

Supplementary information

Supplementary Table S1: List of metabolite derivatives and their biological group used for reference search. MeOX: Methoxyamine hydrochloride. PPP: Pentose phosphate pathway. SCFA: short chain fatty acid. TCA: Tricarboxylic acid cycle. TMS: Trimethylsilyl derivatives.

| Biological group | Metabolite | Detected as |
|---------------------|----------------------------|----------------------|
| Amino acid | Alanine | 2TMS or 3TMS |
| Amino acid | Asparagine | 2TMS |
| Amino acid | Aspartic acid | 2TMS or 3TMS |
| Amino acid | Cysteine | 3TMS |
| Amino acid | Glycine | 2TMS or 3TMS |
| Amino acid | Isoleucine | 1TMS or 2TMS |
| Amino acid | Leucine | 1TMS or 2TMS |
| Amino acid | Lysine | 3TMS |
| Amino acid | Methionine | 1TMS or 2TMS |
| Amino acid | Phenylalanine | 1TMS or 2TMS |
| Amino acid | Proline | 1TMS or 2TMS |
| Amino acid | Serine | 2TMS or 3TMS or 4TMS |
| Amino acid | Threonine | 2TMS or 3TMS |
| Amino acid | Tryptophan | 2TMS |
| Amino acid | Tyrosine | 3TMS |
| Amino acid | Valine | 1TMS |
| Amino acid | Glutamine | 1TMS |
| Amino acid | Homocysteine | 3TMS |
| Amino acid | Arginine | 1TMS |
| Amino acid | Glucosamine N-acetyl | 1MeOx 5TMS |
| Amino acid derivate | Pyroglutamic acid | 2TMS |
| Glycolysis | Fructose-6-phosphate | 1MeOx 6TMS |
| Glycolysis | Glucose-6-phosphate | 1MeOx 6TMS |
| Glycolysis | Glyceric acid-3-phosphate | 4TMS |
| Glycolysis | Lactic acid | 2TMS |
| Glycolysis | Phosphoenolpyruvic acid | 3TMS |
| Glycolysis | Pyruvic acid | 1MeOx 1TMS |
| Glycolysis | Putrescine | 3TMS or 4TMS |
| TCA | Citric acid | 4TMS |
| TCA | Fumaric acid | 2TMS |
| TCA | 2-hydroxy glutaric acid | 3TMS |
| TCA | 2-oxo glutaric acid | 1MeOx 2TMS |
| TCA | Malic acid | 3TMS |
| TCA | Succinic acid | 2TMS |
| TCA | Isocitric acid | 1MeOx 5TMS |
| TCA | Aconitic acid | 3TMS |
| Others (Nucleotide) | Adenine | 2TMS |
| Others (Nucleotide) | Uracil | 2TMS |
| Others (Nucleotide) | Uridine | 3TMS |
| Others (Nucleobase) | Adenosine | 3TMS or 4TMS |
| Others (Nucleobase) | Cytosine | 2TMS |
| Others (Nucleobase) | Thymine | 2TMS |
| Others (Glycerol) | Dihydroxyacetone phosphate | 1MeOx 3TMS |

| | | |
|--------------------------|---------------------------|--------------|
| Others (Glycerol) | Glycerol | 3TMS |
| Others (Glycerol) | Glycerol-3-phosphate | 4TMS |
| Others (Glycerol) | Glyceric acid | 3TMS |
| Others (SCFA) | 3-hydroxy butanoic acid | 2TMS |
| Others (SCFA) | 4-amino butanoic acid | 3TMS |
| Others (SCFA) | 2-amino butanoic acid | 2TMS |
| Others (Sugar alcohol) | Erythritol | 4TMS |
| Others (Sugar alcohol) | Arabitol | 5TMS |
| Others (Alcohol) | Thymine | 2TMS |
| Others (Alcohol) | Sorbitol | 1TMS |
| Others (Carboxylic acid) | Glutaric acid | 2TMS |
| Others (PPP) | Ribose-5-phosphate | 1MeOx 5TMS |
| Others (PPP) | Ribose | 1MeOx 4TMS |
| Others (PPP) | Ribulose-5-phosphate | 1MeOx 5TMS |
| Others (PPP) | Ribitol | 5TMS |
| Others (PPP) | Erythrose-4-phosphate | 1MeOx 4TMS |
| Others (PPP) | Gluconic acid 6-phosphate | 7TMS |
| Others (Urea cycle) | Urea | 2TMS |
| Others (Urea cycle) | Ornithine | 3TMS or 4TMS |
| Others (Sugar) | Trehalose | 8TMS |
| Others (Sugar) | Sucrose | 8TMS |
| Others (Sugar) | Mannose | 1MeOx 5TMS |
| Others (Sugar) | Maltose | 1MeOx 8TMS |
| Others (Sugar) | Glucose | 1MeOx 5TMS |
| Others (Sugar) | Galactitol | 6TMS |
| Others (Sugar) | Acetyl-galactosamine | 1MeOx 4TMS |
| Others (Hydrocarbons) | Xylose | 1MeOx 4TMS |
| Others (Hydrocarbons) | Hypotaurine | 3TMS |
| Others (Vitamin) | Pantothenic acid | 3TMS |
| Others | Maleic Acid | 3TMS |
| Others | Ethanolaminephosphate | 4TMS |

Supplementary Table S2: List of metabolite's RSD values obtained for each of the protocols performed in bone and muscle tissue.

| Metabolite | Bone RSD | | | Muscle RSD | | |
|---------------|----------|---------|------|------------|---------|------|
| | mBD | mBD-low | mMat | mBD | mBD-low | mMat |
| Alanine | 37 | 18 | 8 | 33 | 42 | 64 |
| Asparagine | NA | NA | NA | NA | NA | NA |
| Aspartic acid | 25 | 14 | 15 | 28 | 64 | 40 |
| Cysteine | 17 | 8 | 10 | 25 | 59 | NA |
| Glycine | 30 | 15 | 25 | 18 | 17 | 67 |
| Isoleucine | 17 | NA | NA | 60 | NA | 54 |
| Leucine | 32 | 15 | 23 | 45 | 66 | NA |
| Lysine | 43 | 9 | 20 | 58 | 63 | 20 |
| Methionine | 13 | 35 | 26 | 25 | 34 | 52 |
| Phenylalanine | 13 | 50 | 29 | 48 | 48 | 46 |
| Proline | 34 | 61 | 51 | 89 | 58 | 53 |
| Serine | 25 | NA | NA | 32 | 61 | 56 |
| Threonine | 45 | 44 | 44 | 28 | 37 | 16 |

| | | | | | | |
|----------------------------|----|----|----|-----|----|----|
| Tryptophan | 15 | 12 | 10 | 67 | 63 | 39 |
| Tyrosine | 26 | 22 | 22 | 63 | 35 | 87 |
| Valine | 14 | 27 | 30 | 67 | 40 | 61 |
| Glutamine | NA | NA | NA | NA | NA | NA |
| Homocysteine | 33 | 23 | 52 | 25 | 36 | 26 |
| Arginine | NA | NA | NA | NA | NA | NA |
| Glucosamine N-acetyl | 4 | 10 | 21 | NA | NA | NA |
| Pyroglutamic acid | 26 | 15 | 14 | 3 | 11 | 59 |
| Fructose-6-phosphate | 25 | 33 | 8 | 95 | 69 | 37 |
| Glucose-6-phosphate | 23 | 20 | 24 | 45 | 60 | NA |
| Glyceric acid-3-phosphate | 32 | NA | NA | 41 | 86 | NA |
| Lactic acid | 11 | 4 | 8 | 65 | 7 | 55 |
| Phosphoenolpyruvic acid | 9 | 45 | 46 | 29 | 18 | 57 |
| Pyruvic acid | 18 | 26 | 77 | 29 | 88 | 8 |
| Putrescine | 50 | 31 | 58 | 45 | 55 | 47 |
| Citric acid | 4 | 16 | 3 | 32 | 56 | 58 |
| Fumaric acid | 4 | 4 | 6 | 21 | 58 | 25 |
| 2-hydroxy glutaric acid | 1 | 13 | 2 | 12 | 15 | 96 |
| 2-oxo glutaric acid | 8 | NA | NA | 36 | NA | 25 |
| Malic acid | 3 | 4 | 4 | 15 | 19 | 23 |
| Succinic acid | 4 | 4 | 5 | 67 | 60 | 70 |
| Isocitric acid | 4 | 17 | 3 | 32 | 55 | 58 |
| Aconitic acid | NA | NA | NA | NA | NA | NA |
| Adenine | NA | NA | NA | NA | NA | NA |
| Uracil | 5 | 27 | 21 | 21 | 58 | 42 |
| Uridine | 10 | 12 | 5 | 31 | 59 | 35 |
| Adenosine | 37 | 18 | 8 | 28 | 7 | 24 |
| Cytosine | 31 | 39 | 15 | 27 | 14 | 34 |
| Thymine | 10 | 33 | 15 | 35 | 46 | NA |
| Dihydroxyacetone phosphate | 30 | 46 | 59 | 36 | NA | NA |
| Glycerol | 3 | 4 | 4 | 59 | 82 | 21 |
| Glycerol-3-phosphate | 9 | 13 | 19 | 55 | 37 | 82 |
| Glyceric acid | 4 | 7 | 2 | 13 | 77 | 27 |
| 3-hydroxy butanoic acid | 8 | 18 | 22 | 67 | 20 | 42 |
| 4-amino butanoic acid | NA | NA | NA | NA | NA | NA |
| 2-amino butanoic acid | 16 | 24 | NA | 86 | 74 | 54 |
| Erythritol | NA | NA | NA | NA | NA | NA |
| Arabitol | NA | NA | NA | NA | NA | NA |
| Thymine | 10 | 33 | 15 | 35 | 46 | NA |
| Sorbitol | NA | NA | NA | NA | NA | NA |
| Glutaric acid | 35 | 31 | 3 | 20 | 21 | 24 |
| Ribose-5-phosphate | 33 | 79 | 69 | 56 | 24 | 9 |
| Ribose | 6 | 4 | 3 | 59 | NA | 57 |
| Ribulose-5-phosphate | 16 | 10 | 7 | 97 | 75 | 22 |
| Ribitol | 4 | 18 | 10 | 56 | 83 | 93 |
| Erythrose-4-phosphate | 29 | 5 | 1 | 112 | 84 | NA |
| Gluconic acid 6-phosphate | 13 | 23 | 6 | NA | NA | NA |
| Urea | 4 | 11 | 17 | 23 | 10 | 68 |
| Ornithine | 27 | 60 | 27 | 50 | 69 | 81 |
| Trehalose | 5 | 64 | 5 | 8 | 23 | 60 |
| Sucrose | 16 | 23 | NA | 24 | 28 | 52 |

| | | | | | | |
|-----------------------|----|----|----|----|----|----|
| Mannose | 1 | 4 | 1 | 17 | 53 | 11 |
| Maltose | 4 | NA | 9 | NA | NA | NA |
| Glucose | 2 | 5 | 1 | NA | NA | NA |
| Galactitol | 3 | 22 | 15 | 13 | 13 | 21 |
| Acetyl-galactosamine | 4 | 10 | 21 | NA | NA | NA |
| Xylose | NA | NA | NA | NA | NA | NA |
| Hypotaurine | 24 | 29 | 25 | 37 | 18 | 61 |
| Pantothenic acid | 52 | 57 | 8 | 19 | 16 | 34 |
| Maleic Acid | 3 | 4 | 4 | 18 | 20 | 73 |
| Ethanolaminephosphate | 24 | 21 | 15 | 51 | 35 | 30 |