

Table 2. Metabolites important to the differentiation of treatment and control groups, using PLD-DA analysis (VIP ≥ 1.0 with a jack-knife confidence interval that did not include 0).

Exposure	Increased relative to control	Decreased relative to control
α -HBCD 3 mg/kg	3-hydroxybutyrate Acetoacetate Creatine Leucine Methionine O-Phosphocholine Taurine Tyrosine Valine	Alanine Arginine Glutamate Lactate Pyruvate Serine
α -HBCD 10 mg/kg	3-hydroxybutyrate Acetoacetate Glutamine Methionine O-Phosphocholine Taurine	Lactate Methanol N,N-Dimethylglycine Phenylalanine Pyruvate Glutamate
α -HBCD 30 mg/kg	2-hydroxyisobutyrate 3-hydroxybutyrate Acetoacetate Glutamine Leucine Taurine Valine	Acetate Alanine Choline Citrate Glutamate Lactate Methanol Phenylalanine Pyruvate
γ -HBCD 3 mg/kg	3-hydroxybutyrate Citrate Creatine Glycerol Glycine Serine Taurine	Alanine Asparagine Cysteine Lactate Methanol Phenylalanine Pyruvate
γ -HBCD 30 mg/kg	2-hydroxyisobutyrate 3-hydroxybutyrate Asparagine Citrate Creatine Glucose Glycerol Glycine Taurine	Choline Glutamate Lactate Methanol Phenylalanine Pyruvate Serine Threonine Tyrosine
CM-HBCD 30 mg/kg	3-hydroxybutyrate Asparagine Citrate Creatine Glycerol Lactate Methionine O-Phosphocholine Taurine Valine	Alanine Arginine Glucose Methanol Phenylalanine

Note: VIP, variable influence on projections.