

Supplementary Table 4. The top 50 differentially metabolites based on VIP values identified between WS and SD groups from serum samples.

| Metabolites | Compound ID | Formula | VIP | adj.P-value | log2(FC) |
|--|--------------|--------------|-----------|-------------|-----------|
| PA(17:1(9Z)/22:2(13Z,16Z)) | LMGP10010273 | C42H77O8P | 97.314967 | 0.209804 | -0.895337 |
| LysoPC(18:1(11Z)) | HMDB0010385 | C26H52NO7P | 18.311347 | 0.3165841 | -0.34309 |
| PC(14:0/22:4(7Z,10Z,13Z,16Z)) | HMDB0007889 | C44H80NO8P | 14.032345 | 0.2252829 | 0.649401 |
| PC(16:0/20:5(5Z,8Z,11Z,14Z,17Z)) | HMDB0007984 | C44H78NO8P | 11.516296 | 0.1951097 | -0.955838 |
| PE(19:0/20:2(11Z,14Z)) | LMGP02010783 | C44H84NO8P | 10.620062 | 0.1921897 | 0.7109557 |
| LysoPC(20:1(11Z)) | HMDB0010391 | C28H56NO7P | 10.48363 | 0.1212164 | -0.722421 |
| PE-NMe2(18:0/20:4(5Z,8Z,11Z,14Z)) | HMDB0113999 | C45H82NO8P | 10.160781 | 0.2333785 | -1.244559 |
| LysoPC(18:1(9Z)) | HMDB0002815 | C26H52NO7P | 9.0009403 | 0.2231003 | -0.539019 |
| L-Isoleucine | 23 | C6H13NO2 | 8.9537036 | 0.0824465 | -0.554532 |
| LysoPC(20:5(5Z,8Z,11Z,14Z,17Z)) | HMDB0010397 | C28H48NO7P | 8.6833586 | 0.1888057 | -1.704422 |
| PC(16:0/20:4(5Z,8Z,10E,14Z)(12OH[S])) | LMGP20010002 | C44H80NO9P | 7.8218772 | 0.1745241 | -0.929309 |
| Dihydrocoumarin | 65745 | C9H8O2 | 7.4571693 | 0.1189771 | -0.492561 |
| LysoPC(P-18:0) | HMDB0013122 | C26H54NO6P | 7.4562366 | 0.0474968 | 0.7093557 |
| PC(16:0/18:3(9Z,12Z,15Z)) | HMDB0007975 | C42H78NO8P | 7.0461573 | 0.0307741 | 1.4723047 |
| PE-NMe(16:0/22:4(7Z,10Z,13Z,16Z)) | HMDB0113055 | C44H80NO8P | 6.9274977 | 0.0829941 | -1.494256 |
| LysoPC(16:1(9Z)/0:0) | HMDB0010383 | C24H48NO7P | 6.6465147 | 0.1030072 | -0.947832 |
| PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | HMDB0008057 | C48H84NO8P | 5.7353409 | 0.2631859 | -0.825004 |
| [4-(7-hydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)phenyl]oxidanesulfonic acid | HMDB0141213 | C15H14O6S | 5.5775041 | 0.0012168 | -2.359003 |
| PC(16:0/16:1(9Z)) | HMDB0007969 | C40H78NO8P | 5.1757936 | 0.3061426 | -0.93991 |
| LysoPC(18:3(6Z,9Z,12Z)) | HMDB0010387 | C26H48NO7P | 5.1445447 | 0.2939349 | 1.0303031 |
| PC(18:3(6Z,9Z,12Z)/P-16:0) | HMDB0008192 | C42H78NO7P | 4.8624727 | 0.0309988 | 4.0621769 |
| SM(d16:1/17:0) | LMSP03010037 | C38H77N2O6P | 4.8170665 | 0.175073 | 1.0270691 |
| PS(P-18:0/0:0) | LMGP03070002 | C24H48NO8P | 4.6128137 | 0.2902771 | 1.7678306 |
| PC(19:1(9Z)/0:0) | LMGP01050130 | C27H54NO7P | 4.4287531 | 0.0507577 | -0.998555 |
| 2-Hydroxycinnamic acid | 306 | C9H8O3 | 4.3767768 | 0.1862954 | -0.3715 |
| PS(O-18:0/0:0) | LMGP03060002 | C24H50NO8P | 4.2481394 | 0.2269156 | -2.151201 |
| PE(20:3(5Z,8Z,11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | HMDB0009342 | C47H76NO8P | 3.7751669 | 0.1696274 | -1.398126 |
| PC(O-18:1(11Z)/0:0) | LMGP01060034 | C26H54NO6P | 3.525407 | 0.0056784 | 1.7496163 |
| PS(18:2(9Z,12Z)/0:0) | LMGP03050011 | C24H44NO9P | 3.4711804 | 0.0006819 | 4.0646739 |
| PC(O-20:0/0:0) | LMGP01060041 | C28H60NO6P | 3.1728602 | 0.1396623 | 1.0487906 |
| 2-amino-6-hydroxyhexanoic acid | HMDB0142963 | C6H13NO3 | 3.0204929 | 0.0032674 | 1.1836564 |
| PC(16:0/20:4(5Z,8Z,11Z,14Z)) | HMDB0007982 | C44H80NO8P | 2.9742859 | 0.062752 | -1.379219 |
| 5β-CHOLANIC ACID-3α, 12α-DIOL N-(2-SULPHOETHYL)-AMIDE | 44688 | C26H45NO6S | 2.9194186 | 0.0024679 | 3.4147921 |
| Glu Leu | 44684 | C11H20N2O5 | 2.7882774 | 0.1058725 | -0.790463 |
| 10,11-dihydro-20-trihydroxy-leukotriene B4 | HMDB0012503 | C20H34O7 | 2.7657274 | 0.2583607 | 1.3817179 |
| PE(19:0/20:4(5Z,8Z,11Z,14Z)) | LMGP02010785 | C44H80NO8P | 2.735602 | 0.0588195 | -1.447664 |
| 2-O-methyl PAF C-16 | 43417 | C25H54NO6P | 2.4993142 | 0.0039339 | 2.6908699 |
| 2-Heptanethiol | HMDB0032303 | C7H16S | 2.4603179 | 0.0845367 | -0.562484 |
| LysoPE(0:0/20:5(5Z,8Z,11Z,14Z,17Z)) | HMDB0011489 | C25H42NO7P | 2.455469 | 0.0192129 | -1.376139 |
| Cholesteryl-alpha-D-glucoside | LMST05050029 | C32H54O6 | 2.3441144 | 0.0461908 | -5.753648 |
| {4-[(1E)-3-(4-hydroxy-2-methoxyphenyl)prop-1-en-1-yl]phenyl}oxidanesulfonic acid | HMDB0130353 | C16H16O6S | 2.3387177 | 0.0083457 | -2.38248 |
| 3-(4-Methyl-3-pentenyl)thiophene | 92919 | C10H14S | 2.3260856 | 0.1212665 | -0.491184 |
| PE(P-18:0/20:4(6E,8Z,11Z,14Z)(5OH[S])) | 82394 | C43H78NO8P | 2.2653099 | 0.2514598 | 1.0801764 |
| THTC | 68817 | C5H8O2S | 2.2653005 | 0.1299283 | -0.365755 |
| SM C16:1 | HMDB0029216 | C40H80N2O6P+ | 2.228824 | 0.2024559 | 1.1942671 |
| 17-hydroxy stearic acid | LMFA02000135 | C18H36O3 | 2.1478087 | 0.1745841 | -0.473623 |
| L-Carnitine | 34532 | C7H15NO3 | 2.1361484 | 0.2269156 | 0.290201 |
| PC(21:0/0:0) | 40317 | C29H60NO7P | 2.1260332 | 0.1819852 | 1.0141365 |
| Equol 4'-O-glucuronide | HMDB0041731 | C21H22O9 | 2.0921303 | 0.003526 | -2.94973 |
| L-Proline | 29 | C5H9NO2 | 2.0847472 | 0.2193284 | -0.462759 |