

Table 1S. Comparative table of the discriminant metabolites resulting from the analysis of the S-plot and VIP list of the multivariate models (C vs R, C vs NR and R vs NR). Amount of + indicates the class with higher or lower concentration of the different metabolites.

Metabolites	C	R	NR
Citrate	+++	++	+
Lactate	+++	++	+
Glucose	+++	++	+
Glutamate	++	+	++
Scyllo-Inositol	+	+++	+
2-OH-Butyr/Valerate	+	++	+++
3-OH-Butyrate	+	++	+++
Acetoacetate	+	++	+++
Acetate	+	++	+++
Acetone	+	++	+++
Alanine	+	+	++
Choline	+	++	++