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Table S4. Biochemical reactions and corresponding enzymes (coding sequences – CDSs) potentially catalyzing these reactions. Reactions and CDSs depicted in Figure 4 are indicated.

Reaction number in Figure 4	Reaction identifier defined as in KEGG	Definition of the reaction	Coded equation as in KEGG. C##### is identifier for compound	EC number	Enzyme name
1	R01090	L-Leucine + 2-Oxoglutarate <=> 4-Methyl-2- oxopentanoate + L-Glutamate	C00123 + C00026 <=> C00233 + C00025	2.6.1.42	L-Leucine:2-oxoglutarate aminotransferase
2	R07601	4-Methyl-2-oxopentanoate + Thiamin diphosphate <=> 3-Methyl-1-hydroxybutyl-ThPP + CO2	C00233 + C00068 <=> C15974 + C00011	1.2.4.4	2-oxoisovalerate dehydrogenase E1 component alpha subunit
3	R07602	3-Methyl-1-hydroxybutyl-ThPP + Enzyme N6- (lipoyl)lysine <=> [Dihydrolipoyllysine-residue (2- methylpropanoyl)transferase] S-(3- methylbutanoyl)dihydrolipoyllysine + Thiamin diphosphate	C15974 + C15972 <=> C15975 + C00068	1.2.4.4	2-oxoisovalerate dehydrogenase E1 component alpha subunit
4	R04097	3-Methylbutanoyl-CoA + Enzyme N6- (dihydrolipoyl)lysine <=> CoA + [Dihydrolipoyllysine-residue (2- methylpropanoyl)transferase] S-(3- methylbutanoyl)dihydrolipoyllysine	C02939 + C15973 <=> C00010 + C15975	2.3.1.168	3-methylbutanoyl-CoA:enzyme N6- (dihydrolipoyl)lysine S-(3- methylbutanoyl)transferase
5	R01214	L-Valine + 2-Oxoglutarate <=> 3-Methyl-2- oxobutanoic acid + L-Glutamate	C00183 + C00026 <=> C00141 + C00025	2.6.1.42	L-Valine:2-oxoglutarate aminotransferase
6	R07599	3-Methyl-2-oxobutanoic acid + Thiamin diphosphate <=> 2-Methyl-1-hydroxypropyl-ThPP + CO2	C00141 + C00068 <=> C15976 + C00011	1.2.4.4	2-oxoisovalerate dehydrogenase E1 component alpha subunit

Reaction number in Figure 4	Reaction identifier defined as in KEGG	Definition of the reaction	Coded equation as in KEGG. C##### is identifier for compound	EC number	Enzyme name
7	R07600	2-Methyl-1-hydroxypropyl-ThPP + Enzyme N6- (lipoyl)lysine <=> [Dihydrolipoyllysine-residue (2- methylpropanoyl)transferase] S-(2- methylpropanoyl)dihydrolipoyllysine + Thiamin diphosphate	C15976 + C15972 <=> C15977 + C00068	1.2.4.4	2-oxoisovalerate dehydrogenase E1 component alpha subunit
8	R02662	2-Methylpropanoyl-CoA + Enzyme N6- (dihydrolipoyl)lysine <=> CoA + [Dihydrolipoyllysine-residue (2- methylpropanoyl)transferase] S-(2- methylpropanoyl)dihydrolipoyllysine	C00630 + C15973 <=> C00010 + C15977	2.3.1.168	2-methylpropanoyl-CoA:enzyme N6-(dihydrolipoyl)lysine S-(2- methylpropanoyl)transferase
9	R02199	L-Isoleucine + 2-Oxoglutarate <=> (S)-3-Methyl-2- oxopentanoic acid + L-Glutamate	C00407 + C00026 <=> C00671 + C00025	2.6.1.42	L-Isoleucine:2-oxoglutarate aminotransferase
10	R07603	(S)-3-Methyl-2-oxopentanoic acid + Thiamin diphosphate <=> 2-Methyl-1-hydroxybutyl-ThPP + CO2	C00671 + C00068 <=> C15978 + C00011	1.2.4.4	2-oxoisovalerate dehydrogenase E1 component alpha subunit
11	R07604	2-Methyl-1-hydroxybutyl-ThPP + Enzyme N6- (lipoyl)lysine <=> [Dihydrolipoyllysine-residue (2- methylpropanoyl)transferase] S-(2- methylbutanoyl)dihydrolipoyllysine + Thiamin diphosphate	C15978 + C15972 <=> C15979 + C00068	1.2.4.4	2-oxoisovalerate dehydrogenase E1 component alpha subunit

Reaction number in Figure 4	Reaction identifier defined as in KEGG	Definition of the reaction	Coded equation as in KEGG. C##### is identifier for compound	EC number	Enzyme name
12	R03174	(S)-2-Methylbutanoyl-CoA + Enzyme N6- (dihydrolipoyl)lysine <=> CoA + [Dihydrolipoyllysine-residue (2- methylpropanoyl)transferase] S-(2- methylbutanoyl)dihydrolipoyllysine	C15980 + C15973 <=> C00010 + C15979	2.3.1.168	(S)-2-methylbutanoyl-CoA:enzyme N6-(dihydrolipoyl)lysine S-(2- methylbutanoyl)transferase
13	R00316	ATP + Acetate <=> Diphosphate + Acetyl adenylate	C00002 + C00033 <=> C00013 + C05993	6.2.1.1	ATP:acetate adenylyltransferase
14	R00236	Acetyl adenylate + CoA <=> AMP + Acetyl-CoA	C05993 + C00010 <=> C00020 + C00024	6.2.1.1	acetyl adenylate:CoA acetyltransferase
15	R00710	Acetaldehyde + NAD+ + H2O <=> Acetate + NADH + H+	C00084 + C00003 + C00001 <=> C00033 + C00004 + C00080	1.2.1.3	Acetaldehyde:NAD+ oxidoreductase
16	R00472	(S)-Malate + CoA <=> Acetyl-CoA + H2O + Glyoxylate	C00149 + C00010 <=> C00024 + C00001 + C00048	2.3.3.9	malate synthase
17	R00216	(S)-Malate + NADP+ <=> Pyruvate + CO2 + NADPH + H+	C00149 + C00006 <=> C00022 + C00011 + C00005 + C00080	1.1.1.40	malate dehydrogenase
18	R00341	ATP + Oxaloacetate <=> ADP + Phosphoenolpyruvate + CO2	C00002 + C00036 <=> C00008 + C00074 + C00011	4.1.1.49	phosphoenolpyruvate carboxykinase
19	R00540	Nitrile + 2 H2O <=> Carboxylate + Ammonia	C00726 + 2 C00001 <=> C00060 + C00014	3.5.5.1	nitrilase
20	R00248	L-Glutamate + NADP+ + H2O <=> 2-Oxoglutarate + Ammonia + NADPH + H+	C00025 + C00006 + C00001 <=> C00026 + C00014 + C00005 + C00080	1.4.1.4	glutamate dehydrogenase
21	R00025	Ethylnitronate + Oxygen + Reduced FMN <=> Acetaldehyde + Nitrite + FMN + H2O	C18091 + C00007 + C01847 <=> C00084 + C00088 + C00061 + C00001	1.13.12.16	nitronate monooxygenase

Reaction number in Figure 4	Reaction identifier defined as in KEGG	Definition of the reaction	Coded equation as in KEGG. C##### is identifier for compound	EC number	Enzyme name
22	R10996	2-Oxobutanoate + Thiamin diphosphate <=> 2- (alpha-Hydroxypropyl)thiamine diphosphate + CO2	C00109 + C00068 <=> C21017 + C00011	1.2.4.4	2-oxoisovalerate dehydrogenase E1 component alpha subunit
23	R10997	2-(alpha-Hydroxypropyl)thiamine diphosphate + Enzyme N6-(lipoyl)lysine <=> Enzyme N6-(S- propyldihydrolipoyl)lysine + Thiamin diphosphate	C21017 + C15972 <=> C21018 + C00068	1.2.4.4	2-oxoisovalerate dehydrogenase E1 component alpha subunit
24	R10998	Propanoyl-CoA + Enzyme N6-(dihydrolipoyl)lysine <=> CoA + Enzyme N6-(S- propyldihydrolipoyl)lysine	C00100 + C15973 <=> C00010 + C21018	2.3.1.168	propanoyl-CoA:enzyme N6- (dihydrolipoyl)lysine S- propanoyltransferase
25	R00926	Propionyladenylate + CoA <=> AMP + Propanoyl- CoA	C05983 + C00010 <=> C00020 + C00100	6.2.1.1	Propionyladenylate:CoA propionyltransferase
26	R01354	ATP + Propanoate <=> Diphosphate + Propionyladenylate	C00002 + C00163 <=> C00013 + C05983	6.2.1.1	ATP:propanoate adenylyltransferase
27	R00734	L-Tyrosine + 2-Oxoglutarate <=> 3-(4- Hydroxyphenyl)pyruvate + L-Glutamate	C00082 + C00026 <=> C01179 + C00025	2.6.1.1	L-tyrosine:2-oxoglutarate aminotransferase
28	R02521	3-(4-Hydroxyphenyl)pyruvate + Oxygen <=> Homogentisate + CO2	C01179 + C00007 <=> C00544 + C00011	1.13.11.27	4-Hydroxyphenylpyruvate:oxygen oxidoreductase
29	R03181	4-Maleylacetoacetate <=> 4-Fumarylacetoacetate	C01036 <=> C01061	5.2.1.2	4-Maleylacetoacetate cis-trans- isomerase
30	R01364	Acetoacetate + Fumarate <=> 4-Fumarylacetoacetate + H2O	C00164 + C00122 <=> C01061 + C00001	3.7.1.2	4-fumarylacetoacetate fumarylhydrolase