**Supplemental Table 1. M/z Transitions and Collision Energies**

| Metabolite | m/z(1) | m/z(2) | Polarity | Target Collision Energy |
|---|---|---|---|---|
| Glutathione | 308 | 84.05 | + | -24 |
| NADH | 666 | 649.1 | + | -17 |
| Glycine | 75.9 | 30.1 | + | -12 |
| Aspartic acid | 134 | 74.05 | + | -15 |
| Glutamine | 147.1 | 84.05 | + | -25 |
| Lysine | 147 | 84.1 | + | -25 |
| Threonine | 120.1 | 74.1 | + | -12 |
| L-a-Glycerophosphocholine | 257.7 | 104.1 | + | -16 |
| Glutamic acid | 147.9 | 84.1 | + | -20 |
| Alanine | 89.9 | 44.1 | + | -13 |
| Histidine | 155.9 | 110.05 | + | -20 |
| Arginine | 175.1 | 70.1 | + | -30 |
| Creatine | 132.1 | 90.1 | + | -14 |
| Valine | 118.1 | 72.1 | + | -16 |
| Methionine | 149.9 | 56.1 | + | -20 |
| Nicotinic acid | 124.1 | 78.05 | + | -22 |
| Leucine | 132.1 | 86.15 | + | -15 |
| Adenosine | 268.1 | 136.05 | + | -25 |
| FAD | 786.2 | 136.1 | + | -47 |
| Phenylalanine | 166.1 | 120.1 | + | -20 |
| Tryptophan | 205.1 | 188.15 | + | -10 |
| Uracil | 113 | 70 | + | -17 |
| Carnitine | 162.1 | 103.05 | + | -18 |
| Glucose 6-phosphate_N | 259 | 97 | - | 15 |
| Citric acid_N | 191 | 111.15 | - | 12 |
| Malic Acid | 133.1 | 114.95 | - | 17 |
| Lactic Acid | 89.3 | 89.05 | - | 7 |
| Pyruvate | 86.9 | 87.05 | - | 7 |
| Fumaric Acid | 115.1 | 71 | - | 0 |
| MES | 196.2 | 100.05 | + | -23 |