

Table S1. Case processing summary. NA: value was rejected by automatic sample and measurement quality control; TAG: value cannot be quantified due to detected irregularity in sample. Rejected metabolites are marked in red font. Please note that albumin was rejected due to the quantification uncertainties.

		Valid cases	Missing cases	TAG	NA
Metabolite	Group	N	N	N	N
Glucose	Patients	44	0	0	0
	Controls	14	0	0	0
Lactate	Patients	44	0	0	0
	Controls	14	0	0	0
Pyruvate	Patients	6	38	36	2
	Controls	10	4	0	4
Citrate	Patients	41	3	3	0
	Controls	44	0	0	0
Glycerol	Patients	17	27	9	18
	Controls	6	8	8	0
Alanine	Patients	44	0	0	0
	Controls	14	0	0	0
Glutamine	Patients	8	36	36	0
	Controls	14	0	0	0
Glycine	Patients	44	0	0	0
	Controls	14	0	0	0
Histidine	Patients	44	0	0	0
	Controls	14	0	0	0
Isoleucine	Patients	44	0	0	0
	Controls	14	0	0	0
Leucine	Patients	12	32	32	0
	Controls	14	0	0	0
Valine	Patients	44	0	0	0
	Controls	14	0	0	0
Phenylalanine	Patients	12	32	32	0
	Controls	14	0	0	0
Tyrosine	Patients	44	0	0	0
	Controls	14	0	0	0
Acetate	Patients	10	34	34	0
	Controls	14	0	0	0
Acetoacetate	Patients	12	32	32	0
	Controls	14	0	0	0
3-hydroxybutyrate	Patients	44	0	0	0
	Controls	14	0	0	0
Creatinine	Patients	29	15	15	0
	Controls	14	0	0	0
Albumin	Patients	44	0	0	0
	Controls	14	0	0	0

Glycoprotein acetyls	Patients	44	0	0	0
	Controls	14	0	0	0