

**Metabolomic analysis via reversed-phase ion-pairing liquid chromatography  
coupled to a stand alone orbitrap mass spectrometer**

Supporting Information

Wenyun Lu, Michelle F. Clasquin, Eugene Melamud, Daniel Amador-Noguez, Amy A. Caudy, Joshua D. Rabinowitz

Lewis-Sigler Institute for Integrative Genomics and Department of Chemistry

Princeton University, Princeton, NJ 08544

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Table S-1. LC-MS parameters and method validation results for 87 metabolite standards

| <i>Metabolite</i> | <i>Neutral formula</i>                                          | <i>Theoretical mass</i> | <i>Observed mass</i> | <i>Error (ppm)</i> | <i>Retention time (min)</i> | <i>Limit of detection (ng/mL)</i> | <i>Linear coefficient (<math>R^2</math>)</i> | <i>Linear range (ng/mL)</i> | <i>RSD (%) at 100 ng/mL</i> |
|-------------------|-----------------------------------------------------------------|-------------------------|----------------------|--------------------|-----------------------------|-----------------------------------|----------------------------------------------|-----------------------------|-----------------------------|
| Pyruvate          | C <sub>3</sub> H <sub>4</sub> O <sub>3</sub>                    | 87.0088                 | 87.0088              | 0.00               | 8.30                        | 20                                | 0.9859                                       | 20-2000                     | 4.85                        |
| Alanine           | C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>                   | 88.0404                 | 88.0403              | -1.14              | 1.00                        | 20                                | 0.9996                                       | 20-1000                     | 7.29                        |
| Acetoacetate      | C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>                    | 101.0244                | 101.0242             | -1.98              | 8.00                        | 100                               | 0.9975                                       | 100-2000                    | 5.20                        |
| 4-aminobutyrate   | C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>                   | 102.0561                | 102.056              | -0.98              | 4.50                        | 2                                 | 0.9952                                       | 2-1000                      | 8.71                        |
| Glycerate         | C <sub>3</sub> H <sub>6</sub> O <sub>4</sub>                    | 105.0193                | 105.0194             | 0.95               | 6.30                        | 5                                 | 0.9934                                       | 5-1000                      | 11.16                       |
| uracil            | C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>     | 111.02                  | 111.0199             | -0.90              | 1.50                        | 2                                 | 0.9823                                       | 2-1000                      | 4.64                        |
| fumarate          | C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>                    | 115.0037                | 115.0037             | 0.00               | 13.40                       | 2                                 | 0.9924                                       | 2-500                       | 12.19                       |
| succinate         | C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>                    | 117.0193                | 117.0193             | 0.00               | 11.60                       | 10                                | 0.9906                                       | 10-1000                     | 25.19                       |
| threonine         | C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub>                   | 118.051                 | 118.0509             | -0.85              | 1.00                        | 1                                 | 0.9943                                       | 1-2000                      | 5.32                        |
| cysteine          | C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S                 | 120.0125                | 120.0126             | 0.83               | 1.10                        | 100                               | 0.9862                                       | 100-2000                    | 6.42                        |
| aspartate         | C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S | 132.0302                | 132.03               | -1.51              | 4.40                        | 2                                 | 0.9997                                       | 2-2000                      | 11.40                       |
| malate            | C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>                    | 133.0143                | 133.0142             | -0.75              | 12.70                       | 10                                | 0.9907                                       | 10-2000                     | 4.73                        |
| adenine           | C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>                    | 134.0472                | 134.0469             | -2.24              | 3.70                        | 1                                 | 0.9818                                       | 1-500                       | 4.64                        |
| hypoxanthine      | C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O                  | 135.0312                | 135.0311             | -0.74              | 3.60                        | 1                                 | 0.9922                                       | 1-1000                      | 17.65                       |

| <i>Metabolite</i>            | <i>Neutral formula</i>                                       | <i>Theoretical mass</i> | <i>Observed mass</i> | <i>Error (ppm)</i> | <i>Retention time (min)</i> | <i>Limit of detection (ng/mL)</i> | <i>Linear coefficient (R<sup>2</sup>)</i> | <i>Linear range (ng/mL)</i> | <i>RSD (%) at 100 ng/mL</i> |
|------------------------------|--------------------------------------------------------------|-------------------------|----------------------|--------------------|-----------------------------|-----------------------------------|-------------------------------------------|-----------------------------|-----------------------------|
| p-aminobenzoate              | C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>                | 136.0404                | 136.0404             | 0.00               | 8.70                        | 10                                | 0.9946                                    | 10-2000                     | 5.77                        |
| anthranilate                 | C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>                | 136.0404                | 136.0401             | -2.21              | 13.30                       | 1                                 | 0.9988                                    | 1-200                       | 3.48                        |
| α-ketoglutarate              | C <sub>5</sub> H <sub>6</sub> O <sub>5</sub>                 | 145.0143                | 145.0141             | -1.38              | 13.10                       | 5                                 | 0.9963                                    | 5-1000                      | 15.79                       |
| glutamine                    | C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> | 145.0619                | 145.0617             | -1.38              | 1.00                        | 2                                 | 0.9942                                    | 2-2000                      | 4.51                        |
| lysine                       | C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> | 145.0983                | 145.0981             | -1.38              | 0.80                        | 1                                 | 0.9902                                    | 1-1000                      | 14.21                       |
| glutamate                    | C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>                | 146.0459                | 146.0457             | -1.37              | 4.60                        | 5                                 | 0.9969                                    | 5-1000                      | 4.77                        |
| methionine                   | C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S             | 148.0438                | 148.0436             | -1.35              | 1.60                        | 5                                 | 0.9933                                    | 5-500                       | 6.60                        |
| histidine                    | C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>  | 154.0622                | 154.062              | -1.30              | 0.80                        | 1                                 | 0.9956                                    | 1-1000                      | 13.35                       |
| orotate                      | C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>4</sub>  | 155.0098                | 155.0098             | 0.00               | 8.10                        | 5                                 | 0.9976                                    | 5-2000                      | 5.35                        |
| dihydroorotate               | C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>  | 157.0255                | 157.0254             | -0.64              | 6.80                        | 1                                 | 0.9877                                    | 1-1000                      | 10.55                       |
| phenylpyruvate               | C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>                 | 163.0401                | 163.04               | -0.61              | 15.10                       | 5                                 | 0.9957                                    | 5-2000                      | 10.53                       |
| phenylalanine                | C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>               | 164.0717                | 164.0715             | -1.22              | 4.10                        | 1                                 | 0.9883                                    | 1-1000                      | 6.86                        |
| phosphoenolpyruvate          | C <sub>3</sub> H <sub>5</sub> O <sub>6</sub> P               | 166.9751                | 166.975              | -0.60              | 13.70                       | 10                                | 0.9865                                    | 10-2000                     | 9.98                        |
| D-glyceraldehyde-3-phosphate | C <sub>3</sub> H <sub>7</sub> O <sub>6</sub> P               | 168.9908                | 168.9906             | -1.18              | 7.30                        | 5                                 | 0.9947                                    | 5-1000                      | 17.80                       |

| <i>Metabolite</i>           | <i>Neutral formula</i>                                          | <i>Theoretical mass</i> | <i>Observed mass</i> | <i>Error (ppm)</i> | <i>Retention time (min)</i> | <i>Limit of detection (ng/mL)</i> | <i>Linear coefficient (R<sup>2</sup>)</i> | <i>Linear range (ng/mL)</i> | <i>RSD (%) at 100 ng/mL</i> |
|-----------------------------|-----------------------------------------------------------------|-------------------------|----------------------|--------------------|-----------------------------|-----------------------------------|-------------------------------------------|-----------------------------|-----------------------------|
| dihydroxy-acetone-phosphate | C <sub>3</sub> H <sub>7</sub> O <sub>6</sub> P                  | 168.9908                | 168.9908             | 0.00               | 9.30                        | 50                                | 0.9943                                    | 50-2000                     | 11.31                       |
| sn-glycerol-3-phosphate     | C <sub>3</sub> H <sub>9</sub> O <sub>6</sub> P                  | 171.0064                | 171.0063             | -0.58              | 7.30                        | 1                                 | 0.9931                                    | 1-2000                      | 3.81                        |
| aconitate                   | C <sub>6</sub> H <sub>6</sub> O <sub>6</sub>                    | 173.0092                | 173.009              | -1.16              | 13.80                       | 10                                | 0.9904                                    | 10-1000                     | 24.99                       |
| arginine                    | C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>7</sub> P | 173.1044                | 173.1041             | -1.73              | 0.80                        | 2                                 | 0.9918                                    | 2-1000                      | 13.76                       |
| N-carbamoyl-L-aspartate     | C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>5</sub>     | 175.036                 | 175.0359             | -0.57              | 12.60                       | 2                                 | 0.9961                                    | 2-1000                      | 7.97                        |
| allantoate                  | C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>     | 175.0473                | 175.0469             | -2.29              | 6.10                        | 10                                | 0.9932                                    | 10-2000                     | 17.15                       |
| citrate                     | C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>                    | 191.0197                | 191.0199             | 1.05               | 13.60                       | 200                               | 0.9942                                    | 200-2000                    | N/A                         |
| D-gluconate                 | C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>                   | 195.051                 | 195.051              | 0.00               | 5.80                        | 2                                 | 0.9933                                    | 2-2000                      | 10.47                       |
| tryptophan                  | C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>   | 203.0826                | 203.0823             | -1.48              | 7.60                        | 1                                 | 0.9950                                    | 1-1000                      | 6.26                        |
| pantothenate                | C <sub>9</sub> H <sub>17</sub> NO <sub>5</sub>                  | 218.1034                | 218.1032             | -0.92              | 11.00                       | 1                                 | 0.9931                                    | 1-2000                      | 7.75                        |
| ribose-5-phosphate          | C <sub>5</sub> H <sub>11</sub> O <sub>8</sub> P                 | 229.0119                | 229.0116             | -1.31              | 7.20                        | 1                                 | 0.9995                                    | 1-1000                      | 8.64                        |
| uridine                     | C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub>    | 243.0623                | 243.0618             | -2.06              | 2.10                        | 2                                 | 0.9927                                    | 2-2000                      | 12.31                       |
| biotin                      | C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S | 243.0809                | 243.0802             | -2.88              | 12.60                       | 1                                 | 0.9923                                    | 1-1000                      | 4.32                        |
| D-glucosamine-6-            | C <sub>6</sub> H <sub>14</sub> NO <sub>8</sub> P                | 258.0384                | 258.038              | -1.55              | 1.50                        | 20                                | 0.9897                                    | 20-2000                     | 14.71                       |

| <i>Metabolite</i>              | <i>Neutral formula</i>                                          | <i>Theoretical mass</i> | <i>Observed mass</i> | <i>Error (ppm)</i> | <i>Retention time (min)</i> | <i>Limit of detection (ng/mL)</i> | <i>Linear coefficient (R<sup>2</sup>)</i> | <i>Linear range (ng/mL)</i> | <i>RSD (%) at 100 ng/mL</i> |
|--------------------------------|-----------------------------------------------------------------|-------------------------|----------------------|--------------------|-----------------------------|-----------------------------------|-------------------------------------------|-----------------------------|-----------------------------|
| phosphate                      |                                                                 |                         |                      |                    |                             |                                   |                                           |                             |                             |
| glucose-6-phosphate            | C <sub>6</sub> H <sub>13</sub> O <sub>9</sub> P                 | 259.0224                | 259.0222             | -0.77              | 6.90                        | 1                                 | 0.9866                                    | 1-1000                      | 5.48                        |
| fructose-6-phosphate           | C <sub>6</sub> H <sub>13</sub> O <sub>9</sub> P                 | 259.0224                | 259.0221             | -1.16              | 7.30                        | 2                                 | 0.9990                                    | 2-1000                      | 7.16                        |
| adenosine                      | C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>   | 266.0895                | 266.0898             | 1.13               | 7.00                        | 10                                | 0.9977                                    | 10-2000                     | 20.85                       |
| inosine                        | C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>   | 267.0735                | 267.0731             | -1.50              | 3.60                        | 1                                 | 0.9998                                    | 1-500                       | 18.66                       |
| guanosine                      | C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>   | 282.0844                | 282.084              | -1.42              | 4.20                        | 1                                 | 0.9992                                    | 1-500                       | 8.56                        |
| xanthosine                     | C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>6</sub>   | 283.0684                | 283.0681             | -1.06              | 7.50                        | 1                                 | 0.9859                                    | 1-500                       | 1.99                        |
| glutathione                    | C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub> S | 306.0765                | 306.0771             | 1.96               | 8.00                        | 10                                | 0.9957                                    | 10-2000                     | 15.71                       |
| cytidine-5'-phosphate (CMP)    | C <sub>9</sub> H <sub>14</sub> N <sub>3</sub> O <sub>8</sub> P  | 322.0446                | 322.0444             | -0.62              | 8.70                        | 2                                 | 0.9961                                    | 2-2000                      | 9.50                        |
| Uridine-5'-monophosphate (UMP) | C <sub>9</sub> H <sub>13</sub> N <sub>2</sub> O <sub>9</sub> P  | 323.0286                | 323.0284             | -0.62              | 10.20                       | 1                                 | 0.9997                                    | 1-1000                      | 6.01                        |
| 3',5'-cyclic AMP               | C <sub>10</sub> H <sub>12</sub> N <sub>5</sub> O <sub>6</sub> P | 328.0453                | 328.0445             | -2.44              | 12.60                       | 1                                 | 0.9922                                    | 1-2000                      | 5.05                        |
| fructose-1,6-bisphosphate      | C <sub>6</sub> H <sub>14</sub> O <sub>12</sub> P <sub>2</sub>   | 338.9888                | 338.9889             | 0.29               | 13.50                       | 20                                | 0.9846                                    | 20-2000                     | 6.77                        |

| <i>Metabolite</i>              | <i>Neutral formula</i>                                                        | <i>Theoretical mass</i> | <i>Observed mass</i> | <i>Error (ppm)</i> | <i>Retention time (min)</i> | <i>Limit of detection (ng/mL)</i> | <i>Linear coefficient (R<sup>2</sup>)</i> | <i>Linear range (ng/mL)</i> | <i>RSD (%) at 100 ng/mL</i> |
|--------------------------------|-------------------------------------------------------------------------------|-------------------------|----------------------|--------------------|-----------------------------|-----------------------------------|-------------------------------------------|-----------------------------|-----------------------------|
| adenosine-5'-phosphate (AMP)   | C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>7</sub> P               | 346.0558                | 346.0551             | -2.02              | 11.30                       | 5                                 | 0.9988                                    | 5-2000                      | 4.04                        |
| inosine-5'-phosphate (IMP)     | C <sub>10</sub> H <sub>13</sub> N <sub>4</sub> O <sub>8</sub> P               | 347.0398                | 347.0397             | -0.29              | 10.70                       | 2                                 | 0.9915                                    | 2-2000                      | 9.18                        |
| guanosine-5'-phosphate (GMP)   | C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>8</sub> P               | 362.0507                | 362.0507             | 0.00               | 10.70                       | 1                                 | 0.9966                                    | 1-2000                      | 9.69                        |
| riboflavin                     | C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> O <sub>6</sub>                 | 375.131                 | 375.131              | 0.00               | 12.20                       | 1                                 | 0.9920                                    | 1-500                       | 4.99                        |
| s-adenosyl-l-homocysteine      | C <sub>10</sub> H <sub>12</sub> N <sub>5</sub> O <sub>6</sub> P               | 383.1143                | 383.114              | -0.78              | 6.10                        | 2                                 | 0.9986                                    | 2-2000                      | 6.62                        |
| cytidine-5'-diphosphate (CDP)  | C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>11</sub> P <sub>2</sub>  | 402.0109                | 402.0125             | 3.98               | 13.30                       | 50                                | 0.9925                                    | 50-2000                     | 5.69                        |
| uridine-5'-diphosphate (UDP)   | C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>12</sub> P <sub>2</sub>  | 402.9949                | 402.9959             | 2.48               | 13.50                       | 50                                | 0.9824                                    | 50-2000                     | 11.09                       |
| trehalose-6-Phosphate          | C <sub>12</sub> H <sub>23</sub> O <sub>14</sub> P                             | 421.0753                | 421.0752             | -0.24              | 7.20                        | 1                                 | 0.9958                                    | 1-2000                      | 1.67                        |
| adenosine-5'-diphosphate (ADP) | C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>10</sub> P <sub>2</sub> | 426.0221                | 426.0229             | 1.88               | 13.70                       | 50                                | 0.9829                                    | 50-2000                     | 18.12                       |
| folate                         | C <sub>19</sub> H <sub>19</sub> N <sub>7</sub> O <sub>6</sub>                 | 440.1324                | 440.1332             | 1.82               | 13.80                       | 5                                 | 0.9896                                    | 5-1000                      | 6.03                        |
| guanosine-5'-                  | C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>11</sub> P <sub>2</sub> | 442.0171                | 442.0185             | 3.17               | 13.50                       | 100                               | 0.9915                                    | 100-2000                    | 11.83                       |

| <i>Metabolite</i>               | <i>Neutral formula</i>                                                        | <i>Theoretical mass</i> | <i>Observed mass</i> | <i>Error (ppm)</i> | <i>Retention time (min)</i> | <i>Limit of detection (ng/mL)</i> | <i>Linear coefficient (R<sup>2</sup>)</i> | <i>Linear range (ng/mL)</i> | <i>RSD (%) at 100 ng/mL</i> |
|---------------------------------|-------------------------------------------------------------------------------|-------------------------|----------------------|--------------------|-----------------------------|-----------------------------------|-------------------------------------------|-----------------------------|-----------------------------|
| diphosphate (GDP)               |                                                                               |                         |                      |                    |                             |                                   |                                           |                             |                             |
| flavin mononucleotide (FMN)     | C <sub>17</sub> H <sub>21</sub> N <sub>4</sub> O <sub>9</sub> P               | 455.0974                | 455.0976             | 0.44               | 14.20                       | 2                                 | 0.9967                                    | 2-2000                      | 2.51                        |
| cytidine-5'-triphosphate (CTP)  | C <sub>9</sub> H <sub>16</sub> N <sub>3</sub> O <sub>14</sub> P <sub>3</sub>  | 481.9772                | 481.9777             | 1.04               | 14.80                       | 200                               | 0.9939                                    | 200-5000                    | N/A                         |
| uridine-5'-triphosphate (UTP)   | C <sub>9</sub> H <sub>15</sub> N <sub>2</sub> O <sub>15</sub> P <sub>3</sub>  | 482.9612                | 482.9617             | 1.04               | 15.00                       | 200                               | 0.9939                                    | 200-10000                   | N/A                         |
| adenosine-5'-triphosphate (ATP) | C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>13</sub> P <sub>3</sub> | 505.9885                | 505.9888             | 0.59               | 15.10                       | 200                               | 0.9938                                    | 200-10000                   | N/A                         |
| guanosine-5'-triphosphate (GTP) | C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>14</sub> P <sub>3</sub> | 521.9834                | 521.9836             | 0.38               | 15.00                       | 200                               | 0.9969                                    | 200-5000                    | N/A                         |
| UDP-D-glucose                   | C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>17</sub> P <sub>2</sub> | 565.0477                | 565.049              | 2.30               | 13.25                       | 2                                 | 0.9996                                    | 2-2000                      | 3.63                        |
| UDP-D-glucuronate               | C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>18</sub> P <sub>2</sub> | 579.027                 | 579.0273             | 0.52               | 14.70                       | 1                                 | 0.9967                                    | 1-2000                      | 5.05                        |
| ADP-D-glucose                   | C <sub>16</sub> H <sub>25</sub> N <sub>5</sub> O <sub>15</sub> P <sub>2</sub> | 588.075                 | 588.0747             | -0.51              | 13.50                       | 5                                 | 0.9891                                    | 5-2000                      | 4.86                        |
| UDP-N-acetyl-glucosamine        | C <sub>17</sub> H <sub>27</sub> N <sub>3</sub> O <sub>17</sub> P <sub>2</sub> | 606.0743                | 606.0754             | 1.81               | 13.27                       | 2                                 | 0.9892                                    | 2-2000                      | 4.49                        |
| glutathione disulfide           | C <sub>20</sub> H <sub>32</sub> N <sub>6</sub> O <sub>12</sub> S <sub>2</sub> | 611.1447                | 611.1465             | 2.95               | 12.80                       | 20                                | 0.9962                                    | 20-1000                     | 23.13                       |

| <i>Metabolite</i>                                                | <i>Neutral formula</i>                                                          | <i>Theoretical mass</i> | <i>Observed mass</i> | <i>Error (ppm)</i> | <i>Retention time (min)</i> | <i>Limit of detection (ng/mL)</i> | <i>Linear coefficient (R<sup>2</sup>)</i> | <i>Linear range (ng/mL)</i> | <i>RSD (%) at 100 ng/mL</i> |
|------------------------------------------------------------------|---------------------------------------------------------------------------------|-------------------------|----------------------|--------------------|-----------------------------|-----------------------------------|-------------------------------------------|-----------------------------|-----------------------------|
| nicotinamide adenine dinucleotide (NAD <sup>+</sup> )            | C <sub>21</sub> H <sub>27</sub> N <sub>7</sub> O <sub>14</sub> P <sub>2</sub>   | 662.1019                | 662.104              | 3.17               | 8.60                        | 10                                | 0.9998                                    | 10-2000                     | 7.94                        |
| NADH                                                             | C <sub>21</sub> H <sub>29</sub> N <sub>7</sub> O <sub>14</sub> P <sub>2</sub>   | 664.1175                | 664.1193             | 2.71               | 13.90                       | 20                                | 0.9973                                    | 20-1000                     | 8.44                        |
| dephospho-CoA                                                    | C <sub>21</sub> H <sub>35</sub> N <sub>7</sub> O <sub>13</sub> P <sub>2</sub> S | 686.1416                | 686.1436             | 2.91               | 14.80                       | 5                                 | 0.9941                                    | 5-2000                      | 5.85                        |
| cyclic bis(3'->5') dimeric GMP                                   | C <sub>20</sub> H <sub>24</sub> N <sub>10</sub> O <sub>14</sub> P <sub>2</sub>  | 689.0876                | 689.0905             | 4.21               | 13.90                       | 20                                | 0.9989                                    | 20-2000                     | 12.97                       |
| nicotinamide adenine dinucleotide phosphate (NADP <sup>+</sup> ) | C <sub>21</sub> H <sub>28</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub>   | 742.0682                | 742.0701             | 2.56               | 13.50                       | 100                               | 0.9914                                    | 100-2000                    | 20.74                       |
| coenzyme A                                                       | C <sub>21</sub> H <sub>36</sub> N <sub>7</sub> O <sub>16</sub> P <sub>3</sub> S | 766.1079                | 766.1105             | 3.39               | 15.50                       | 100                               | 0.9826                                    | 100-2000                    | 25.86                       |
| flavin adenine dinucleotide (FAD)                                | C <sub>27</sub> H <sub>33</sub> N <sub>9</sub> O <sub>15</sub> P <sub>2</sub>   | 784.1498                | 784.1522             | 3.06               | 15.00                       | 1                                 | 0.9947                                    | 1-2000                      | 2.67                        |
| acetyl-CoA                                                       | C <sub>23</sub> H <sub>38</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub> S | 808.1185                | 808.1208             | 2.85               | 15.60                       | 10                                | 0.9885                                    | 10-1000                     | 11.73                       |
| butyryl-CoA                                                      | C <sub>25</sub> H <sub>42</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub> S | 836.1498                | 836.1541             | 5.14               | 16.00                       | 10                                | 0.9983                                    | 10-2000                     | 3.05                        |
| acetoacetyl-CoA                                                  | C <sub>25</sub> H <sub>40</sub> N <sub>7</sub> O <sub>18</sub> P <sub>3</sub> S | 850.1291                | 850.1317             | 3.06               | 15.60                       | 50                                | 0.9877                                    | 50-2000                     | 21.19                       |
| malonyl-coA                                                      | C <sub>24</sub> H <sub>38</sub> N <sub>7</sub> O <sub>19</sub> P <sub>3</sub> S | 852.1083                | 852.1121             | 4.46               | 15.60                       | 50                                | 0.9928                                    | 50-2000                     | 22.64                       |

| <i>Metabolite</i>    | <i>Neutral formula</i>                                                          | <i>Theoretical mass</i> | <i>Observed mass</i> | <i>Error (ppm)</i> | <i>Retention time (min)</i> | <i>Limit of detection (ng/mL)</i> | <i>Linear coefficient (R<sup>2</sup>)</i> | <i>Linear range (ng/mL)</i> | <i>RSD (%) at 100 ng/mL</i> |
|----------------------|---------------------------------------------------------------------------------|-------------------------|----------------------|--------------------|-----------------------------|-----------------------------------|-------------------------------------------|-----------------------------|-----------------------------|
| 3-hydroxybutyryl-CoA | C <sub>25</sub> H <sub>42</sub> N <sub>7</sub> O <sub>18</sub> P <sub>3</sub> S | 852.1483                | 852.1478             | -0.59              | 15.60                       | 10                                | 0.9955                                    | 10-2000                     | 12.52                       |
| succinyl-coA         | C <sub>25</sub> H <sub>40</sub> N <sub>7</sub> O <sub>19</sub> P <sub>3</sub> S | 866.124                 | 866.1271             | 3.58               | 15.60                       | 50                                | 0.9818                                    | 50-2000                     | 9.70                        |

Table S-2. LC-MS parameters for an additional 127 metabolites (\* indicates structural isomers that are not separated with current method)

| <i>Metabolite</i>        | <i>Neutral formula</i>                                      | <i>Theoretical mass</i> | <i>Retention time (min)</i> |
|--------------------------|-------------------------------------------------------------|-------------------------|-----------------------------|
| 2-oxobutanoate           | C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>                | 101.0244                | 10.95                       |
| serine                   | C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>               | 104.0353                | 1.00                        |
| cytosine                 | C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O              | 110.0360                | 1.00                        |
| proline                  | C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>               | 114.0561                | 1.12                        |
| 2-keto-isovalerate       | C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>                | 115.0401                | 13.06                       |
| guanidoacetic acid       | C <sub>3</sub> H <sub>7</sub> N <sub>3</sub> O <sub>2</sub> | 116.0466                | 1.14                        |
| indole                   | C <sub>8</sub> H <sub>7</sub> N                             | 116.0506                | 7.50                        |
| valine                   | C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>              | 116.0717                | 1.00                        |
| 3-S-methylthiopropionate | C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S              | 119.0172                | 11.92                       |
| nicotinate               | C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>               | 122.0248                | 11.20                       |
| taurine                  | C <sub>2</sub> H <sub>7</sub> NO <sub>3</sub> S             | 124.0074                | 0.82                        |
| thymine                  | C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> | 125.0357                | 2.60                        |
| pipecolic acid           | C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub>              | 128.0717                | 1.20                        |
| citraconic acid          | C <sub>5</sub> H <sub>6</sub> O <sub>4</sub>                | 129.0193                | 12.95                       |
| hydroxyproline           | C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>               | 130.0510                | 1.10                        |

| <i>Metabolite</i>                  | <i>Neutral formula</i>                                       | <i>Theoretical mass</i> | <i>Retention time (min)</i> |
|------------------------------------|--------------------------------------------------------------|-------------------------|-----------------------------|
| N-acetyl-L-alanine                 | C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>                | 130.0510                | 7.97                        |
| leucine/isoleucine*                | C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 130.0874                | 1.90                        |
| oxaloacetate                       | C <sub>4</sub> H <sub>4</sub> O <sub>5</sub>                 | 130.9986                | 13.64                       |
| asparagine                         | C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>  | 131.0462                | 1.00                        |
| hydroxyisocaproic acid             | C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>                | 131.0714                | 14.35                       |
| ornithine                          | C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> | 131.0826                | 1.00                        |
| homocysteine                       | C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> S              | 134.0281                | 1.00                        |
| p-hydroxybenzoate                  | C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>                 | 137.0244                | 10.88                       |
| acetylphosphate                    | C <sub>2</sub> H <sub>5</sub> O <sub>5</sub> P               | 138.9802                | 12.38                       |
| carbamoyl phosphate                | CH <sub>4</sub> NO <sub>5</sub> P                            | 139.9754                | 12.06                       |
| histidinol                         | C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O              | 140.0829                | 0.80                        |
| phenylpropionic acid               | C <sub>9</sub> H <sub>6</sub> O <sub>2</sub>                 | 145.0295                | 15.50                       |
| O-acetyl-L-serine                  | C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>                | 146.0459                | 1.10                        |
| 2-oxo-4-methylthiobutanoate        | C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> S               | 147.0122                | 13.75                       |
| 2-hydroxy-2-methylbutanedioic acid | C <sub>5</sub> H <sub>8</sub> O <sub>5</sub>                 | 147.0299                | 12.60                       |
| 3-methylphenylacetic acid          | C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>                | 149.0608                | 15.93                       |
| guanine                            | C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O               | 150.0421                | 3.40                        |

| <i>Metabolite</i>         | <i>Neutral formula</i>                                       | <i>Theoretical mass</i> | <i>Retention time (min)</i> |
|---------------------------|--------------------------------------------------------------|-------------------------|-----------------------------|
| xanthine                  | C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>  | 151.0262                | 1.18                        |
| hydroxyphenylacetic acid  | C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>                 | 151.0401                | 14.80                       |
| 2,3-dihydroxybenzoic acid | C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>                 | 153.0193                | 13.58                       |
| allantoin                 | C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub>  | 157.0367                | 0.82                        |
| 2-aminooctanoic acid      | C <sub>8</sub> H <sub>17</sub> NO <sub>2</sub>               | 158.1187                | 11.80                       |
| indole-3-carboxylic acid  | C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub>                | 160.0404                | 14.40                       |
| aminoadipic acid          | C <sub>6</sub> H <sub>11</sub> NO <sub>4</sub>               | 160.0615                | 4.33                        |
| carnitine                 | C <sub>7</sub> H <sub>15</sub> NO <sub>3</sub>               | 160.0979                | 1.00                        |
| phenyllactic acid         | C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>                | 165.0557                | 14.82                       |
| quinolinate               | C <sub>7</sub> H <sub>5</sub> NO <sub>4</sub>                | 166.0146                | 13.58                       |
| uric acid                 | C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>  | 167.0211                | 5.00                        |
| pyridoxamine              | C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> | 167.0826                | 0.82                        |
| pyridoxine                | C <sub>8</sub> H <sub>11</sub> NO <sub>3</sub>               | 168.0666                | 1.80                        |
| 1-methyl-histidine        | C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> | 168.0779                | 1.00                        |
| shikimate                 | C <sub>7</sub> H <sub>10</sub> O <sub>5</sub>                | 173.0456                | 10.92                       |
| N-acetyl-L-ornithine      | C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> | 173.0932                | 1.00                        |
| citrulline                | C <sub>6</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> | 174.0884                | 0.90                        |

| <i>Metabolite</i>       | <i>Neutral formula</i>                                       | <i>Theoretical mass</i> | <i>Retention time (min)</i> |
|-------------------------|--------------------------------------------------------------|-------------------------|-----------------------------|
| ascorbic acid           | C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>                 | 175.0248                | 6.59                        |
| 2-isopropylmalic acid   | C <sub>7</sub> H <sub>12</sub> O <sub>5</sub>                | 175.0612                | 13.94                       |
| glucono-δ-lactone       | C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>                | 177.0405                | 6.59                        |
| glucosamine             | C <sub>6</sub> H <sub>13</sub> NO <sub>5</sub>               | 178.0721                | 0.70                        |
| hydroxyphenylpyruvate   | C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>                 | 179.0350                | 13.58                       |
| tyrosine                | C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>               | 180.0666                | 2.00                        |
| homocysteic acid        | C <sub>4</sub> H <sub>9</sub> NO <sub>5</sub> S              | 182.0129                | 4.80                        |
| 4-pyridoxic acid        | C <sub>8</sub> H <sub>9</sub> NO <sub>4</sub>                | 182.0459                | 14.00                       |
| 3-phospho-serine        | C <sub>3</sub> H <sub>8</sub> NO <sub>6</sub> P              | 184.0017                | 8.20                        |
| 3-phosphoglycerate      | C <sub>3</sub> H <sub>7</sub> O <sub>7</sub> P               | 184.9857                | 13.58                       |
| indoleacrylic acid      | C <sub>11</sub> H <sub>9</sub> NO <sub>2</sub>               | 186.0561                | 15.50                       |
| N-acetyl-glutamine      | C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> | 187.0724                | 7.00                        |
| acetyllysine            | C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> | 187.1088                | 1.20                        |
| kynurenic acid          | C <sub>10</sub> H <sub>7</sub> NO <sub>3</sub>               | 188.0353                | 14.22                       |
| N-acetyl-glutamate      | C <sub>7</sub> H <sub>11</sub> NO <sub>5</sub>               | 188.0564                | 13.00                       |
| 2-dehydro-D-gluconate   | C <sub>6</sub> H <sub>10</sub> O <sub>7</sub>                | 193.0354                | 5.00                        |
| D-erythrose-4-phosphate | C <sub>4</sub> H <sub>9</sub> O <sub>7</sub> P               | 199.0013                | 7.45                        |

| <i>Metabolite</i>               | <i>Neutral formula</i>                                         | <i>Theoretical mass</i> | <i>Retention time (min)</i> |
|---------------------------------|----------------------------------------------------------------|-------------------------|-----------------------------|
| xanthurenic acid                | C <sub>10</sub> H <sub>7</sub> NO <sub>4</sub>                 | 204.0302                | 13.90                       |
| kynurenine                      | C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>  | 207.0775                | 3.87                        |
| D-glucarate                     | C <sub>6</sub> H <sub>10</sub> O <sub>8</sub>                  | 209.0303                | 13.00                       |
| deoxyribose-5-phosphate         | C <sub>5</sub> H <sub>11</sub> O <sub>7</sub> P                | 213.0170                | 7.74                        |
| N-acetyl-D-glucosamine          | C <sub>8</sub> H <sub>15</sub> NO <sub>6</sub>                 | 220.0827                | 2.00                        |
| cystathionine                   | C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S | 221.0602                | 1.00                        |
| prephenate                      | C <sub>10</sub> H <sub>10</sub> O <sub>6</sub>                 | 225.0405                | 13.87                       |
| deoxyuridine                    | C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>   | 227.0674                | 3.54                        |
| 5-methoxytryptophan             | C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>  | 233.0932                | 8.95                        |
| thymidine                       | C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub>  | 241.0830                | 5.40                        |
| cytidine                        | C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub>   | 242.0783                | 1.20                        |
| deoxyadenosine                  | C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>3</sub>  | 250.0946                | 8.00                        |
| deoxyinosine                    | C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>4</sub>  | 251.0786                | 3.90                        |
| shikimate-3-phosphate           | C <sub>7</sub> H <sub>11</sub> O <sub>8</sub> P                | 253.0119                | 13.44                       |
| D-glucono-δ-lactone-6-phosphate | C <sub>6</sub> H <sub>11</sub> O <sub>9</sub> P                | 257.0068                | 6.17                        |
| thiamine                        | C <sub>12</sub> H <sub>16</sub> N <sub>4</sub> OS              | 263.0972                | 0.80                        |
| 1,3-diphosphoglycerate          | C <sub>3</sub> H <sub>8</sub> O <sub>10</sub> P <sub>2</sub>   | 264.9520                | 13.87                       |

| <i>Metabolite</i>                     | <i>Neutral formula</i>                                           | <i>Theoretical mass</i> | <i>Retention time (min)</i> |
|---------------------------------------|------------------------------------------------------------------|-------------------------|-----------------------------|
| 2,3-diphosphoglycerate                | C <sub>3</sub> H <sub>8</sub> O <sub>10</sub> P <sub>2</sub>     | 264.9520                | 14.68                       |
| S-ribosyl-L-homocysteine              | C <sub>9</sub> H <sub>17</sub> NO <sub>6</sub> S                 | 266.0704                | 0.68                        |
| deoxyguanosine                        | C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>    | 266.0895                | 4.80                        |
| 6-phospho-D-gluconate                 | C <sub>6</sub> H <sub>13</sub> O <sub>10</sub> P                 | 275.0174                | 13.38                       |
| 1-methyladenosine                     | C <sub>11</sub> H <sub>15</sub> N <sub>5</sub> O <sub>4</sub>    | 280.1051                | 1.00                        |
| L-arginino-succinate                  | C <sub>10</sub> H <sub>18</sub> N <sub>4</sub> O <sub>6</sub>    | 289.1154                | 7.70                        |
| S-methyl-5'-thioadenosine             | C <sub>11</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub> S  | 296.0823                | 11.60                       |
| 7-methylguanosine                     | C <sub>11</sub> H <sub>16</sub> N <sub>5</sub> O <sub>5</sub>    | 297.1079                | 1.16                        |
| N-acetyl-D-glucosamine-1/6-phosphate* | C <sub>8</sub> H <sub>16</sub> NO <sub>9</sub> P                 | 300.0490                | 7.30                        |
| dCMP                                  | C <sub>9</sub> H <sub>14</sub> N <sub>3</sub> O <sub>7</sub> P   | 306.0497                | 9.80                        |
| dUMP                                  | C <sub>9</sub> H <sub>13</sub> N <sub>2</sub> O <sub>8</sub> P   | 307.0337                | 10.28                       |
| geranyl-diphosphate                   | C <sub>10</sub> H <sub>20</sub> O <sub>7</sub> P <sub>2</sub>    | 313.0612                | 16.46                       |
| thymidine-5'-phosphate (dTMP)         | C <sub>10</sub> H <sub>15</sub> N <sub>2</sub> O <sub>8</sub> P  | 321.0493                | 11.27                       |
| dAMP                                  | C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>6</sub> P  | 330.0609                | 12.00                       |
| trehalose/sucrose/cellobiose*         | C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>                  | 341.1090                | 1.18                        |
| thiamine-phosphate                    | C <sub>12</sub> H <sub>17</sub> N <sub>4</sub> O <sub>4</sub> PS | 343.0635                | 3.30                        |
| dGMP                                  | C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>7</sub> P  | 346.0558                | 11.00                       |

| <i>Metabolite</i>                 | <i>Neutral formula</i>                                                        | <i>Theoretical mass</i> | <i>Retention time (min)</i> |
|-----------------------------------|-------------------------------------------------------------------------------|-------------------------|-----------------------------|
| S-adenosyl-L-methioninamine       | C <sub>14</sub> H <sub>23</sub> N <sub>6</sub> O <sub>3</sub> S               | 354.1480                | 1.00                        |
| xanthosine-5-phosphate            | C <sub>10</sub> H <sub>13</sub> N <sub>4</sub> O <sub>9</sub> P               | 363.0347                | 12.70                       |
| orotidine-5'-phosphate            | C <sub>10</sub> H <sub>13</sub> N <sub>2</sub> O <sub>11</sub> P              | 367.0184                | 13.58                       |
| trans, trans-farnesyl diphosphate | C <sub>15</sub> H <sub>28</sub> O <sub>7</sub> P <sub>2</sub>                 | 381.1238                | 16.74                       |
| dCDP                              | C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>10</sub> P <sub>2</sub>  | 386.0160                | 13.58                       |
| 5-phosphoribosyl-1-pyrophosphate  | C <sub>5</sub> H <sub>13</sub> O <sub>14</sub> P <sub>3</sub>                 | 388.9446                | 14.94                       |
| S-adenosyl-L-methionine           | C <sub>15</sub> H <sub>22</sub> N <sub>6</sub> O <sub>5</sub> S               | 397.1300                | 0.90                        |
| thymidine-5'-diphosphate (dTDP)   | C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>11</sub> P <sub>2</sub> | 401.0157                | 13.58                       |
| cholic acid                       | C <sub>24</sub> H <sub>40</sub> O <sub>5</sub>                                | 407.2803                | 18.00                       |
| adenosine 5'-phosphosulfate       | C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>10</sub> PS             | 426.0126                | 13.58                       |
| dGDP                              | C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>10</sub> P <sub>2</sub> | 426.0221                | 14.00                       |
| inosine diphosphate (IDP)         | C <sub>10</sub> H <sub>14</sub> N <sub>4</sub> O <sub>11</sub> P <sub>2</sub> | 427.0062                | 13.90                       |
| 7,8-dihydrofolate                 | C <sub>19</sub> H <sub>21</sub> N <sub>7</sub> O <sub>6</sub>                 | 442.1480                | 13.60                       |
| CDP-ethanolamine                  | C <sub>11</sub> H <sub>20</sub> N <sub>4</sub> O <sub>11</sub> P <sub>2</sub> | 445.0531                | 6.38                        |
| deoxycholic acid                  | C <sub>26</sub> H <sub>43</sub> NO <sub>5</sub>                               | 448.3069                | 17.90                       |
| 5-methyl-tetrahydrofolate         | C <sub>20</sub> H <sub>25</sub> N <sub>7</sub> O <sub>6</sub>                 | 458.1794                | 14.10                       |
| dCTP                              | C <sub>9</sub> H <sub>16</sub> N <sub>3</sub> O <sub>13</sub> P <sub>3</sub>  | 465.9823                | 14.80                       |

| <i>Metabolite</i>                                           | <i>Neutral formula</i>                                                          | <i>Theoretical mass</i> | <i>Retention time (min)</i> |
|-------------------------------------------------------------|---------------------------------------------------------------------------------|-------------------------|-----------------------------|
| dUTP                                                        | C <sub>9</sub> H <sub>15</sub> N <sub>2</sub> O <sub>14</sub> P <sub>3</sub>    | 466.9663                | 14.81                       |
| thymidine 5'-triphosphate (dTTP)                            | C <sub>10</sub> H <sub>17</sub> N <sub>2</sub> O <sub>14</sub> P <sub>3</sub>   | 480.9820                | 14.94                       |
| CDP-choline                                                 | C <sub>14</sub> H <sub>27</sub> N <sub>4</sub> O <sub>11</sub> P <sub>2</sub>   | 488.1079                | 6.33                        |
| dATP                                                        | C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>12</sub> P <sub>3</sub>   | 489.9936                | 14.94                       |
| taurodeoxycholic acid                                       | C <sub>26</sub> H <sub>45</sub> NO <sub>6</sub> S                               | 498.2895                | 17.73                       |
| dGTP                                                        | C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>13</sub> P <sub>3</sub>   | 505.9885                | 15.46                       |
| guanosine 5'-diphosphate,3'-diphosphate                     | C <sub>10</sub> H <sub>11</sub> N <sub>5</sub> O <sub>17</sub> P <sub>4</sub>   | 595.9028                | 15.40                       |
| nicotinamide adenine dinucleotide phosphate reduced (NADPH) | C <sub>21</sub> H <sub>30</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub>   | 744.0838                | 14.87                       |
| propionyl-CoA                                               | C <sub>24</sub> H <sub>40</sub> N <sub>7</sub> O <sub>17</sub> P <sub>3</sub> S | 822.1342                | 15.64                       |
| 3-hydroxy-3-methylglutaryl-CoA                              | C <sub>27</sub> H <sub>44</sub> N <sub>7</sub> O <sub>20</sub> P <sub>3</sub> S | 910.1502                | 15.72                       |