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| **Metabolite** | **δH /ppm (multiplicity)** |
| 4-hydroxyphenylacetate | 3.46 (s), 6.87 (dd), 7.16 (dd), |
| Acetate | 1.92 (s) |
| Acetoacetate | 2.27 (s), 3.46 (s) |
| Acetone | 2.23 (s) |
| Alanine | 1.48 (d), 3.78 (q) |
| Aspartate | 2.69 (dd), 2.82 (dd), 3.91 (dd) |
| Bile acids a | 0.68 (s), 0.70 (s), 0.72 (s) |
| Butyrate | 0.90 (t), 1.57 (m), 2.17 (t) |
| Choline | 3.20 (s), 3.52 (m), 4.08 (m) |
| Ethanol | 1.19 (t), 3.65 (q) |
| Formate | 8.46 (s) |
| Fructose | 3.58 (m), 3.66 (dd), 3.70 (m), 3.81 (dd), 3.83 (m), 3.90 (dd), 3.95 (m), 4.01 (m), 4.04 (m), 4.06 (m), 4.12 (m) |
| Fumarate | 6.53 (s) |
| Galactose | 3.49 (dd), 3.64 (dd), 3.75 (m), 3.83 (m), 3.93 (d), 3.98 (d), 4.10 (t, C1H), 4.60 (d, CH2), 5.28 (d, C5H) |
| Glutamate | 2.04 (m), 2.12 (m), 2.34 (m), 3.75 (dd) |
| Glutamine | 2.15 (m), 2.47 (m), 3.79 (t) |
| α-Glucose | 3.42 (t), 3.54 (dd), 3.71 (t), 3.77 (dd), 3.84 (m), 5.23 (d) |
| β-Glucose | 3.23 (dd); 3.44 (m), 3.50 (t), 3.72 (dd), 3.90 (m), 4.65 (d) |
| Glycerol | 3.55 (m), 3.65 (dd), 3.78 (m) |
| Glycine | 3.56 (s) |
| Hypoxanthine | 8.19 (s), 8.21 (s) |
| Isoleucine | 0.94 (t), 1.01 (d), 1.26 (m), 1.47(m), 1.98 (m), 3.62 (d) |
| Lactate | 1.34 (d), 4.11 (q) |
| Leucine | 0.96 (t), 1.73 (m) |
| Lysine | 1.48 (m), 1.73 (m), 1.92 (m), 3.03 (t), 3.77 (t) |
| Methanol | 3.36 (s) |
| Phenylalanine | 3.13(dd), 3,29(dd), 4.00(dd), 7.34(m), 7.38(m), 7.44(m) |
| *N*-acetyl residue a | 2.05 (s) |
| Propionate | 1.06 (t), 2.18 (q) |
| Pyruvate | 2.38 (s) |
| Succinate | 2.41 (s) |
| Sucrose | 3.48 (t), 3.56 (dd), 3.63 (s), 3.77 (t), 3.83 (dd), 3.85 (m), 3.89 (m), 4.06 (t), 4.22 (d), 5.41 (d) |
| Taurine | 3.26 (t), 3.43 (t) |
| TMA | 2.88 (s) |
| TMAO | 3.28 (s) |
| Threonine | 1.33 (d), 3.61 (d), 4.26 (dd) |
| Tyrosine | 6.98 (dd), 7.20 (dd), 3.95 (dd), 3.20 (dd), 3.06 (dd) |
| Uracil | 5.78 (d), 7.54 (d) |
| Urea | 5.80 (s,br) |
| Valine | 0.99 (d), 1.04 (d), 2.27 (m), 3.61 (d) |
| Xylose | 3.23 (dd), 3.33 (dd), 3.42 (t), 3.53 (dd), 3.63 (m), 3.93 (dd), 4.59 (d), 5.21 (d) |
| **Unassigned spin systems varying significantly between groups** | |
| U1 | 5.93 (d), 5.98 (d), 6.07 (d), 6.11 (d), 8.03 (s), 8.27 (s), 8.38 (s) |
| U2 | 8.63 (s) |
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