

Table 1. Compounds identified in GC-MS and <sup>1</sup>H NMR. L: by library; Std: with the corresponding standard.

| COMPOUNDS              | GC-MS  | <sup>1</sup> H NMR |
|------------------------|--------|--------------------|
| 11-Cis-Odecanoate      | L      | -                  |
| 11-Trans-Octadecenoate | L      | -                  |
| 2,3,4-Tri-OH-Butyrate  | L      | -                  |
| 2-Aminobutyrate        | L/Std  | -                  |
| 2-OH-Butyrate          | L/Std  | -                  |
| 3-OH-Butyrate          | L/Std  | Std                |
| 4-OH-Proline           | L/Std  | -                  |
| Acetate                | -      | L                  |
| Acetoacetate           | -      | L                  |
| Acetone                | -      | Std                |
| Alanine                | L/Std  | L                  |
| Aminomalonate          | L      | -                  |
| Arginine               | -      | L                  |
| Asparagine             | L/Std  | -                  |
| Aspartate              | L/Std  | -                  |
| BHT <sup>a</sup>       | L      | -                  |
| Cholesterol            | L/Std  | -                  |
| Citrate                | L/Std  | L                  |
| Creatine               | -      | L                  |
| Creatinine             | L/Std  | L                  |
| Dehydrated citrate     | L/Std  | -                  |
| EDTA                   | L/Std  | Std                |
| Ethanol                | -      | Std                |
| Formate                | -      | L                  |
| Fructose               | L/Std  | Std                |
| Galactofuranose        | L      | -                  |
| Gluconate              | L      | -                  |
| Glucopyranose          | L      | -                  |
| Glucose                | L/Std  | Std                |
| Glucose oxime          | L      | -                  |
| Glutamate              | L/Std  | -                  |
| Glutamine              | L/Std  | Std                |
| Glycerate              | L      | -                  |
| Glycerol               | L      | Std                |
| Glycine                | L/Std  | Std                |
| Glycolate              | L /Std | -                  |
| Hexanoate              | Std    | -                  |
| Histidine              | -      | Std                |

| COMPOUNDS                        | GC-MS | <sup>1</sup> H NMR |
|----------------------------------|-------|--------------------|
| Inositol                         | L     | -                  |
| Isocitrate                       | L/Std | -                  |
| Isoleucine                       | L/Std | Std                |
| Ketoglutarate                    | Std   | -                  |
| Lactate                          | Std   | L                  |
| Laurate                          | Std   | -                  |
| LDL/VLDL                         | -     | L                  |
| Leucine                          | -     | Std                |
| Linoleate                        | L     | -                  |
| Lysine                           | L     | L                  |
| Malate                           | L/Std | -                  |
| MeOH                             | -     | Std                |
| Methionine                       | L/Std | -                  |
| Myo-inositol                     | L/Std | Std                |
| Myristate                        | Std   | -                  |
| NAC (glycoproteins) <sup>b</sup> | -     | L                  |
| Ornithine                        | L/Std | -                  |
| Oxalate                          | Std   | -                  |
| Palmitate                        | L/Std | -                  |
| Phenylalanine                    | L/Std | -                  |
| Phenylpyruvate                   | Std   | -                  |
| Proline                          | L/Std | Std                |
| Pyroglutamate                    | L/Std | -                  |
| Pyruvate                         | L/Std | L                  |
| Ribofuranose                     | L     | -                  |
| Scyllo-inositol                  | -     | Std                |
| Serine                           | L/Std | Std                |
| Sorbitol                         | L     | -                  |
| Stearate                         | L/Std | -                  |
| Succinate                        | Std   | -                  |
| Threonine                        | L/Std | Std                |
| Tryptophan                       | L/Std | -                  |
| Tyrosine                         | L/Std | Std                |
| Urate                            | L/Std | -                  |
| Urea                             | L/Std | -                  |
| Valine                           | L/Std | Std                |
| Xylitol                          | L     | -                  |

<sup>b</sup> BHT is not a metabolite, appears from exogenous sources

<sup>a</sup> NAC refers to composite acetyl signals from  $\alpha$ 1-acid glycoprotein<sup>12</sup>.