Supplementary Table S3 General statistics of the Serum Dataset

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | ILW 1 | | | | ID2 | | | |
| Metabolites | Mean | SD | Min | Max | Mean | SD | Min | Max |
| C0 | 6.871 | 0.598 | 5.710 | 7.610 | 6.605 | 0.602 | 5.460 | 7.570 |
| C10 | 0.073 | 0.009 | 0.060 | 0.091 | 0.070 | 0.010 | 0.058 | 0.092 |
| C10:2 | 0.027 | 0.004 | 0.019 | 0.034 | 0.029 | 0.004 | 0.023 | 0.034 |
| C12 | 0.037 | 0.007 | 0.027 | 0.050 | 0.035 | 0.005 | 0.028 | 0.043 |
| C12-DC | 0.104 | 0.005 | 0.096 | 0.112 | 0.104 | 0.006 | 0.092 | 0.114 |
| C14 | 0.017 | 0.004 | 0.011 | 0.024 | 0.017 | 0.010 | 0.010 | 0.049 |
| C14:1 | 0.035 | 0.004 | 0.027 | 0.041 | 0.031 | 0.009 | 0.022 | 0.048 |
| C14:1-OH | 0.009 | 0.002 | 0.005 | 0.011 | 0.008 | 0.002 | 0.006 | 0.012 |
| C14:2 | 0.006 | 0.002 | 0.003 | 0.008 | 0.005 | 0.001 | 0.003 | 0.006 |
| C16 | 0.026 | 0.006 | 0.017 | 0.038 | 0.023 | 0.010 | 0.013 | 0.046 |
| C16-OH | 0.008 | 0.001 | 0.006 | 0.010 | 0.007 | 0.001 | 0.006 | 0.011 |
| C16:1 | 0.023 | 0.004 | 0.018 | 0.029 | 0.021 | 0.005 | 0.017 | 0.032 |
| C16:2-OH | 0.006 | 0.001 | 0.004 | 0.007 | 0.006 | 0.001 | 0.003 | 0.008 |
| C18 | 0.020 | 0.005 | 0.013 | 0.028 | 0.018 | 0.006 | 0.011 | 0.031 |
| C18:1 | 0.031 | 0.011 | 0.015 | 0.053 | 0.026 | 0.012 | 0.010 | 0.051 |
| C18:2 | 0.011 | 0.004 | 0.007 | 0.019 | 0.008 | 0.003 | 0.005 | 0.013 |
| C2 | 1.419 | 0.215 | 1.030 | 1.690 | 1.719 | 0.713 | 1.080 | 3.800 |
| C3 | 0.091 | 0.018 | 0.070 | 0.140 | 0.079 | 0.024 | 0.051 | 0.144 |
| C3-DC (C4-OH) | 0.061 | 0.006 | 0.053 | 0.072 | 0.062 | 0.009 | 0.049 | 0.079 |
| C3-OH | 0.034 | 0.004 | 0.028 | 0.042 | 0.038 | 0.003 | 0.033 | 0.044 |
| C3:1 | 0.011 | 0.001 | 0.009 | 0.014 | 0.012 | 0.003 | 0.009 | 0.017 |
| C4 | 0.045 | 0.007 | 0.034 | 0.057 | 0.042 | 0.007 | 0.030 | 0.054 |
| C4:1 | 0.027 | 0.004 | 0.023 | 0.034 | 0.028 | 0.005 | 0.020 | 0.037 |
| C5 | 0.031 | 0.005 | 0.025 | 0.042 | 0.029 | 0.005 | 0.021 | 0.041 |
| C5-DC (C6-OH) | 0.013 | 0.003 | 0.010 | 0.018 | 0.012 | 0.001 | 0.009 | 0.014 |
| C5-M-DC | 0.034 | 0.003 | 0.028 | 0.040 | 0.031 | 0.003 | 0.026 | 0.035 |
| C5-OH (C3-DC-M) | 0.060 | 0.006 | 0.052 | 0.075 | 0.059 | 0.005 | 0.049 | 0.068 |
| C5:1 | 0.022 | 0.004 | 0.015 | 0.028 | 0.022 | 0.003 | 0.017 | 0.026 |
| C6 (C4:1-DC) | 0.033 | 0.004 | 0.028 | 0.041 | 0.037 | 0.006 | 0.030 | 0.050 |
| C6:1 | 0.018 | 0.003 | 0.012 | 0.021 | 0.018 | 0.003 | 0.014 | 0.023 |
| C8 | 0.075 | 0.007 | 0.064 | 0.086 | 0.075 | 0.007 | 0.061 | 0.084 |
| C9 | 0.020 | 0.005 | 0.015 | 0.030 | 0.024 | 0.002 | 0.020 | 0.028 |
| PC aa C28:1 | 0.984 | 0.336 | 0.629 | 1.820 | 0.803 | 0.224 | 0.553 | 1.200 |
| PC aa C30:0 | 1.603 | 0.325 | 1.110 | 2.380 | 1.279 | 0.185 | 0.990 | 1.730 |
| PC aa C32:0 | 5.100 | 1.126 | 3.930 | 8.280 | 4.258 | 0.575 | 3.560 | 5.340 |
| PC aa C32:1 | 1.827 | 0.379 | 1.200 | 2.540 | 1.776 | 0.352 | 1.360 | 2.680 |
| PC aa C32:2 | 0.661 | 0.125 | 0.467 | 0.904 | 0.588 | 0.105 | 0.442 | 0.776 |
| PC aa C32:3 | 0.221 | 0.078 | 0.136 | 0.381 | 0.178 | 0.061 | 0.130 | 0.332 |
| PC aa C34:1 | 77.950 | 15.460 | 50.400 | 99.900 | 71.950 | 10.306 | 62.600 | 91.200 |
| PC aa C34:2 | 110.658 | 20.102 | 80.800 | 153.000 | 95.875 | 16.550 | 75.600 | 129.000 |
| PC aa C34:3 | 3.538 | 0.657 | 2.740 | 5.070 | 3.272 | 0.593 | 2.490 | 4.620 |
| PC aa C34:4 | 0.247 | 0.040 | 0.183 | 0.302 | 0.219 | 0.024 | 0.191 | 0.262 |
| PC aa C36:1 | 41.917 | 5.844 | 30.400 | 51.700 | 41.433 | 6.470 | 34.100 | 54.500 |
| PC aa C36:2 | 131.250 | 15.286 | 108.000 | 156.000 | 121.458 | 20.834 | 97.500 | 161.000 |
| PC aa C36:3 | 27.633 | 5.616 | 23.200 | 44.200 | 24.925 | 4.427 | 18.700 | 33.500 |
| PC aa C36:4 | 66.808 | 10.449 | 50.800 | 80.400 | 59.242 | 8.201 | 43.400 | 75.300 |
| PC aa C36:5 | 1.990 | 0.322 | 1.490 | 2.460 | 1.715 | 0.231 | 1.380 | 2.240 |
| PC aa C36:6 | 0.146 | 0.037 | 0.086 | 0.215 | 0.110 | 0.028 | 0.076 | 0.160 |
| PC aa C38:0 | 0.558 | 0.121 | 0.405 | 0.859 | 0.426 | 0.077 | 0.296 | 0.568 |
| PC aa C38:3 | 21.817 | 2.414 | 18.700 | 27.200 | 19.083 | 4.479 | 13.800 | 27.900 |
| PC aa C38:4 | 159.667 | 26.095 | 134.000 | 220.000 | 159.000 | 27.366 | 134.000 | 210.000 |
| PC aa C38:5 | 35.175 | 5.355 | 26.000 | 44.200 | 32.250 | 4.433 | 27.500 | 42.100 |
| PC aa C38:6 | 14.775 | 3.456 | 10.400 | 21.100 | 11.383 | 2.932 | 6.880 | 17.000 |
| PC aa C40:1 | 0.315 | 0.056 | 0.222 | 0.427 | 0.284 | 0.060 | 0.213 | 0.418 |
| PC aa C40:2 | 0.344 | 0.056 | 0.244 | 0.461 | 0.348 | 0.045 | 0.266 | 0.437 |
| PC aa C40:3 | 0.540 | 0.083 | 0.426 | 0.650 | 0.535 | 0.101 | 0.399 | 0.725 |
| PC aa C40:4 | 10.833 | 2.286 | 6.210 | 14.100 | 10.350 | 2.192 | 6.690 | 13.300 |
| PC aa C40:5 | 22.483 | 3.960 | 15.400 | 28.100 | 21.358 | 4.010 | 17.100 | 31.000 |
| PC aa C40:6 | 13.887 | 3.440 | 8.460 | 18.800 | 10.917 | 4.276 | 6.550 | 20.700 |
| PC aa C42:0 | 0.147 | 0.031 | 0.106 | 0.216 | 0.126 | 0.024 | 0.094 | 0.169 |
| PC aa C42:1 | 0.107 | 0.025 | 0.069 | 0.152 | 0.097 | 0.016 | 0.072 | 0.122 |
| PC aa C42:2 | 0.128 | 0.023 | 0.101 | 0.170 | 0.103 | 0.015 | 0.076 | 0.139 |
| PC aa C42:4 | 0.179 | 0.023 | 0.131 | 0.226 | 0.150 | 0.029 | 0.105 | 0.208 |
| PC aa C42:5 | 0.214 | 0.026 | 0.153 | 0.245 | 0.184 | 0.042 | 0.109 | 0.272 |
| PC aa C42:6 | 0.595 | 0.084 | 0.485 | 0.763 | 0.500 | 0.076 | 0.389 | 0.610 |
| PC ae C30:0 | 0.453 | 0.103 | 0.312 | 0.660 | 0.361 | 0.082 | 0.267 | 0.517 |
| PC ae C32:1 | 1.607 | 0.349 | 1.230 | 2.420 | 1.399 | 0.291 | 1.030 | 1.920 |
| PC ae C34:0 | 0.661 | 0.147 | 0.484 | 0.987 | 0.525 | 0.131 | 0.353 | 0.743 |
| PC ae C34:1 | 5.094 | 0.742 | 3.620 | 6.370 | 4.597 | 0.627 | 3.640 | 5.700 |
| PC ae C34:2 | 5.763 | 1.007 | 3.800 | 7.530 | 5.566 | 0.983 | 4.080 | 7.750 |
| PC ae C34:3 | 2.706 | 0.442 | 1.900 | 3.180 | 2.863 | 0.360 | 2.080 | 3.330 |
| PC ae C36:1 | 3.274 | 0.717 | 2.160 | 4.930 | 2.888 | 0.546 | 2.080 | 3.710 |
| PC ae C36:2 | 6.034 | 1.224 | 4.210 | 9.210 | 5.258 | 0.971 | 4.130 | 6.920 |
| PC ae C36:3 | 3.903 | 0.646 | 2.620 | 4.980 | 3.702 | 0.645 | 2.620 | 4.760 |
| PC ae C36:4 | 4.114 | 0.917 | 2.620 | 5.850 | 3.753 | 0.512 | 2.970 | 4.550 |
| PC ae C36:5 | 1.806 | 0.234 | 1.420 | 2.240 | 1.701 | 0.242 | 1.260 | 1.980 |
| PC ae C38:0 | 0.556 | 0.038 | 0.495 | 0.618 | 0.499 | 0.076 | 0.360 | 0.614 |
| PC ae C38:1 | 0.680 | 0.106 | 0.536 | 0.909 | 0.553 | 0.157 | 0.291 | 0.851 |
| PC ae C38:2 | 1.115 | 0.174 | 0.851 | 1.500 | 0.966 | 0.178 | 0.665 | 1.350 |
| PC ae C38:3 | 1.392 | 0.263 | 0.967 | 1.990 | 1.145 | 0.272 | 0.832 | 1.650 |
| PC ae C38:4 | 8.358 | 1.532 | 5.750 | 11.300 | 7.053 | 1.273 | 5.450 | 10.400 |
| PC ae C38:5 | 4.387 | 0.843 | 3.090 | 5.750 | 3.874 | 0.560 | 3.050 | 4.940 |
| PC ae C38:6 | 1.028 | 0.192 | 0.707 | 1.430 | 0.893 | 0.126 | 0.701 | 1.090 |
| PC ae C40:1 | 1.021 | 0.136 | 0.848 | 1.290 | 0.834 | 0.137 | 0.627 | 1.120 |
| PC ae C40:2 | 0.370 | 0.050 | 0.283 | 0.482 | 0.333 | 0.054 | 0.270 | 0.445 |
| PC ae C40:3 | 0.559 | 0.088 | 0.417 | 0.701 | 0.502 | 0.088 | 0.398 | 0.659 |
| PC ae C40:4 | 1.891 | 0.303 | 1.440 | 2.420 | 1.635 | 0.240 | 1.330 | 2.140 |
| PC ae C40:5 | 2.072 | 0.353 | 1.540 | 2.700 | 1.721 | 0.302 | 1.290 | 2.310 |
| PC ae C40:6 | 1.280 | 0.288 | 0.756 | 1.760 | 0.943 | 0.201 | 0.614 | 1.350 |
| PC ae C42:0 | 0.550 | 0.106 | 0.416 | 0.812 | 0.479 | 0.055 | 0.425 | 0.600 |
| PC ae C42:1 | 1.315 | 0.357 | 0.657 | 2.020 | 1.178 | 0.295 | 0.844 | 1.770 |
| PC ae C42:2 | 0.472 | 0.087 | 0.277 | 0.581 | 0.421 | 0.057 | 0.310 | 0.509 |
| PC ae C42:3 | 0.343 | 0.145 | 0.189 | 0.673 | 0.230 | 0.075 | 0.144 | 0.437 |
| PC ae C42:4 | 0.254 | 0.052 | 0.160 | 0.336 | 0.209 | 0.040 | 0.148 | 0.292 |
| PC ae C42:5 | 0.606 | 0.095 | 0.502 | 0.794 | 0.530 | 0.083 | 0.408 | 0.715 |
| PC ae C44:4 | 0.173 | 0.061 | 0.103 | 0.330 | 0.134 | 0.031 | 0.099 | 0.203 |
| PC ae C44:5 | 0.244 | 0.073 | 0.171 | 0.412 | 0.195 | 0.047 | 0.120 | 0.264 |
| PC ae C44:6 | 0.224 | 0.064 | 0.155 | 0.353 | 0.195 | 0.053 | 0.101 | 0.276 |
| lysoPC a C14:0 | 1.527 | 0.145 | 1.350 | 1.810 | 1.569 | 0.098 | 1.450 | 1.770 |
| lysoPC a C16:0 | 43.817 | 5.433 | 35.100 | 51.200 | 42.442 | 5.504 | 33.500 | 50.200 |
| lysoPC a C16:1 | 1.127 | 0.143 | 0.832 | 1.330 | 1.175 | 0.171 | 0.988 | 1.500 |
| lysoPC a C17:0 | 0.974 | 0.180 | 0.632 | 1.280 | 0.858 | 0.170 | 0.606 | 1.210 |
| lysoPC a C18:0 | 27.850 | 2.722 | 25.100 | 33.600 | 28.092 | 3.930 | 19.200 | 32.400 |
| lysoPC a C18:1 | 14.629 | 2.530 | 9.550 | 18.600 | 14.092 | 1.928 | 10.400 | 16.700 |
| lysoPC a C18:2 | 19.950 | 3.787 | 12.300 | 24.900 | 16.050 | 2.495 | 12.200 | 20.100 |
| lysoPC a C20:3 | 1.224 | 0.323 | 0.700 | 1.850 | 0.913 | 0.214 | 0.670 | 1.350 |
| lysoPC a C20:4 | 9.844 | 2.657 | 6.020 | 14.400 | 7.854 | 1.369 | 5.490 | 9.840 |
| lysoPC a C26:1 | 2.882 | 0.427 | 2.360 | 3.740 | 2.738 | 0.432 | 2.260 | 3.740 |
| SM (OH) C14:1 | 1.743 | 0.213 | 1.300 | 2.220 | 1.369 | 0.176 | 1.080 | 1.670 |
| SM (OH) C16:1 | 2.434 | 0.390 | 1.910 | 3.190 | 1.826 | 0.286 | 1.480 | 2.420 |
| SM (OH) C22:1 | 3.403 | 0.310 | 2.770 | 3.880 | 3.341 | 0.343 | 2.860 | 3.940 |
| SM (OH) C22:2 | 1.486 | 0.156 | 1.250 | 1.840 | 1.304 | 0.168 | 1.060 | 1.630 |
| SM (OH) C24:1 | 0.306 | 0.049 | 0.222 | 0.370 | 0.302 | 0.034 | 0.232 | 0.343 |
| SM C16:0 | 74.358 | 7.120 | 60.500 | 84.700 | 61.775 | 5.134 | 53.800 | 69.800 |
| SM C16:1 | 4.868 | 0.523 | 4.180 | 6.030 | 4.155 | 0.611 | 3.240 | 5.640 |
| SM C18:0 | 15.242 | 1.834 | 11.200 | 17.800 | 13.667 | 1.952 | 11.300 | 17.300 |
| SM C18:1 | 3.822 | 0.503 | 3.070 | 4.750 | 3.320 | 0.427 | 2.450 | 3.850 |
| SM C20:2 | 0.196 | 0.030 | 0.147 | 0.267 | 0.164 | 0.015 | 0.139 | 0.195 |
| SM C24:0 | 10.762 | 0.969 | 8.540 | 11.900 | 9.700 | 1.035 | 7.660 | 12.100 |
| SM C24:1 | 16.575 | 2.073 | 12.500 | 20.900 | 13.867 | 1.726 | 11.300 | 16.900 |
| H1 | 5349.250 | 595.848 | 4385.000 | 6221.000 | 5782.000 | 1739.606 | 3901.000 | 9726.000 |
| Ala | 452.000 | 73.308 | 321.000 | 577.000 | 522.250 | 108.610 | 366.000 | 723.000 |
| Arg | 229.417 | 29.980 | 180.000 | 310.000 | 228.000 | 23.733 | 194.000 | 266.000 |
| Asn | 54.150 | 9.180 | 39.100 | 70.700 | 59.058 | 12.108 | 41.900 | 91.500 |
| Cit | 76.817 | 14.025 | 53.600 | 102.000 | 81.942 | 17.880 | 47.000 | 110.000 |
| Gln | 618.167 | 89.120 | 511.000 | 767.000 | 708.167 | 125.893 | 530.000 | 1010.000 |
| Glu | 264.833 | 43.401 | 200.000 | 334.000 | 230.083 | 51.796 | 156.000 | 347.000 |
| Gly | 925.000 | 107.463 | 649.000 | 1060.000 | 1030.917 | 143.013 | 789.000 | 1220.000 |
| His | 121.092 | 18.202 | 99.100 | 153.000 | 125.917 | 19.335 | 94.200 | 161.000 |
| Ile | 147.083 | 21.890 | 106.000 | 178.000 | 136.667 | 21.744 | 112.000 | 183.000 |
| Leu | 245.083 | 34.964 | 186.000 | 294.000 | 229.583 | 33.835 | 190.000 | 307.000 |
| Lys | 332.833 | 47.530 | 235.000 | 416.000 | 360.583 | 51.318 | 317.000 | 496.000 |
| Met | 51.758 | 10.120 | 31.100 | 65.700 | 53.858 | 9.505 | 42.300 | 77.700 |
| Orn | 97.842 | 18.710 | 67.000 | 127.000 | 111.150 | 21.194 | 86.500 | 163.000 |
| Phe | 95.783 | 13.969 | 72.500 | 113.000 | 96.267 | 12.674 | 84.300 | 127.000 |
| Pro | 210.333 | 35.041 | 159.000 | 275.000 | 236.250 | 41.687 | 190.000 | 348.000 |
| Ser | 139.250 | 22.736 | 108.000 | 182.000 | 136.583 | 16.747 | 107.000 | 163.000 |
| Thr | 150.208 | 26.405 | 94.500 | 191.000 | 172.417 | 24.284 | 153.000 | 240.000 |
| Trp | 73.250 | 11.667 | 56.000 | 91.400 | 63.392 | 10.913 | 47.800 | 78.300 |
| Tyr | 99.625 | 18.783 | 65.200 | 124.000 | 100.792 | 26.368 | 76.100 | 173.000 |
| Val | 327.833 | 45.279 | 230.000 | 390.000 | 297.583 | 46.381 | 246.000 | 388.000 |
| Ac-Orn | 6.238 | 3.475 | 1.820 | 13.200 | 12.976 | 2.357 | 8.710 | 16.000 |
| Carnosine | 39.425 | 9.406 | 30.800 | 64.300 | 50.583 | 18.235 | 32.700 | 92.900 |
| Creatinine | 174.500 | 25.232 | 146.000 | 241.000 | 199.500 | 34.031 | 144.000 | 264.000 |
| Kynurenine | 0.557 | 0.198 | 0.000 | 0.722 | 1.091 | 0.418 | 0.641 | 2.130 |
| Met-SO | 0.935 | 0.419 | 0.333 | 1.790 | 0.813 | 0.339 | 0.378 | 1.510 |
| Putrescine | 1.316 | 0.350 | 0.945 | 2.170 | 1.311 | 0.302 | 0.973 | 2.160 |
| Sarcosine | 11.933 | 2.856 | 8.210 | 17.300 | 13.850 | 2.640 | 11.500 | 19.600 |
| Serotonin | 5.892 | 2.387 | 1.720 | 10.100 | 4.766 | 1.340 | 2.790 | 7.010 |
| Spermidine | 0.558 | 0.118 | 0.412 | 0.745 | 0.697 | 0.330 | 0.421 | 1.650 |
| Spermine | 0.376 | 0.028 | 0.325 | 0.416 | 0.415 | 0.104 | 0.329 | 0.729 |
| Taurine | 206.083 | 25.314 | 174.000 | 262.000 | 206.167 | 23.794 | 150.000 | 238.000 |
| alpha-AAA | 25.527 | 11.462 | 9.720 | 45.900 | 21.725 | 8.809 | 11.100 | 43.200 |
| total DMA | 1.052 | 0.131 | 0.924 | 1.300 | 1.173 | 0.238 | 0.856 | 1.620 |

Mean = Mean computed after quality control; SD = Standard Deviation; Min = minimum concentration measured; Max = maximum concentration measured.

1 Statistics of the metabolites concentrations considering only the Italian Large White Dataset.

2 Statistics of the metabolites concentrations considering only the Italian Duroc Dataset.

3 Metabolites are named according with abbreviations provided by Biocrates.