

Supplementary Table 2. Internal standards selected based on the group classification produced in experiment A

| Group    | 1st  | 2nd   | 3rd   |
|----------|--|---|---|
| Group 1  | lactic acid- <sup>13</sup> C <sub>3</sub>            | isoleucine-d <sub>10</sub>  | alanine- <sup>13</sup> C <sub>3</sub>           |
| Group 2  | glucose- <sup>13</sup> C <sub>6</sub>                | taurine- <sup>13</sup> C <sub>2</sub>                                 | taurine- <sup>13</sup> C <sub>2</sub>           |
| Group 3  | tryptophan- <sup>13</sup> C <sub>11</sub>            | 3-aminopropanoic acid- <sup>13</sup> C <sub>3</sub> - <sup>15</sup> N | ornithine-d <sub>7</sub>                        |
| Group 4  | sarcosine-d <sub>3</sub>                             | sarcosine-d <sub>3</sub>  | sarcosine-d <sub>3</sub>                        |
| Group 5  | tyrosine- <sup>13</sup> C <sub>6</sub>               | valine-d <sub>8</sub>   | glutamic acid- <sup>13</sup> C <sub>5</sub>     |
| Group 6  | glutamine- <sup>13</sup> C <sub>5</sub>              | palmitoleic acid- <sup>13</sup> C <sub>16</sub>                       | palmitoleic acid- <sup>13</sup> C <sub>16</sub> |
| Group 7  | lauric acid-d <sub>3</sub>                           | ribose- <sup>13</sup> C <sub>5</sub>                                  | succinic acid- <sup>13</sup> C <sub>4</sub>     |
| Group 8  | 2-IPMA   | 2-IPMA  | 2-IPMA  |
| Group 9  | 3-hydroxyisovaleric acid-d <sub>8</sub>              | 3-hydroxyisovaleric acid-d <sub>8</sub>                               | 3-hydroxyisovaleric acid-d <sub>8</sub>         |
| Group 10 | 1,5-anhydro-D-glucitol- <sup>13</sup> C <sub>6</sub> | histidine- <sup>13</sup> C <sub>6</sub>                               | citric acid-d <sub>4</sub>                      |
| Group 11 | palmitic acid- <sup>13</sup> C <sub>16</sub>         | palmitic acid- <sup>13</sup> C <sub>16</sub>                          | palmitic acid- <sup>13</sup> C <sub>16</sub>    |
| Group 12 | 2-IPMA   | 2-IPMA  | 2-IPMA  |

Internal standards selected based on the group classification produced in experiment A are listed, and these internal standards were used in experiment B.