

## Supplementary material:

**Table 1:** Unique enzymes, which are only present in *T. gondii* and homologs are absent in humans.

S. No.	Metabolic Pathway	Enzyme	Enzyme Detail	<i>T. gondii</i> Gene I.D.
1.	Glycolysis Gluconeogenesis	[EC:4.1.1.49]	Phosphoenolpyruvate carboxykinase	TGME49_089930
2.	Citrate Cycle (TCA cycle)	[EC:4.1.1.49]	Phosphoenolpyruvate carboxykinase	TGME49_089650
3.	Fatty Acid Biosynthesis	[EC:2.3.1.180] [EC: 4.2.1.-] [EC:1.3.1.9]	3-Oxoacyl-(acyl-carrier-protein) synthase III family protein; (3R)-Hydroxymyristoyl ACP dehydratase; Enoyl-acyl carrier reductase	TGME49_031890 TGME49_121570 TGME49_051930
4.	Oxidative Phosphorylation	[EC:1.6.99.3] [EC:3.6.3.6]	Mitochondrial alternative NADH dehydrogenase 1; Pyridine nucleotide-disulphide oxidoreductase; Plasma-membrane H <sup>+</sup> -ATPase	TGME49_009150 TGME49_088830 TGME49_052640 TGME49_084600
5.	Purine Metabolism	(EC:3.2.1.3) [EC:2.7.7.4]	SIN-like domain-containing protein; Sulfate adenyltransferase-adenylsulfate kinase	TGME49_064460 TGME49_082230
6.	Pyrimidine Metabolism	[EC:3.5.2.3] (EC:3.2.1.3); [EC:2.1.1.451.5.1.3]	Dihydroorotase protein; SIN-like domain-containing protein; Bifunctional dihydrofolate reductase / thymidylate synthase	TGME49_093610 TGME49_064460 TGME49_049180
7.	Alanine, Aspartate and Glutamate Metabolism	[EC:2.1.3.2] [EC:1.4.1.2] [EC:1.4.1.4]	Aspartate carbamoyltransferase; NAD-specific glutamate dehydrogenase	TGME49_091640 TGME49_049390 TGME49_093180
8.	Glycine, Serine and Threonine Metabolism	[EC:2.7.2.4] [EC:1.2.1.11] [EC:2.7.1.39] [EC:4.2.3.1]	Aspartate kinase; Aspartate-semialdehyde dehydrogenase; Homoserine kinase; Threonine synthase	TGME49_027090 TGME49_005420 TGME49_016640 TGME49_020840
9.	Cysteine and Methionine Metabolism	[EC:2.5.1.47] [EC:2.1.1.10] [EC:2.7.2.4] [EC:1.2.1.11] [EC:2.3.1.31]	O-acetylserine (thiol) lyase; Cysteine synthase A; Homocysteine S-methyltransferase-1; Aspartate kinase; Aspartate-semialdehyde dehydrogenase; Homoserine O-acetyltransferase	TGME49_078910 TGME49_057750 TGME49_027090 TGME49_005420 TGME49_120730
10.	Lysine Biosynthesis	[EC:2.7.2.4] [EC:1.2.1.11]	Aspartate kinase; Aspartate-semialdehyde dehydrogenase	TGME49_027090 TGME49_005420
11.	Arginine and Proline Metabolism	[EC:1.4.1.4]	NADP-specific glutamate dehydrogenase	TGME49_093180
12.	Phenylalanine, Tyrosine and Tryptophan Biosynthesis	[EC:4.2.3.5] [EC:2.5.1.54]	Chorismate synthase; DAHP synthetase	TGME49_001380 TGME49_021260
13.	Beta-Alanine Metabolism	[EC:6.3.2.1]	Pantoate--beta-alanine ligase	TGME49_065870
14.	Seleno-compound Metabolism	[EC:2.7.7.4]	Sulfate adenyltransferase-adenylsulfate kinase	TGME49_082230
15.	Starch and Sucrose Metabolism	[EC:2.4.1.34] [EC:2.4.1.15] [EC:2.4.1.21]	1,3-beta-glucan synthase; Trehalose-6-phosphate synthase domain-containing protein; Glycogen synthase	TGME49_078110 TGME49_097720 TGME49_022720
16.	Amino Sugar and Nucleotide Sugar Metabolism	[EC:2.7.7.64]	UDP-N-acetylglucosamine pyrophosphorylase	TGME49_018200
17.	Glycosphingolipid Biosynthesis - globo series	[EC: 2.3.1.-]	Acetyl-CoA transporter	TGME49_015940
18.	Pyruvate Metabolism	[EC:4.4.1.5] [EC:4.1.1.49]	Lactoylglycyl-L-homoserine lyase; Phosphoenolpyruvate carboxykinase	TGME49_048400 TGME49_089930 TGME49_089650
19.	Butanoate Metabolism	[EC:1.1.1.157]	3-Hydroxybutyryl-CoA dehydrogenase	TGME49_032090
20.	Vitamin B6 Metabolism	[EC:2.7.1.35] [EC:4.2.3.1] [EC: 4.-.-] [EC: 2.6.-.-]	Hypothetical protein; Threonine synthase; Ethylene inducible protein; Glutamine amidotransferase	TGME49_097080 TGME49_020840 TGME49_037140 TGME49_081490
21.	Nicotinate and Nicotinamide Metabolism	[EC:2.7.1.23] [EC:1.6.1.1]	ATP-NAD kinase domain-containing protein; Transhydrogenase	TGME49_044700 TGME49_118650
22.	Pantothenate and CoA-Biosynthesis	[EC:6.3.2.1]	Pantoate--beta-alanine ligase	TGME49_065870
23.	Lipoic acid Metabolism	[EC:2.7.7.63]	Lipoate-protein ligase A	TGME49_071820
24.	Folate Biosynthesis	[EC:2.5.1.15] [EC:2.7.6.3] [EC:2.6.1.85]	Hydroxymethyl-dihydropterin; Pyrophosphokinase-dihydropteroate synthase; Para-aminobenzoate synthase	TGME49_059550 TGME49_002920
25.	Porphyrin and Chlorophyll Metabolism	[EC:1.3.99.22] [EC:4.4.1.17]	Radical SAM domain containing protein; Coproporphyrinogen III oxidase; Cytochrome c heme lyase;	TGME49_088640 TGME49_114040

26.	Terpenoid Biosynthesis	Backbone	[EC:2.2.1.7] [EC:1.1.1.267] [EC:4.6.1.12] [EC:1.17.1.2]	1-deoxy-D-xylulose 5-phosphate synthase; 1-deoxy-D-xylulose 5-phosphate reductoisomerase; 2C-methyl-D-erythritol 2; lytB domain-containing protein, Hydroxy-3-methylbut-2-enyl diphosphate reductase	TGME49_008820 TGME49_014850 TGME49_055690 TGME49_027420
27.	Nitrogen Metabolism		[EC:1.4.1.4]	NADP-specific glutamate dehydrogenase	TGME49_093180
28.	Sulfur Metabolism		[EC:2.3.1.31] [EC:2.5.1.47]	Homoserine O-acetyltransferase; O-acetylserine (thiol) lyase	TGME49_120730 TGME49_078910
29.	Biosynthesis of Unsaturated Fatty Acids		[EC:1.1.1.100]	Oxoacyl-ACP reductase	TGME49_017740

**Table 2:** Enzymes, which are present in more than one pathway in *T. gondii* and absent in humans.

S. No.	<i>T. gondii</i> Gene I.D.	Enzyme	Metabolic Pathway	Function
1.	TGME49_089930	Phosphoenolpyruvate Carboxykinase	1. Glycolysis / Gluconeogenesis 2. Pyruvate Metabolism	Phosphoenolpyruvate carboxykinase (PEPCK) is an enzyme in the lyase family used in the metabolic pathway of gluconeogenesis. It converts oxaloacetate into phosphoenolpyruvate and carbon dioxide.
2.	TGME49_089650	Phosphoenolpyruvate Carboxykinase	1. Citrate cycle (TCA cycle) 2. Pyruvate Metabolism	Phosphoenolpyruvate carboxykinase (PEPCK) is an enzyme in the lyase family used in the metabolic pathway of gluconeogenesis. It converts oxaloacetate into phosphoenolpyruvate and carbon dioxide.
3.	TGME49_093180	NAD-specific glutamate dehydrogenase	1. Alanine, Aspartate and Glutamate Metabolism 2. Arginine and Proline Metabolism 3. Nitrogen Metabolism	(GLDH) is an enzyme, present in most microbes and the mitochondria of eukaryotes, required for urea synthesis, that converts glutamate to $\alpha$ -Ketoglutarate, and vice versa.
4.	TGME49_027090	Aspartate kinase	1. Glycine, Serine and threonine Metabolism 2. Cysteine and Methionine Metabolism 3. Lysine Biosynthesis	Catalyzes the phosphorylation of the amino acid aspartate. This reaction is the first step in the biosynthesis of three essential amino acids: methionine, lysine, and threonine, known as the "aspartate family".
5.	TGME49_005420	Aspartate-semialdehyde dehydrogenase	1. Glycine, Serine and Threonine Metabolism 2. Cysteine and Methionine Metabolism 3. Lysine Biosynthesis	It forms an early branch point in the metabolic pathway forming lysine, methionine, leucine and isoleucine from aspartate. This enzyme belongs to the family of oxidoreductases, specifically those acting on the aldehyde or oxo group of donor with NAD+ or NADP+ as acceptor.
6.	TGME49_020840	Threonine synthase	1. Glycine, Serine and Threonine Metabolism 2. Vitamin B6 Metabolism	This enzyme belongs to the family of lyases, specifically those carbon-oxygen lyases acting on phosphates.
7.	TGME49_078910	O-acetylserine (thiol) lyase	1. Cysteine and Methionine Metabolism 2. Sulfur Metabolism	The enzyme O-acetylserine (thiol)-lyase, using sulfide sources, converts O-acetylserine ester into cysteine, releasing acetate
8.	TGME49_120730	Homoserine O-acetyltransferase	1. Cysteine and Methionine Metabolism 2. Sulfur Metabolism	This enzyme belongs to the family of transferases, specifically those acyltransferases transferring groups other than aminoacyl groups. The two substrates of this enzyme are acetyl-CoA and L-homoserine, whereas its two products are CoA and O-acetyl-L-homoserine.
9.	TGME49_065870	Pantoate--beta-alanine ligase	1. Beta-Alanine Metabolism 2. Pantothenate and CoA biosynthesis	This enzyme belongs to the family of ligases, specifically those forming carbon-nitrogen bonds as acid-D-amino-acid ligases (peptide synthases). The 3 substrates of this enzyme are ATP, (R)- pantoate, and beta-alanine, whereas its 3 products are AMP, diphosphate, and (R)- pantothenate.
10.	TGME49_082230	Sulfate adenyltransferase-adenylsulfate kinase	1. Purine Metabolism 2. Selenocompound Metabolism	This enzyme belongs to the family of transferases, specifically those transferring phosphorus-containing nucleotide groups (nucleotidyltransferases). The two substrates of this enzyme are ATP and sulfate, whereas its two products are diphosphate and adenylsulfate.
11.	TGME49_064460	SIN-like domain-containing protein	1. Purine Metabolism 2. Pyrimidine Metabolism	Utilizes a DNA template, i.e. the catalysis of DNA-template-directed extension of the 3'-end of an RNA strand by one nucleotide at a time.

**Table 3:** Top ten ligand molecules identified from NCI diversity subset II of the ZINC database after virtual screening

S. No.	ZINC ID of the screened molecules	Energy score (Kcal/Mol)	No. of Hydrogen Interaction of ligand with active site residues	No. Hydrophobic Interaction of ligand with active site residues	Molecular Weight (g/mol)	Log P value
1.	ZINC01690699	-9.1	2	9	548.59336	6.0
2.	ZINC17465979	-8.1	5	5	546.52144	5.9
3.	ZINC17465983	-7.9	4	5	546.52144	5.9
4.	ZINC18141294_03	-7.9	3	8	453.47264	5.3
5.	ZINC05462670	-7.9	4	5	546.52144	5.9
6.	ZINC01572309	-7.9	3	5	474.55802	5.0
7.	ZINC18055497_01	-7.8	1	7	479.67574	4.7
8.	ZINC18141294	-7.8	1	12	453.47264	5.3
9.	ZINC05462674	-7.8	4	6	546.52144	5.9
10.	ZINC13152284_01	-7.8	1	7	392.4492	6.7