysteic acid | [M-H]- | 182.0128 | 182.0135 | 3.8459 | 1.29E+08 | 9.93E+07 |
| L-Glutamic acid | [M-H]- | 146.0459 | 146.0458 | -0.6847 | 1.21E+09 | 8.78E+08 |
| N-Undecanoylglycine | [M-H]- | 242.1761 | 242.1761 | 0.0000 | 7.80E+07 | 8.20E+07 |
| Serine | [M-H]- | 104.0353 | 104.0352 | -0.9612 | 3.02E+07 | 4.40E+07 |
| Threonine;allo-threonine | [M-H]- | 118.0509 | 118.0509 | 0.0000 | 4.91E+07 | 9.44E+07 |
| Organic acids and derivatives | | | | | | |
| Citric acid I | [M-H]- | 191.0197 | 191.0199 | 1.0470 | | 7.43E+06 |
| Citric acid II | [M-H]- | 191.0197 | 191.0197 | 0.0000 | | 2.97E+08 |
| Glycerophosphoglycerol | [M-H]- | 245.0432 | 245.0431 | -0.4081 | 8.88E+07 | 3.53E+09 |
| L-lactic acid; 3-hydroxypropionic acid | [M-H]- | | | | 2.56E+07 | 3.20E+07 |
| Malic acid | [M-H]- | 133.0142 | 133.0142 | 0.0000 | 4.37E+08 | 9.12E+08 |
| Succinic acid; methylmalonic acid III | [M-H]- | 117.0193 | 117.0193 | 0.0000 | 1.21E+09 | 1.81E+09 |
| Carbohydrates and carbohydrate conjugates | | | | | | |
| Arabinonic acid; D-Lyxonic acid; D-Ribulose; Ribonic acid; D-xylonic acid | [M-H]- | 165.0404 | 165.0404 | 0.0000 | 2.95E+08 | 5.23E+08 |
| Cytidine-3'-monophosphate | [M-H]- | 322.0446 | 322.0447 | 0.3105 | 1.94E+06 | 2.84E+07 |
| D-Glucosamine 6-phosphate | [M-H]- | 258.0384 | 258.0385 | 0.3875 | 1.31E+07 | 1.48E+08 |
| Disaccharide | [M+HCOO]- | 387.1144 | 387.1142 | -0.5166 | 2.76E+09 | 1.51E+09 |
| D-Threonic acid | [M-H]- | 135.0299 | 135.0315 | 11.8492 | | 2.60E+08 |
| Gluconic acid I | [M-H]- | 195.0510 | 195.0510 | 0.0000 | 1.32E+08 | 7.55E+07 |
| Gluconic acid II | [M-H]- | 195.0510 | 195.0510 | 0.0000 | 3.27E+07 | 2.46E+07 |
| L-Threonic acid | [M-H]- | 135.0299 | 135.0299 | 0.0000 | 7.02E+08 | 7.55E+08 |
| | | | | | | 6.23E+08 |

Roman numbering represents different isomers; FA, fatty acid, DGDG, digalactosyldiacylglycerol; DGMG, digalactosylmonoacylglycerol; DGTS, diacylglyceryl-O-4'-(N,N,N-trimethyl) homoserine; LPA, monoacylglycerophosphate; LPC, lysophosphatidylcholine, LPE, lysophosphatidylethanolamine; MGMG, Monogalactosyl monoacylglycerol; MGDG, Monogalactosyldiacylglycerol; MGTS, monoacylglyceryl-O-4'-(N,N,N-trimethyl) homoserine; PE, phosphatidylethanolamine.

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