Supplementary Table S2 General statistics of the Plasma Dataset

|  |  |  |
| --- | --- | --- |
|  | ILW 1 | ID2 |
| Metabolites | Mean | SD | Min | Max | Mean | SD | Min | Max |
| C0 | 6.354 | 0.710 | 5.120 | 7.750 | 6.422 | 0.913 | 5.390 | 7.760 |
| C10 | 0.071 | 0.008 | 0.056 | 0.087 | 0.070 | 0.011 | 0.059 | 0.091 |
| C10:2 | 0.022 | 0.004 | 0.017 | 0.030 | 0.020 | 0.003 | 0.013 | 0.024 |
| C12 | 0.039 | 0.004 | 0.031 | 0.044 | 0.036 | 0.006 | 0.029 | 0.048 |
| C12:DC | 0.104 | 0.008 | 0.090 | 0.119 | 0.101 | 0.006 | 0.091 | 0.113 |
| C14 | 0.015 | 0.004 | 0.007 | 0.022 | 0.017 | 0.004 | 0.012 | 0.024 |
| C14:1 | 0.031 | 0.007 | 0.023 | 0.044 | 0.033 | 0.006 | 0.024 | 0.046 |
| C14:1-OH | 0.008 | 0.001 | 0.006 | 0.010 | 0.009 | 0.001 | 0.006 | 0.010 |
| C14:2 | 0.006 | 0.002 | 0.003 | 0.010 | 0.006 | 0.001 | 0.004 | 0.008 |
| C16 | 0.022 | 0.008 | 0.009 | 0.036 | 0.026 | 0.006 | 0.016 | 0.034 |
| C16-OH | 0.008 | 0.002 | 0.005 | 0.011 | 0.007 | 0.002 | 0.003 | 0.009 |
| C16:1 | 0.021 | 0.002 | 0.017 | 0.026 | 0.022 | 0.003 | 0.018 | 0.027 |
| C16:2-OH | 0.006 | 0.001 | 0.003 | 0.008 | 0.005 | 0.001 | 0.003 | 0.007 |
| C18 | 0.016 | 0.007 | 0.009 | 0.027 | 0.018 | 0.004 | 0.010 | 0.025 |
| C18:1 | 0.025 | 0.011 | 0.013 | 0.046 | 0.029 | 0.006 | 0.017 | 0.038 |
| C18:2 | 0.008 | 0.003 | 0.003 | 0.014 | 0.012 | 0.005 | 0.006 | 0.021 |
| C2 | 1.623 | 0.650 | 0.991 | 3.460 | 1.282 | 0.240 | 0.977 | 1.750 |
| C3 | 0.075 | 0.018 | 0.058 | 0.116 | 0.083 | 0.015 | 0.063 | 0.114 |
| C3-DC (C4:OH) | 0.054 | 0.008 | 0.040 | 0.068 | 0.049 | 0.009 | 0.035 | 0.059 |
| C3-OH | 0.036 | 0.005 | 0.024 | 0.043 | 0.034 | 0.005 | 0.025 | 0.040 |
| C3:1 | 0.010 | 0.002 | 0.007 | 0.014 | 0.011 | 0.002 | 0.009 | 0.013 |
| C4 | 0.041 | 0.007 | 0.030 | 0.052 | 0.043 | 0.007 | 0.032 | 0.054 |
| C4:1 | 0.028 | 0.004 | 0.023 | 0.036 | 0.025 | 0.002 | 0.022 | 0.027 |
| C5 | 0.029 | 0.003 | 0.022 | 0.035 | 0.027 | 0.003 | 0.022 | 0.034 |
| C5-DC (C6:OH) | 0.013 | 0.003 | 0.008 | 0.018 | 0.011 | 0.003 | 0.006 | 0.017 |
| C5-M-DC | 0.031 | 0.003 | 0.024 | 0.036 | 0.033 | 0.003 | 0.028 | 0.039 |
| C5-OH (C3-DC-M) | 0.059 | 0.008 | 0.044 | 0.074 | 0.057 | 0.005 | 0.049 | 0.065 |
| C5:1 | 0.021 | 0.002 | 0.018 | 0.024 | 0.022 | 0.004 | 0.017 | 0.027 |
| C6 (C4:1-DC) | 0.031 | 0.005 | 0.025 | 0.043 | 0.033 | 0.004 | 0.027 | 0.038 |
| C6:1 | 0.018 | 0.003 | 0.012 | 0.023 | 0.016 | 0.002 | 0.013 | 0.020 |
| C8 | 0.067 | 0.006 | 0.051 | 0.078 | 0.069 | 0.005 | 0.059 | 0.076 |
| C9 | 0.024 | 0.004 | 0.017 | 0.034 | 0.020 | 0.003 | 0.014 | 0.026 |
| PC aa C28:1 | 1.177 | 0.286 | 0.646 | 1.880 | 1.163 | 0.265 | 0.767 | 1.650 |
| PC aa C30:0 | 1.436 | 0.247 | 0.995 | 2.000 | 1.657 | 0.215 | 1.390 | 2.020 |
| PC aa C32:0 | 4.333 | 0.602 | 3.680 | 5.490 | 4.816 | 0.974 | 3.690 | 7.430 |
| PC aa C32:1 | 1.543 | 0.242 | 1.060 | 1.980 | 1.573 | 0.271 | 1.230 | 2.050 |
| PC aa C32:2 | 0.651 | 0.075 | 0.576 | 0.812 | 0.630 | 0.129 | 0.417 | 0.906 |
| PC aa C32:3 | 0.232 | 0.055 | 0.135 | 0.330 | 0.238 | 0.054 | 0.146 | 0.322 |
| PC aa C34:1 | 66.483 | 8.559 | 53.400 | 81.800 | 68.775 | 13.834 | 47.800 | 87.800 |
| PC aa C34:2 | 86.542 | 13.320 | 68.000 | 110.000 | 97.092 | 20.851 | 72.600 | 146.000 |
| PC aa C34:3 | 2.963 | 0.543 | 2.190 | 4.150 | 3.103 | 0.624 | 2.010 | 4.550 |
| PC aa C34:4 | 0.232 | 0.032 | 0.187 | 0.312 | 0.245 | 0.037 | 0.196 | 0.308 |
| PC aa C36:1 | 38.817 | 7.084 | 27.700 | 54.500 | 36.817 | 4.602 | 29.500 | 44.500 |
| PC aa C36:2 | 109.242 | 16.745 | 81.900 | 138.000 | 114.183 | 15.950 | 85.100 | 142.000 |
| PC aa C36:3 | 22.842 | 3.618 | 17.200 | 29.400 | 24.383 | 5.659 | 18.000 | 40.600 |
| PC aa C36:4 | 54.125 | 7.644 | 39.000 | 66.400 | 58.400 | 9.898 | 43.100 | 70.200 |
| PC aa C36:5 | 1.613 | 0.223 | 1.310 | 2.060 | 1.783 | 0.251 | 1.340 | 2.180 |
| PC aa C36:6 | 0.159 | 0.042 | 0.070 | 0.225 | 0.167 | 0.030 | 0.120 | 0.221 |
| PC aa C38:0 | 0.498 | 0.097 | 0.385 | 0.697 | 0.560 | 0.092 | 0.454 | 0.774 |
| PC aa C38:3 | 17.425 | 3.667 | 11.800 | 22.800 | 19.092 | 2.389 | 15.000 | 23.500 |
| PC aa C38:4 | 147.167 | 25.301 | 115.000 | 203.000 | 142.692 | 24.253 | 99.300 | 188.000 |
| PC aa C38:5 | 30.167 | 3.763 | 26.100 | 37.100 | 31.342 | 5.511 | 22.700 | 39.900 |
| PC aa C38:6 | 11.137 | 2.597 | 7.960 | 16.200 | 13.268 | 2.828 | 8.600 | 17.200 |
| PC aa C40:1 | 0.363 | 0.050 | 0.257 | 0.446 | 0.362 | 0.047 | 0.260 | 0.404 |
| PC aa C40:2 | 0.399 | 0.044 | 0.336 | 0.462 | 0.376 | 0.057 | 0.259 | 0.454 |
| PC aa C40:3 | 0.573 | 0.056 | 0.468 | 0.680 | 0.544 | 0.092 | 0.370 | 0.682 |
| PC aa C40:4 | 9.651 | 1.903 | 6.560 | 12.400 | 9.780 | 2.566 | 6.280 | 14.600 |
| PC aa C40:5 | 19.500 | 3.370 | 16.500 | 27.800 | 19.975 | 3.853 | 13.800 | 25.100 |
| PC aa C40:6 | 10.601 | 4.080 | 6.090 | 19.600 | 12.721 | 3.067 | 7.600 | 18.300 |
| PC aa C42:0 | 0.181 | 0.028 | 0.120 | 0.222 | 0.174 | 0.034 | 0.111 | 0.222 |
| PC aa C42:1 | 0.125 | 0.020 | 0.092 | 0.160 | 0.129 | 0.020 | 0.092 | 0.159 |
| PC aa C42:2 | 0.127 | 0.022 | 0.094 | 0.170 | 0.132 | 0.025 | 0.090 | 0.173 |
| PC aa C42:4 | 0.161 | 0.025 | 0.120 | 0.207 | 0.168 | 0.027 | 0.124 | 0.215 |
| PC aa C42:5 | 0.181 | 0.043 | 0.124 | 0.287 | 0.197 | 0.026 | 0.152 | 0.234 |
| PC aa C42:6 | 0.596 | 0.066 | 0.525 | 0.729 | 0.638 | 0.070 | 0.492 | 0.735 |
| PC ae C30:0 | 0.493 | 0.105 | 0.295 | 0.736 | 0.500 | 0.090 | 0.335 | 0.639 |
| PC ae C32:1 | 1.664 | 0.366 | 0.961 | 2.510 | 1.673 | 0.260 | 1.240 | 2.070 |
| PC ae C34:0 | 0.597 | 0.145 | 0.430 | 0.876 | 0.646 | 0.119 | 0.489 | 0.911 |
| PC ae C34:1 | 4.369 | 0.623 | 3.340 | 5.210 | 4.582 | 0.717 | 3.740 | 6.240 |
| PC ae C34:2 | 5.188 | 0.867 | 3.590 | 6.870 | 5.014 | 1.008 | 3.640 | 6.750 |
| PC ae C34:3 | 2.738 | 0.345 | 1.970 | 3.170 | 2.542 | 0.375 | 2.070 | 3.480 |
| PC ae C36:1 | 2.852 | 0.558 | 2.060 | 3.740 | 3.113 | 0.641 | 2.300 | 4.840 |
| PC ae C36:2 | 4.824 | 0.860 | 3.560 | 6.060 | 5.303 | 1.117 | 4.170 | 8.430 |
| PC ae C36:3 | 3.403 | 0.643 | 2.220 | 4.410 | 3.461 | 0.648 | 2.520 | 4.950 |
| PC ae C36:4 | 3.457 | 0.434 | 2.670 | 4.060 | 3.687 | 0.662 | 2.680 | 4.760 |
| PC ae C36:5 | 1.673 | 0.217 | 1.300 | 1.920 | 1.642 | 0.186 | 1.370 | 1.930 |
| PC ae C38:0 | 0.537 | 0.087 | 0.428 | 0.665 | 0.547 | 0.050 | 0.445 | 0.652 |
| PC ae C38:1 | 0.698 | 0.170 | 0.366 | 0.962 | 0.720 | 0.114 | 0.529 | 0.938 |
| PC ae C38:2 | 0.998 | 0.171 | 0.734 | 1.280 | 1.102 | 0.166 | 0.931 | 1.490 |
| PC ae C38:3 | 1.092 | 0.228 | 0.820 | 1.490 | 1.259 | 0.228 | 1.060 | 1.890 |
| PC ae C38:4 | 6.513 | 1.025 | 4.910 | 8.830 | 7.257 | 1.073 | 5.810 | 9.320 |
| PC ae C38:5 | 3.665 | 0.515 | 2.820 | 4.490 | 3.918 | 0.606 | 2.790 | 4.840 |
| PC ae C38:6 | 0.872 | 0.144 | 0.643 | 1.110 | 0.937 | 0.124 | 0.737 | 1.180 |
| PC ae C40:1 | 0.931 | 0.164 | 0.735 | 1.310 | 1.017 | 0.157 | 0.786 | 1.300 |
| PC ae C40:2 | 0.375 | 0.053 | 0.292 | 0.490 | 0.386 | 0.046 | 0.323 | 0.466 |
| PC ae C40:3 | 0.600 | 0.094 | 0.453 | 0.752 | 0.586 | 0.075 | 0.462 | 0.689 |
| PC ae C40:4 | 1.591 | 0.262 | 1.220 | 2.150 | 1.731 | 0.226 | 1.460 | 2.290 |
| PC ae C40:5 | 1.624 | 0.244 | 1.240 | 2.080 | 1.865 | 0.286 | 1.450 | 2.410 |
| PC ae C40:6 | 0.914 | 0.191 | 0.603 | 1.290 | 1.143 | 0.186 | 0.870 | 1.520 |
| PC ae C42:0 | 0.561 | 0.064 | 0.479 | 0.724 | 0.602 | 0.103 | 0.459 | 0.807 |
| PC ae C42:1 | 1.640 | 0.373 | 1.020 | 2.370 | 1.584 | 0.369 | 0.887 | 2.030 |
| PC ae C42:2 | 0.537 | 0.108 | 0.409 | 0.751 | 0.518 | 0.133 | 0.330 | 0.736 |
| PC ae C42:3 | 0.355 | 0.107 | 0.184 | 0.547 | 0.392 | 0.100 | 0.225 | 0.573 |
| PC ae C42:4 | 0.229 | 0.046 | 0.154 | 0.320 | 0.247 | 0.030 | 0.197 | 0.286 |
| PC ae C42:5 | 0.538 | 0.080 | 0.417 | 0.707 | 0.593 | 0.063 | 0.525 | 0.699 |
| PC ae C44:4 | 0.171 | 0.039 | 0.119 | 0.255 | 0.181 | 0.036 | 0.121 | 0.236 |
| PC ae C44:5 | 0.231 | 0.051 | 0.167 | 0.352 | 0.256 | 0.042 | 0.186 | 0.317 |
| PC ae C44:6 | 0.199 | 0.050 | 0.124 | 0.314 | 0.220 | 0.039 | 0.171 | 0.287 |
| lysoPC a C14:0 | 1.560 | 0.087 | 1.400 | 1.690 | 1.530 | 0.153 | 1.370 | 1.820 |
| lysoPC a C16:0 | 46.525 | 4.564 | 37.200 | 53.600 | 45.750 | 7.006 | 31.500 | 57.300 |
| lysoPC a C16:1 | 1.291 | 0.139 | 0.989 | 1.500 | 1.175 | 0.155 | 0.941 | 1.450 |
| lysoPC a C17:0 | 1.049 | 0.212 | 0.864 | 1.540 | 1.081 | 0.230 | 0.708 | 1.490 |
| lysoPC a C18:0 | 30.517 | 4.218 | 23.100 | 36.600 | 29.400 | 3.186 | 22.200 | 33.600 |
| lysoPC a C18:1 | 14.383 | 1.452 | 12.100 | 16.700 | 14.617 | 2.122 | 11.100 | 18.400 |
| lysoPC a C18:2 | 16.100 | 1.960 | 12.800 | 19.700 | 19.300 | 3.386 | 13.500 | 23.700 |
| lysoPC a C20:3 | 0.919 | 0.156 | 0.731 | 1.250 | 1.157 | 0.260 | 0.805 | 1.610 |
| lysoPC a C20:4 | 7.674 | 1.203 | 5.650 | 9.840 | 9.359 | 2.181 | 6.030 | 12.400 |
| lysoPC a C26:1 | 3.159 | 0.418 | 2.300 | 3.990 | 3.138 | 0.423 | 2.460 | 3.870 |
| SM (OH) C14:1 | 1.398 | 0.147 | 1.190 | 1.600 | 1.685 | 0.179 | 1.400 | 1.950 |
| SM (OH) C16:1 | 1.880 | 0.303 | 1.550 | 2.630 | 2.298 | 0.299 | 2.030 | 2.920 |
| SM (OH) C22:1 | 3.209 | 0.355 | 2.720 | 3.880 | 3.163 | 0.402 | 2.540 | 3.760 |
| SM (OH) C22:2 | 1.273 | 0.211 | 1.060 | 1.860 | 1.346 | 0.158 | 1.030 | 1.530 |
| SM (OH) C24:1 | 0.302 | 0.048 | 0.220 | 0.377 | 0.288 | 0.061 | 0.214 | 0.436 |
| SM C16:0 | 60.358 | 5.058 | 51.700 | 69.400 | 68.800 | 7.460 | 55.700 | 79.800 |
| SM C16:1 | 3.909 | 0.672 | 3.100 | 5.670 | 4.466 | 0.536 | 3.500 | 5.380 |
| SM C18:0 | 13.433 | 1.857 | 10.600 | 16.700 | 14.325 | 1.260 | 12.000 | 15.800 |
| SM C18:1 | 3.043 | 0.363 | 2.440 | 3.520 | 3.513 | 0.462 | 2.660 | 4.270 |
| SM C20:2 | 0.169 | 0.033 | 0.127 | 0.234 | 0.181 | 0.042 | 0.107 | 0.263 |
| SM C24:0 | 9.432 | 1.031 | 8.010 | 11.100 | 10.402 | 1.332 | 8.390 | 12.100 |
| SM C24:1 | 13.317 | 1.821 | 10.000 | 15.800 | 15.558 | 2.036 | 12.400 | 18.000 |
| H1 | 5989.250 | 1505.605 | 4441.000 | 9622.000 | 5387.250 | 504.794 | 4158.000 | 5943.000 |
| Ala | 509.167 | 122.564 | 311.000 | 760.000 | 439.000 | 97.561 | 255.000 | 623.000 |
| Arg | 150.833 | 19.711 | 109.000 | 178.000 | 132.083 | 27.596 | 102.000 | 196.000 |
| Asn | 53.867 | 10.917 | 40.300 | 84.500 | 48.700 | 10.313 | 28.600 | 65.500 |
| Cit | 82.117 | 19.857 | 50.800 | 113.000 | 78.392 | 15.766 | 48.700 | 103.000 |
| Gln | 681.417 | 92.316 | 458.000 | 833.000 | 558.167 | 108.358 | 418.000 | 840.000 |
| Glu | 207.250 | 55.860 | 112.000 | 312.000 | 239.667 | 38.969 | 199.000 | 302.000 |
| Gly | 982.500 | 135.139 | 681.000 | 1160.000 | 840.917 | 148.586 | 473.000 | 1000.000 |
| His | 115.242 | 18.857 | 78.500 | 143.000 | 104.817 | 18.159 | 77.500 | 145.000 |
| Ile | 128.500 | 17.349 | 103.000 | 153.000 | 131.792 | 22.869 | 98.500 | 166.000 |
| Leu | 211.000 | 27.713 | 171.000 | 265.000 | 217.917 | 31.816 | 168.000 | 259.000 |
| Lys | 359.500 | 56.484 | 273.000 | 472.000 | 319.250 | 53.899 | 246.000 | 433.000 |
| Met | 49.783 | 7.145 | 36.400 | 62.900 | 45.467 | 11.207 | 22.900 | 65.700 |
| Orn | 107.683 | 17.746 | 79.200 | 132.000 | 95.375 | 17.697 | 72.000 | 125.000 |
| Phe | 86.975 | 8.074 | 77.700 | 104.000 | 79.900 | 12.739 | 60.400 | 106.000 |
| Pro | 215.833 | 28.152 | 183.000 | 293.000 | 180.333 | 34.639 | 115.000 | 235.000 |
| Ser | 122.033 | 14.933 | 88.400 | 143.000 | 114.767 | 21.534 | 68.900 | 149.000 |
| Thr | 159.833 | 27.286 | 124.000 | 224.000 | 138.092 | 34.224 | 73.100 | 187.000 |
| Trp | 59.125 | 7.080 | 46.100 | 68.700 | 64.333 | 12.129 | 48.200 | 94.000 |
| Tyr | 90.792 | 18.040 | 67.600 | 135.000 | 86.367 | 18.967 | 52.800 | 124.000 |
| Val | 283.250 | 39.370 | 237.000 | 361.000 | 300.667 | 42.322 | 243.000 | 359.000 |
| Ac-Orn | 14.112 | 3.067 | 8.940 | 18.400 | 6.933 | 3.620 | 1.890 | 14.100 |
| Carnosine | 49.833 | 16.058 | 29.800 | 81.300 | 37.642 | 8.257 | 30.000 | 61.000 |
| Creatinine | 191.750 | 28.550 | 159.000 | 254.000 | 166.000 | 24.797 | 112.000 | 200.000 |
| Kynurenine | 1.010 | 0.272 | 0.675 | 1.580 | 0.475 | 0.253 | 0.000 | 0.819 |
| Met-SO | 0.990 | 0.361 | 0.385 | 1.570 | 0.781 | 0.309 | 0.346 | 1.390 |
| Putrescine | 0.990 | 0.281 | 0.747 | 1.800 | 0.826 | 0.188 | 0.477 | 1.140 |
| Sarcosine | 11.823 | 1.945 | 9.450 | 15.400 | 10.748 | 2.606 | 5.480 | 16.100 |
| Serotonin | 1.114 | 0.997 | 0.141 | 3.740 | 1.634 | 1.290 | 0.061 | 3.900 |
| Spermidine | 0.903 | 0.382 | 0.623 | 1.790 | 0.738 | 0.192 | 0.419 | 1.090 |
| Spermine | 0.599 | 0.135 | 0.440 | 0.862 | 0.510 | 0.124 | 0.388 | 0.845 |
| Taurine | 157.667 | 29.974 | 123.000 | 232.000 | 161.408 | 39.119 | 99.900 | 222.000 |
| alpha-AAA | 22.392 | 7.700 | 11.400 | 38.300 | 26.692 | 12.029 | 10.300 | 47.900 |
| total-DMA | 1.222 | 0.251 | 0.958 | 1.740 | 1.063 | 0.257 | 0.693 | 1.510 |

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.