**Supplementary Table** **2**.Differential metabolites

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| modle | NO | HMDB ID | Retention  time | Name | Formula | Experimental  Mass | Ion Mode | Mass Error | MS/MS quantity | levels |
| ESI- | P1 | 0003871 | 6.72 | **13-L-Hydroperoxylinoleic acid** | C18H32O4 | 333.205145 | M+Na-2H | 1.33761043 | 12 | ↑ |
|  | P2 | 0003871 | 6.23 | **13-L-Hydroperoxylinoleic acid** | C18H32O4 | 333.2045847 | M+Na-2H | -0.456798865 | 14 | ↑ |
|  | P3 | 0004701 | 9.41 | 9,10-EOA | C18H32O3 | 295.2277627 | M-H | -0.35696978 | 8 | ↑ |
|  | P4 | 0004702 | 9.41 | 12,13-EpOME | C18H32O3 | 295.2277627 | M-H | -0.35696978 | 8 | ↑ |
|  | P5 | 0001256 | 8.42 | **Spermine** | C10H26N4 | 239.164631 | M+K-2H | 1.379597855 | 2 | ↑ |
|  | P6 | 0005050 | 6.90 | 15H-11,12-EETA | C20H32O4 | 371.2025 | M+Cl | -0.060850098 | 18 | ↓ |
|  | P7 | 0004673 | 18.15 | **11,12-Epoxyeicosatrienoic acid** | C20H32O3 | 365.2282 | M+Na | 3.620233869 | 6 | ↑ |
|  | P8 | 0011134 | 18.15 | **5-HETE** | C20H32O3 | 365.2282 | M+Na | 3.620233869 | 6 | ↑ |
|  | P9 | 0003080 | 20.00 | **Leukotriene D4** | C25H40N2O6S | 533.2077227 | M+K-2H | -3.204984531 | 3 | ↑ |
|  | P10 | 0013040 | 6.12 | **Prostaglandin H3** | C20H30O5 | 331.1900557 | M-H2O-H | -4.0754055 | 19 | ↑ |
|  | P11 | 0004673 | 5.82 | **11,12-Epoxyeicosatrienoic acid** | C20H32O3 | 365.2318088 | M-H | -4.80572325 | 16 | ↑ |
|  | P12 | 0011136 | 11.06 | 19(S)-HETE | C20H32O3 | 319.2269203 | M-H | -2.960685962 | 3 | ↓ |
|  | P13 | 0013461 | 19.75 | SM(d18:1/26:1(17Z)) | C49H97N2O6P | 877.6558603 | M+K-2H | -1.392091422 | 2 | ↑ |
|  | P14 | 0003759 | 18.60 | **5a-Pregnane-3,20-dione** | C21H32O2 | 677.4522447 | M-H | -0.312038182 | 4 | ↑ |
|  | P15 | 0060382 | 5.40 | **3beta-Hydroxypregn-5-en-20-one sulfate** | C21H32O5S | 415.1942706 | M+F | -1.401950917 | 5 | ↑ |
|  | P16 | 0006765 | 19.99 | **2-Methoxy-estradiol-17b 3-glucuronide** | C25H34O9 | 459.2041349 | M-H2O-H | 3.540906446 | 3 | ↑ |
|  | P17 | 0001032 | 20.74 | **Dehydroepiandrosterone sulfate** | C19H28O5S | 367.1572338 | M-H | -3.353725684 | 4 | ↑ |
|  | P18 | 0000063 | 5.58 | [Cortisol](https://hmdb.ca/metabolites/HMDB0000063) | C21H30O5 | 361.200367 | M-H | -4.63983385 | 9 | ↑ |
|  | P19 | 0006754 | 5.96 | [11b,21-Dihydroxy-3,20-oxo-5b-pregnan-18-al](https://hmdb.ca/metabolites/HMDB0006754) | C21H32O5 | 363.2161356 | M-H | -4.28880625 | 14 | ↑ |
|  | P20 | 0000145 | 5.94 | [Estrone](https://hmdb.ca/metabolites/HMDB0000145) | C18H22O2 | 329.1792614 | M-H | 0.88782721 | 7 | ↑ |
|  | P21 | 0000063 | 5.58 | [Cortisol](https://hmdb.ca/metabolites/HMDB0000063) | C21H30O5 | 429.1874587 | M-H | -4.92991872 | 9 | ↑ |
|  | P22 | 0000063 | 14.33 | [Cortisol](https://hmdb.ca/metabolites/HMDB0000063) | C21H30O5 | 361.1990629 | M-H | -4.63983385 | 5 | ↓ |
|  | P23 | 0006754 | 9.91 | [11b,21-Dihydroxy-3,20-oxo-5b-pregnan-18-al](https://hmdb.ca/metabolites/HMDB0006754) | C21H32O5 | 385.1982038 | M+Na-2H | -3.948506422 | 7 | ↑ |
|  | P24 | 0004195 | 4.51 | 5-L-Glutamyl-taurine | C7H14N2O6S | 253.0511982 | M-H | 2.719435723 | 10 | ↓ |
|  | P25 | 0000036 | 5.61 | Taurocholic acid | C26H45NO7S | 514.283118 | M-H | -3.485294884 | 7 | ↑ |
|  | P26 | 0004195 | 5.11 | 5-L-Glutamyl-taurine | C7H14N2O6S | 253.0507985 | M-H | 3.218921065 | 10 | ↓ |
|  | P27 | 0004096 | 4.47 | 5-Methoxyindoleacetate | C11H11NO3 | 204.0659817 | M-H | -3.096997856 | 12 | ↑ |
|  | P28 | 0010396 | 9.92 | LysoPC(20:4(8Z,11Z,14Z,17Z)/0:0) | C28H50NO7P | 578.3002386 | M+Cl | -3.041022578 | 2 | ↑ |
|  | P29 | 0001190 | 4.49 | Indoleacetaldehyde | C10H9NO | 158.0603531 | M-H | -3.99269806 | 3 | ↑ |
|  | P30 | 0060484 | 1.05 | Indolepyruvate | C11H9NO3 | 238.0232464 | M+Cl | -1.564934306 | 2 | ↓ |
|  | P31 | 0003337 | 16.56 | Oxidized glutathione | C20H32N6O12S2 | 611.1341823 | M-H | -0.249004006 | 2 | ↑ |
|  | P32 | 0000806 | 18.62 | Myristic acid | C14H28O2 | 249.1832989 | M+Na-2H | -1.310307239 | 2 | ↑ |
|  | P33 | 0000218 | 1.03 | Orotidylic acid | C10H13N2O11P | 402.9869625 | M+Cl | 4.172100199 | 6 | ↑ |
|  | P34 | 0060423 | 18.44 | 7,8-Dihydro-7-hydroxy-8-S-glutathionyl-benzo[a]pyrene | C30H29N3O7S | 610.1423377 | M+Cl | 0.547817024 | 12 | ↑ |
|  | P35 | 0010384 | 17.03 | LysoPC(18:0) | C26H54NO7P | 522.3553686 | M-H | -2.187111707 | 2 | ↓ |
|  | P36 | 0003556 | 17.38 | Chitobiose | C15H26N2O12 | 425.1417596 | M-H | 1.083517545 | 7 | ↑ |
|  | P37 | 0006547 | 18.44 | Stearidonic acid | C18H28O2 | 597.40825 | M-H | 0.449710047 | 3 | ↑ |
|  | P38 | 0006733 | 22.64 | CE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | C49H76O2 | 717.5681936 | M-H | 1.063394566 | 7 | ↓ |
|  | P39 | 0001294 | 22.30 | 2,3-Diphosphoglyceric acid | C3H8O10P2 | 286.9382879 | M+H | -3.307086773 | 13 | ↑ |
|  | P40 | 0000085 | 22.29 | Deoxyguanosine | C10H13N5O4 | 288.0703242 | M+Na-2H | -4.108974939 | 8 | ↑ |
|  | P41 | 0009116 | 23.08 | PE(18:2(9Z,12Z)/P-18:1(11Z)) | C41H76NO7P | 746.5109327 | M+Na-2H | 0.447270627 | 4 | ↓ |
|  | P42 | 0009117 | 23.08 | PE(18:2(9Z,12Z)/P-18:1(9Z)) | C41H76NO7P | 746.5109327 | M+Na-2H | 0.447270627 | 4 | ↓ |
|  | P43 | 0008198 | 24.28 | PC(18:3(9Z,12Z,15Z)/15:0) | C41H76NO8P | 722.5097498 | M-H2O-H | -4.401917206 | 12 | ↓ |
|  | P44 | 0009453 | 24.23 | PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:0) | C43H76NO8P | 746.5125641 | M-H2O-H | -0.587595458 | 2 | ↓ |
|  | P45 | 0009700 | 23.42 | PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:1(13Z)) | C49H84NO8P | 958.5646492 | M-H | -1.731683401 | 3 | ↓ |
|  | P46 | 0009540 | 23.42 | PE(22:1(13Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | C49H84NO8P | 958.5646492 | M-H | -1.731683401 | 3 | ↓ |
|  | P47 | 0009281 | 24.21 | PE(20:1(11Z)/P-18:1(11Z)) | C43H82NO7P | 776.5556462 | M+Na-2H | -2.530737761 | 3 | ↓ |
|  | P48 | 0009282 | 24.21 | PE(20:1(11Z)/P-18:1(9Z)) | C43H82NO7P | 776.5556462 | M+Na-2H | -2.530737762 | 3 | ↓ |
|  | P49 | 0009313 | 24.21 | PE(20:2(11Z,14Z)/P-18:0) | C43H82NO7P | 776.5556462 | M+Na-2H | -2.530737762 | 3 | ↓ |
|  | P50 | 0009576 | 24.21 | PE(22:2(13Z,16Z)/P-16:0) | C43H82NO7P | 776.5556462 | M+Na-2H | -2.530737762 | 3 | ↓ |
|  | P51 | 0006825 | 22.06 | Tetrahydrofolyl-[Glu](2) | C24H30N8O9 | 593.212969 | M-H | -1.796408905 | 6 | ↓ |
|  | P52 | 0001557 | 0.76 | Riboflavin reduced | C15H16N4O6 | 367.1032806 | M-H | -0.476009031 | 2 | ↑ |
|  | P53 | 0002925 | 21.07 | **Dihomo-gamma-linolenic acid** | C20H34O2 | 305.2485881 | M-H | -0.051570628 | 10 | ↑ |
|  | P54 | 0006791 | 6.40 | **Melibiitol** | C12H24O11 | 343.1250448 | M-H | 1.335537469 | 2 | ↑ |
|  | P55 | 0000951 | 6.19 | **Taurochenodesoxycholic acid** | C26H45NO6S | 498.2872855 | M-H | -4.40055667 | 12 | ↑ |
|  | P56 | 0000195 | 4.50 | **Inosine** | C10H12N4O5 | 313.0782323 | M+FA-H | -2.760455674 | 10 | ↑ |
|  | P57 | 0000663 | 4.33 | **Glucaric acid** | C6H10O8 | 269.0482727 | M+Hac-H | -1.64100219 | 3 | ↓ |
|  | P58 | 0000806 | 13.52 | **Myristic acid** | C14H28O2 | 249.1842291 | M+Na-2H | 2.765671018 | 3 | ↑ |
|  | P59 | 0010381 | 10.09 | LysoPC(15:0) | C23H48NO7P | 480.3076509 | M-H | -3.9728778 | 4 | ↓ |
|  | P60 | 0007855 | 9.91 | **LysoPA(18:1(9Z)/0:0)** | C21H41O7P | 457.2339923 | M+Na-2H | 0.765980412 | 2 | ↑ |
|  | P61 | 0000197 | 2.82 | Indoleacetic acid | C10H9NO2 | 242.0478595 | M-H | 4.239021692 | 6 | ↑ |
|  | P62 | 0002925 | 10.41 | **Dihomo-gamma-linolenic acid** | C20H34O2 | 305.2471548 | M-H | -4.731588045 | 5 | ↑ |
| ESI+ | P63 | 0002995 | 21.26 | **12-Keto-tetrahydro-leukotriene B4** | C20H34O4 | 371.2784315 | M+K | -2.274127534 | 7 | ↓ |
|  | P64 | 0003208 | 13.49 | **Thromboxane** | C20H40O | 360.3239269 | M+ACN+Na | 0.813966482 | 13 | ↓ |
|  | P65 | 0004876 | 23.81 | **LacCer(d18:1/25:0)** | C55H105NO13 | 1029.7939 | M+ACN+H | 1.530017275 | 7 | ↑ |
|  | P66 | 0012317 | 23.81 | **3-O-Sulfogalactosylceramide (d18:1/18:1(9Z))** | C42H79NO11S | 838.5610 | M+Na | 2.112738547 | 6 | ↑ |
|  | P67 | 0004949 | 23.50 | Cer(d18:1/16:0) | C34H67NO3 | 502.4968369 | M+H-2H2O | -2.61430559 | 2 | ↑ |
|  | P68 | 0004837 | 23.72 | **Galabiosylceramide (d18:1/24:1(15Z))** | C54H101NO13 | 994.7154136 | M+Na | -1.131331338 | 21 | ↑ |
|  | P69 | 0001547 | 6.05 | **Corticosterone** | C21H30O4 | 347.2218899 | M+H | 0.589437874 | 13 | ↓ |
|  | P70 | 0004096 | 3.75 | 5-Methoxyindoleacetate | C11H11NO3 | 250.0450217 | M+Na | 0.060563635 | 4 | ↑ |
|  | P71 | 0000122 | 0.71 | **D-Glucose** | C6H12O6 | 203.0522236 | M+H-H2O | -2.138878061 | 8 | ↑ |
|  | P72 | 0006547 | 20.12 | Stearidonic acid | C18H28O2 | 259.2059895 | M+H | 1.258637786 | 4 | ↑ |
|  | P73 | 0000175 | 0.66 | **Inosinic acid** | C10H13N4O8P | 355.0578571 | M+2Na-H | 0.034110709 | 5 | ↓ |
|  | P74 | 0005358 | 23.80 | **TG(16:0/16:0/20:0)** | C55H106O6 | 907.7710875 | M+Na | 1.137490066 | 7 | ↓ |
|  | P75 | 0005389 | 23.80 | **TG(16:0/18:2(9Z,12Z)/20:1(11Z))** | C57H104O6 | 907.7710875 | M+H-2H2O | -1.609728224 | 7 | ↓ |
|  | P76 | 0001070 | 23.57 | **Octanoyl-CoA** | C29H50N7O17P3S | 858.2050251 | M+H | -0.891124617 | 4 | ↑ |
|  | P77 | 0009379 | 23.57 | **PE(20:3(8Z,11Z,14Z)/P-18:0)** | C43H80NO7P | 753.5874621 | M+Na | -0.867300072 | 9 | ↑ |
|  | P78 | 0009346 | 23.57 | **PE(20:3(5Z,8Z,11Z)/P-18:0)** | C43H80NO7P | 753.5874621 | M+H | -0.867300072 | 9 | ↑ |
|  | P79 | 0009314 | 23.57 | **PE(20:2(11Z,14Z)/P-18:1(11Z))** | C43H80NO7P | 753.5874621 | M+H | -0.867300072 | 9 | ↑ |
|  | P80 | 0009315 | 23.57 | **PE(20:2(11Z,14Z)/P-18:1(9Z))** | C43H80NO7P | 753.5874621 | M+2Na-H | -0.867300072 | 9 | ↑ |
|  | P81 | 0004041 | 0.70 | **L-Allothreonine** | C4H9NO3 | 164.0293778 | M+H | -0.254434235 | 18 | ↓ |
|  | P82 | 0000883 | 0.71 | **L-Valine** | C5H11NO2 | 118.0859574 | M+Na | -2.542403153 | 21 | ↓ |
|  | P83 | 0006857 | 0.72 | **Dextrin** | C18H32O16 | 527.1581486 | M+H | -0.212347364 | 16 | ↓ |
|  | P84 | 0006519 | 23.22 | **Stearidonoyl CoA** | C39H62N7O17P3S | 1026.318768 | M+H | -2.031738961 | 16 | - |
|  | P85 | 0000290 | 23.69 | **Uridine diphosphate-N-acetylglucosamine** | C17H27N3O17P2 | 649.124109 | M+NH4 | -0.181965764 | 17 | ↓ |
|  | P86 | 0004305 | 12.89 | **Farnesol** | C15H26O | 240.2322209 | M+Na | 0.134490285 | 12 | ↑ |
|  | P87 | 0012453 | 14.99 | **3beta-Hydroxy-5-cholestenoic acid** | C27H44O3 | 417.3362571 | M+Na | -0.155186646 | 27 | ↑ |
|  | P88 | 0011154 | 14.09 | **LysoPA(P-16:0/0:0)** | C19H39O6P | 417.3362571 | M+H-2H2O | -0.897790707 | 18 | ↓ |
|  | P89 | 0003141 | 13.85 | **Retinoyl b-glucuronide** | C26H36O8 | 441.2252953 | M+H-2H2O | -3.926386828 | 20 | ↓ |
|  | P90 | 0010318 | 4.99 | Pregnanediol 3-O-glucuronide | C27H44O8 | 535.2693022 | M+Na | -1.993791678 | 10 | ↑ |
|  | P91 | 0011105 | 6.35 | **5-Acetylamino-6-formylamino-3-methyluracil** | C12H21NO4S2 | 290.0870709 | M+ACN+Na | -2.738468232 | 23 | ↑ |
|  | P92 | 0011105 | 6.35 | **5-Acetylamino-6-formylamino-3-methyluracil** | C8H10N4O4 | 290.0870709 | M+ACN+Na | 4.84959473 | 23 | ↑ |
|  | P93 | 0008652 | 20.77 | **PC(22:4(7Z,10Z,13Z,16Z)/P-16:0)** | C46H84NO7P | 838.5584053 | M+Na | -1.021520748 | 7 | ↑ |
|  | P94 | 0008456 | 20.77 | **PC(20:4(5Z,8Z,11Z,14Z)/P-18:0)** | C46H84NO7P | 838.5584053 | M+Na | -1.021520748 | 7 | ↑ |
|  | P95 | 0001409 | 0.87 | **dUMP** | C9H13N2O8P | 353.0119925 | M+Na | -0.404122646 | 8 | ↓ |
|  | P96 | 0009710 | 21.80 | PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/P-18:1(11Z)) | C45H76NO7P | 818.5098938 | M+Na | 3.604809015 | 15 | ↑ |
|  | P96 | 0009711 | 21.80 | **PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/P-18:1(9Z))** | C45H76NO7P | 818.5098938 | M+Na | 3.604809015 | 15 | ↑ |
|  | P97 | 0001496 | 21.38 | 7alpha-Hydroxycholesterol | C27H46O2 | 243.2104078 | M+H | -1.148116411 | 3 | ↓ |
|  | P98 | 0006228 | 18.39 | **24-Hydroxycalcitriol** | C27H44O4 | 415.3185396 | M+H | -4.931676159 | 7 | ↑ |
|  | P99 | 0000827 | 17.84 | **Stearic acid** | C18H36O2 | 285.2797433 | M+Na | 3.29424837 | 3 | ↑ |
|  | P101 | 0001227 | 1.17 | **5-Thymidylic acid** | C10H15N2O8P | 401.0761598 | M+H | -4.279794928 | 13 | ↑ |
|  | P102 | 0001517 | 23.53 | **AICAR** | C9H15N4O8P | 371.1018086 | M+H | -0.286035627 | 23 | ↓ |
|  | P103 | 0000254 | 8.00 | **Succinic acid** | C4H6O4 | 237.0586719 | M+H | 0.292131609 | 9 | ↑ |
|  | P104 | 0006556 | 1.01 | **L-4-Hydroxyglutamate semialdehyde** | C5H9NO4 | 136.0717 | M+H | -2.291133552 | 5 | ↓ |
|  | P105 | 0007942 | 23.13 | **PC(15:0/18:3(9Z,12Z,15Z))** | C41H76NO8P | 786.4966373 | M+H | 3.504142032 | 7 | ↑ |
|  | P106 | 0000570 | 11.75 | **Coproporphyrin III** | C36H38N4O8 | 619.2576422 | M+H-2H2O | 3.868397252 | 3 | ↓ |
|  | P107 | 0007850 | 10.88 | **LysoPA(0:0/18:0)** | C21H43O7P | 502.2929364 | M+H | -4.885840007 | 18 | ↑ |
|  | P108 | 0000732 | 9.48 | **Hydroxykynurenine** | C10H12N2O4 | 285.1440173 | M+H | 2.656410522 | 5 | ↑ |
|  | P109 | 0005779 | 21.80 | PE(P-18:0/20:4(5Z,8Z,11Z,14Z)) | C43H78NO7P | 751.5695842 | M+H | -3.92743375 | 12 | ↑ |