

Table S4. Pre-specified metabolite groups included in stage one of the statistical plan.

Metabolite group	Metabolite name
Short-chain acylcarnitines	Acetylcarnitine (C2)
	Propionylcarnitine (C3)
	Butyrylcarnitine + Isobutyrylcarnitine (C4)
	Isovalerylcarnitine + Methylbutyrylcarnitine (C5)
Medium-chain acylcarnitines	Hexanoylcarnitine (C6)
	Octanoylcarnitine (C8)
	Decanoylcarnitine (C10)
	Decenoylcarnitine (C10:1)
Long-chain acylcarnitines	Tetradecanoylcarnitine (C14)
	Tetradecenoylcarnitine (C14:1)
	Palmitoylcarnitine (C16)
	Palmitoylcarnitine (C16:1)
	Stearoylcarnitine (C18)
	Oleoylecarnitine (C18:1)
	Linoleoylcarnitine (C18:2)
Amino acids	Arginine (ARG)
	Argininosuccinate (ASA) ^a
	Citrulline (CIT)
	Glycine (GLY)
	Leucine (LEU) ^a
	Methionine (MET)

Ornithine (ORN)

Phenylalanine (PHE)

Tyrosine (TYR)

Valine (VAL)

^aMetabolite was not collected in replication cohort and, therefore, not included in replication analyses.