

Supplementary Table S1. Significantly metabolic pathways (FDR < 0.05) for the metabolites associated with feed efficiency using *Bos taurus* as the library.

Pathway name	Matched metabolite ratio	Metabolite	P-value	-Log(P-value)	False discovery rate (FDR)	Pathway impact value
Aminoacyl-tRNA biosynthesis	6/48	Glutamate, Glycine, Lysine, Phenylalanine, Threonine, Tyrosine	3.78×10^{-5}	4.42	2.64×10^{-3}	0
Glyoxylate and dicarboxylate metabolism	5/32	Acetate, Citrate, Formate, Glutamate, Glycine	6.28×10^{-5}	4.20	2.64×10^{-3}	0.138
Phenylalanine metabolism	3/12	Hippurate, Phenylalanine, Tyrosine	5.41×10^{-4}	3.27	0.0115	0.357
Alanine, aspartate and glutamate metabolism	4/28	α -ketoglutarate, Citrate, Glutamate, Succinate	5.48×10^{-4}	3.26	0.0115	0.245
Butanoate metabolism	3/15	α -ketoglutarate, Glutamate, Succinate	1.09×10^{-3}	2.96	0.0143	0
Glycine, serine and threonine metabolism	4/34	Betaine, Creatine, Glycine, Threonine	1.17×10^{-3}	2.93	0.0143	0.342
Phenylalanine, tyrosine and tryptophan biosynthesis	2/4	Phenylalanine, Tyrosine	1.19×10^{-3}	2.92	0.0143	1.0
D-Glutamine and D-glutamate metabolism	2/5	α -ketoglutarate, Glutamate	1.97×10^{-3}	2.71	0.0207	1.0
Citrate cycle (TCA cycle)	3/20	α -ketoglutarate, Citrate, Succinate	2.60×10^{-3}	2.59	0.0243	0.182

Note: The pathway impact value is calculated using the sum of importance measures of the matched metabolites divided by the sum of the importance measures of all metabolites.

