

Supplementary Table S2. Metabolite identifications of the 97 replicated features

The red features represent the most intense feature belonging to a compound.

| cpd# | monoisotopic mass@retention time | Compound name | Level according to the Metabolomics Standards Initiative |
|---------------------|----------------------------------|----------------------|--|
| 1 | 122.9206@0.56447005 | Unknown | 4 |
| | 205.8796@0.5669058 | | |
| | 207.8776@0.56648636 | | |
| | 273.8663@0.56767327 | | |
| | 289.8411@0.5683634 | | |
| | 341.8549@0.56762207 | | |
| | 357.8274@0.56829727 | | |
| | 409.8426@0.56771487 | | |
| | 425.8154@0.5682527 | | |
| | 445.8809@0.56495804 | | |
| | 493.8012@0.56823456 | | |
| | 513.8702@0.5653107 | | |
| | 561.7904@0.5682394 | | |
| | 565.8809@0.56176305 | | |
| | 581.8576@0.56466657 | | |
| | 623.8351@0.5579561 | | |
| | 629.7794@0.56837577 | | |
| | 649.8467@0.5632472 | | |
| | 657.8285@0.55736333 | | |
| | 691.8246@0.556467 | | |
| | 697.7639@0.56842214 | | |
| | 717.8281@0.5610313 | | |
| | 765.7508@0.56839013 | | |
| 785.8171@0.5577929 | | | |
| 853.8052@0.5547323 | | | |
| 921.7903@0.55131626 | | | |
| 937.7639@0.559643 | | | |
| 2 | 136.0636@0.58916837 | 1-methylnicotinamide | 1 |
| 3 | 125.0146@0.6277308 | Taurine | 1 |
| 4 | 71.074@0.8027233 | Valine | 1 |

139.0611@0.80280536

| | | | |
|----|--|---------------------|---|
| 5 | 157.1107@0.8299292 | Unknown | 4 |
| 6 | 190.0061@0.83498704 | Unknown | 4 |
| 7 | 136.0381@1.1621803 | Hypoxanthine | 1 |
| 7 | 136.0384@0.85686004 | | |
| 8 | 85.0889@1.4623561 | Leucine | 1 |
| 9 | 279.1473@2.7668757 | Unknown | 4 |
| 10 | 171.0292@2.8578448 | Unknown | 4 |
| 11 | 143.0166@3.3154876 200.0362@3.3102927 214.0152@3.31054 231.9886@3.3105862 232.0561@3.3086596 232.0574@3.310062 245.0312@3.3104632 246.0422@3.310548 247.0286@3.3104632 250.0351@3.310955 261.0059@3.3104744 264.0146@3.3119278 282.0348@3.3101916 | Unknown | 4 |
| 12 | 181.1113@5.475981 | Unknown | 4 |
| 13 | 266.1351@6.8201194 | LysoPC(16:1) | 2 |
| 14 | 481.3159@6.8777747 | LysoPC(15:0) | 2 |
| 15 | 525.2864@6.888085 | LysoPE(22:6) | 2 |

| | | | |
|----|--|---------------------|---|
| 16 | 501.285@6.8980646 523.2694@6.8969865 | LysoPE(20:4) | 2 |
| 17 | 495.3333@6.9326496 | LyosPC(16:0) isomer | 2 |
| 18 | 523.2949@6.996259 523.7955@6.9962544 522.2939@6.9969144 522.7951@6.996832 762.478@6.997659 770.46@6.997441 761.976@6.99754 769.9581@6.9974766 517.3147@6.9961543 506.3191@6.9973693 495.3327@6.9956923 990.6655@6.9950514 | LysoPC (16:0) | 2 |
| 19 | 527.312@7.05021 527.8146@7.050606 535.2997@7.0497603 | Unknown | 4 |
| 20 | 479.3405@7.1102185 | LysoPC(P-16:0) | 2 |
| 21 | 509.3468@7.1235833 | LysoPC(17:0) | 2 |
| 22 | 602.9412@7.1884513 597.4188@7.187734 610.9343@7.191048 611.4359@7.191536 | Unknown | 4 |
| 23 | 103.0997@7.241595 523.364@7.2414613 534.8485@7.241308 534.3476@7.2410583 542.3386@7.2418456 542.8411@7.2418675 | LysoPC(18:0) | 2 |

550.3265@7.2414513
550.8254@7.2414603

| | | | |
|----|--|------------------|---|
| 24 | 545.3467@7.2500143 | Unknown | 4 |
| 25 | 452.8025@7.3067145 | Unknown | 4 |
| 26 | 639.4673@7.4324927 638.9663@7.4319897 | Unknown | 4 |
| 27 | 428.3615@7.4910417 | Unknown | 4 |
| 28 | 284.1159@7.9399796 314.1271@7.94182 580.232@7.9397755 612.2575@7.940997 644.2827@7.9412355 | Bilirubin | 1 |