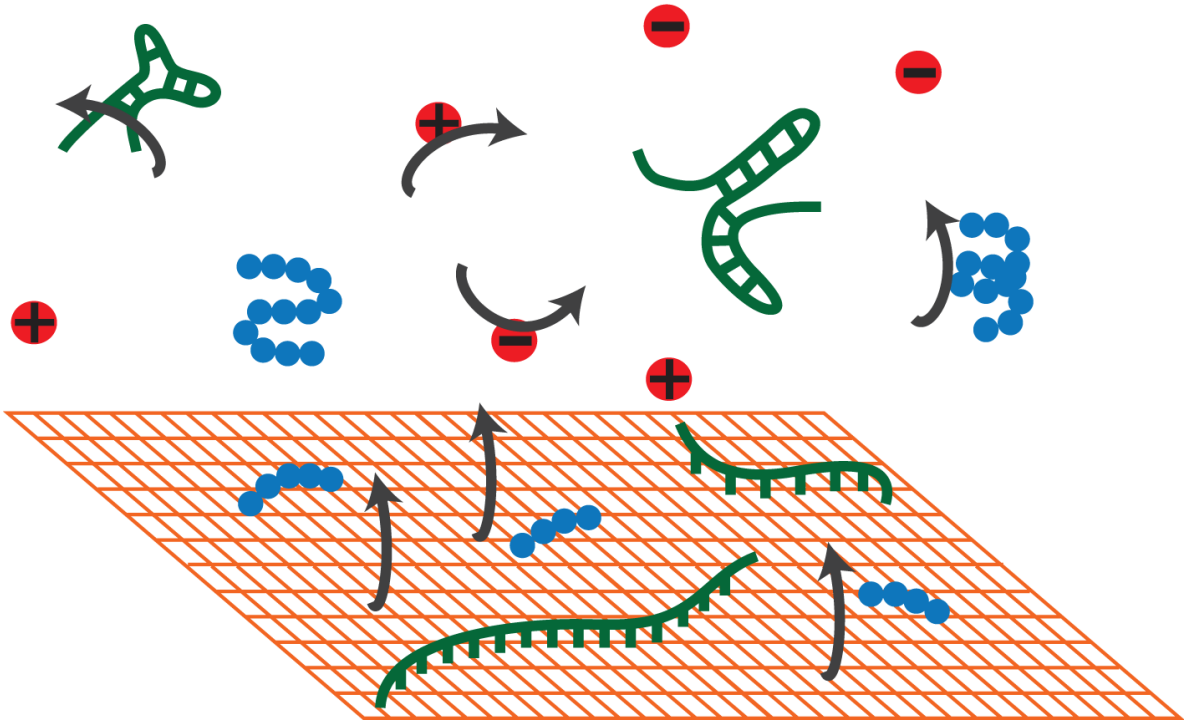
Ancient Metabolic Pathways within the Modern Protein Repertoire

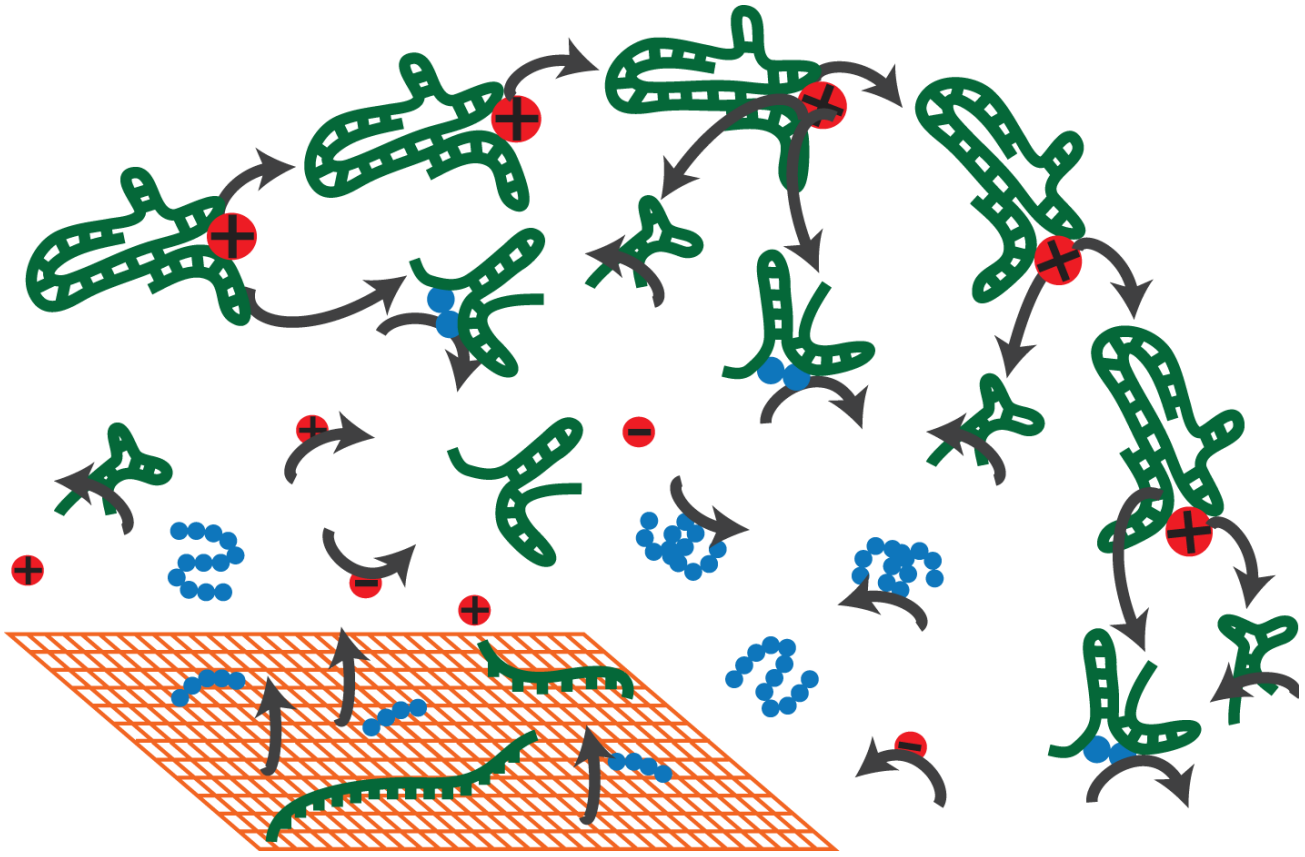
Aaron Goldman

March 28rd, 2013

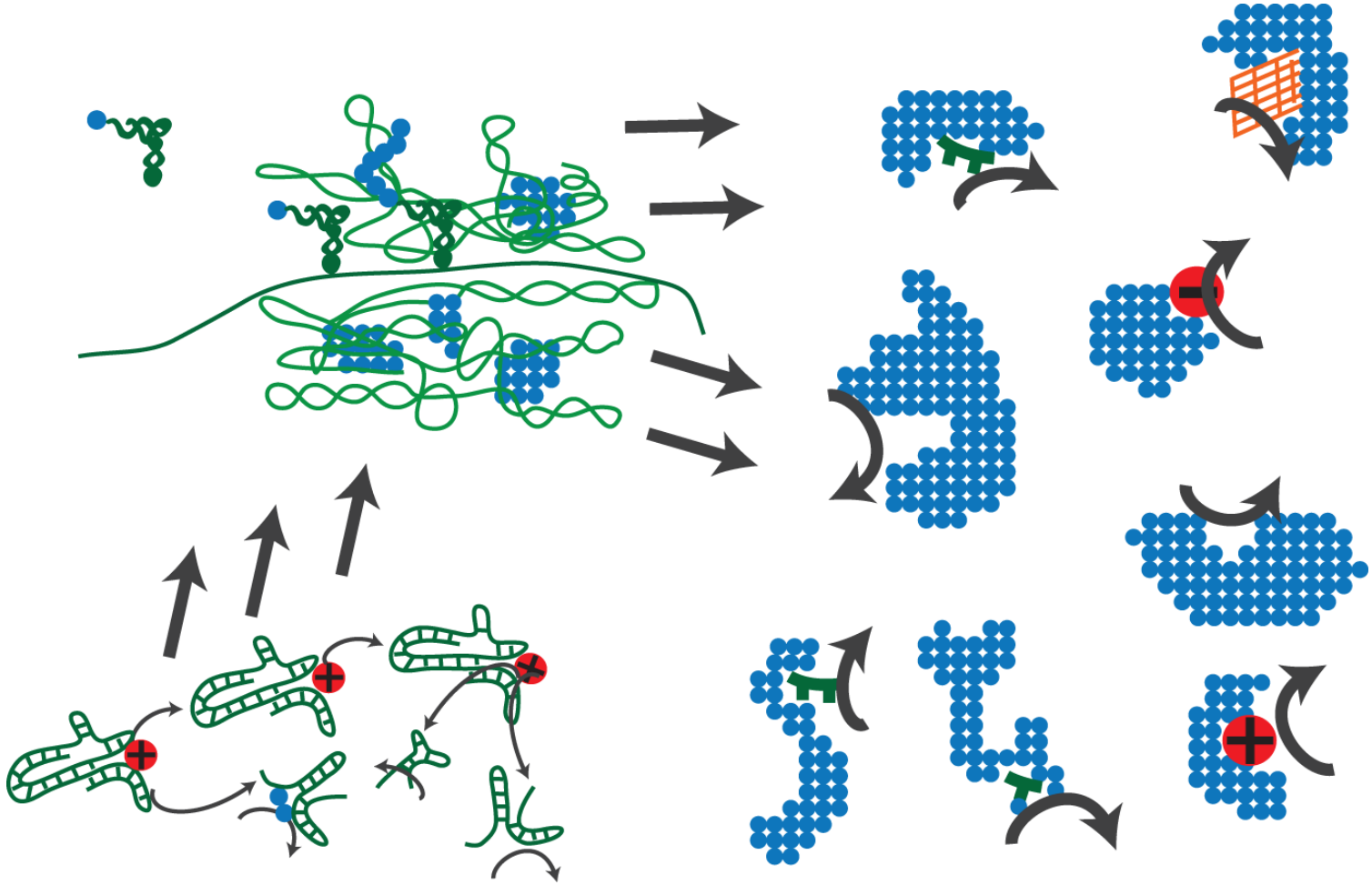
Prebiotic chemistry



“RNA world”

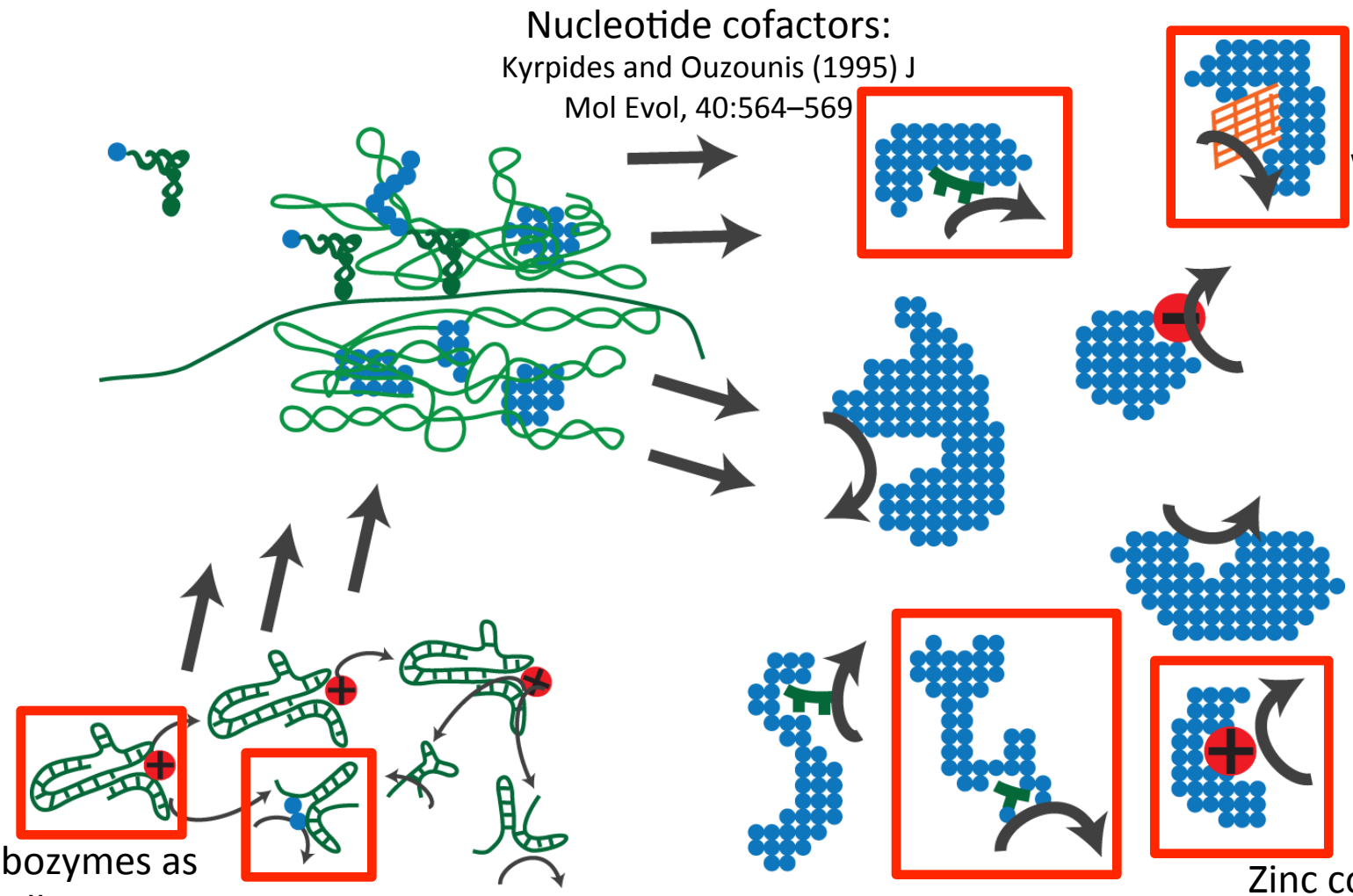


Protein-mediated metabolism

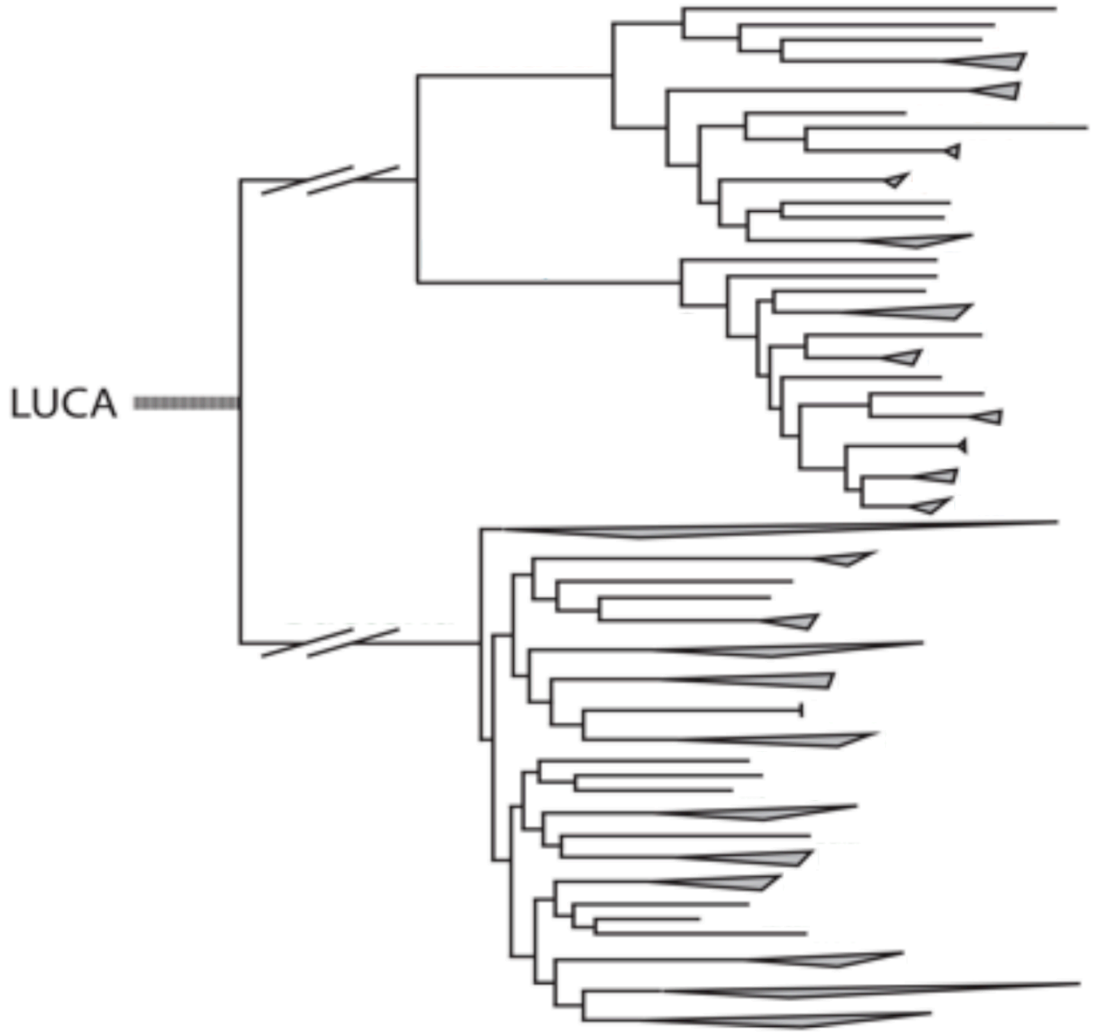


Cofactors reflect ancient catalysis:

White (1976) J Mol Evol 7:101–104

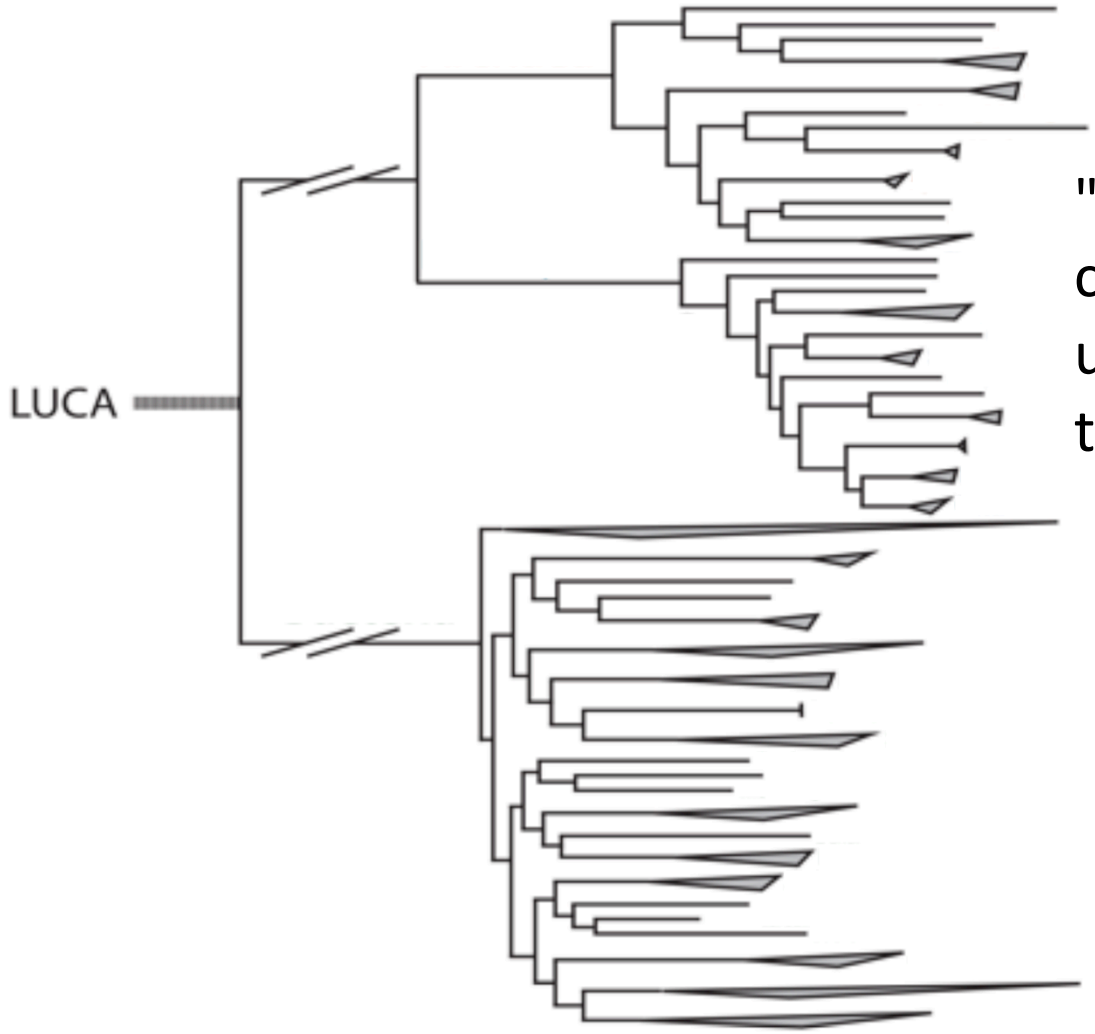


Last Universal Common Ancestor



Tree from Ciccarelli *et al.* (2006) Science 311:1283–1287

Last Universal Common Ancestor



"What we have been calling the root of the universal tree is in fact the tip of its trunk."

- Becerra *et al*. (2007) Annu Rev Ecol Evol Syst, 38:361–79

Tree from Ciccarelli *et al.* (2006) Science 311:1283–1287

Last Universal Common Ancestor

1. Compare genomes or proteomes across species representing the whole tree of life

Tree from Ciccarelli *et al.* (2006) Science 311:1283–1287

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2. Extrapolate presence in LUCA based on evolutionary models

Tree from Ciccarelli *et al.* (2006) Science 311:1283–1287

Last Universal Common Ancestor

Harris *et al.* (2003): 80 gene families (COGs)

Mirkin *et al.* (2003): 571 gene families (COGs)

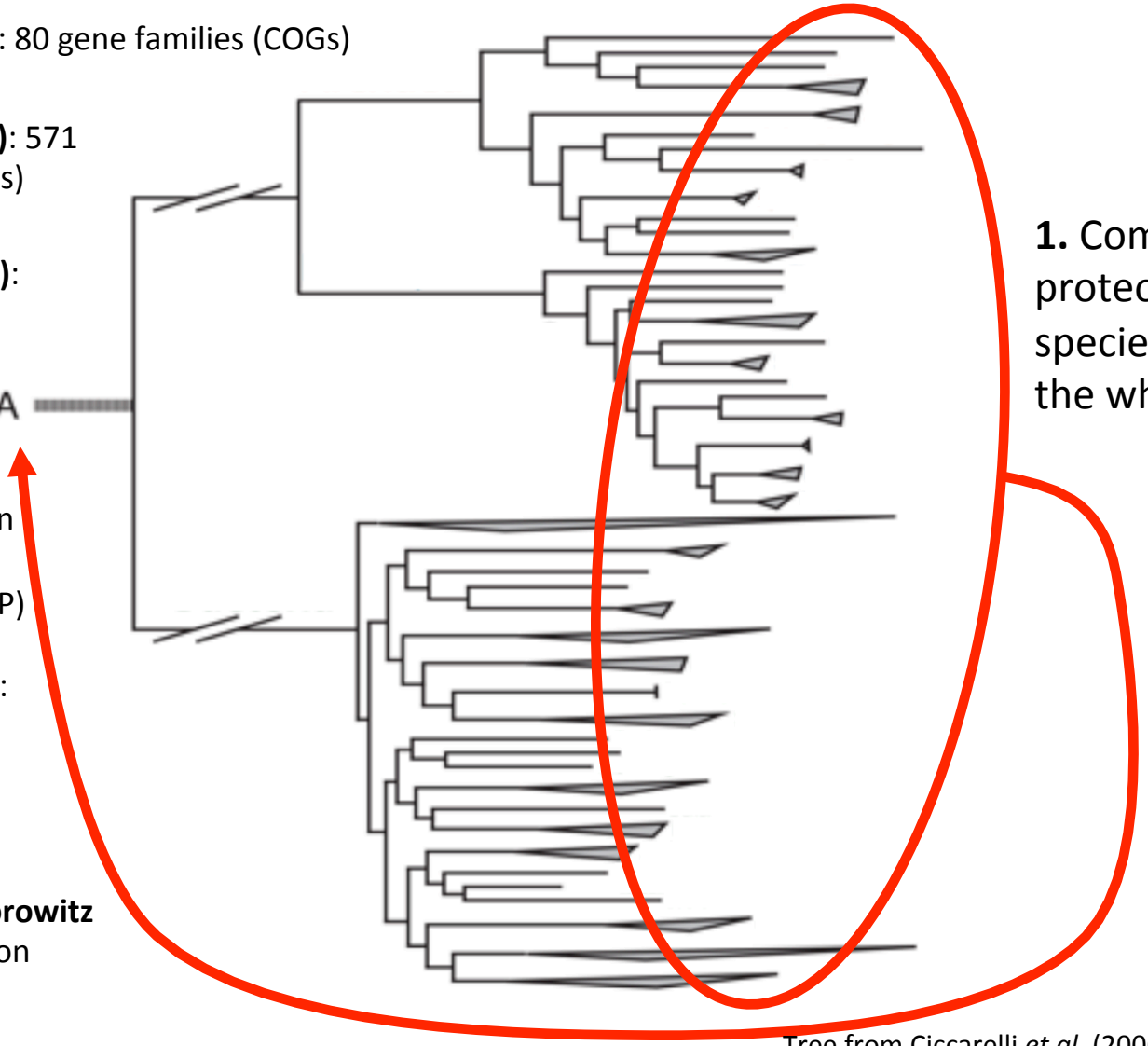
Delaye *et al*. (2005): 115 protein motifs (Pfam)

LUCA

Yang *et al*. (2005): 66 universal protein structural superfamilies (SCOP)

Wang *et al.* (2007): 165 universal protein structural folds (SCOP)

Srinivasan and Morowitz (2009): 286 common reactions (KEGG)



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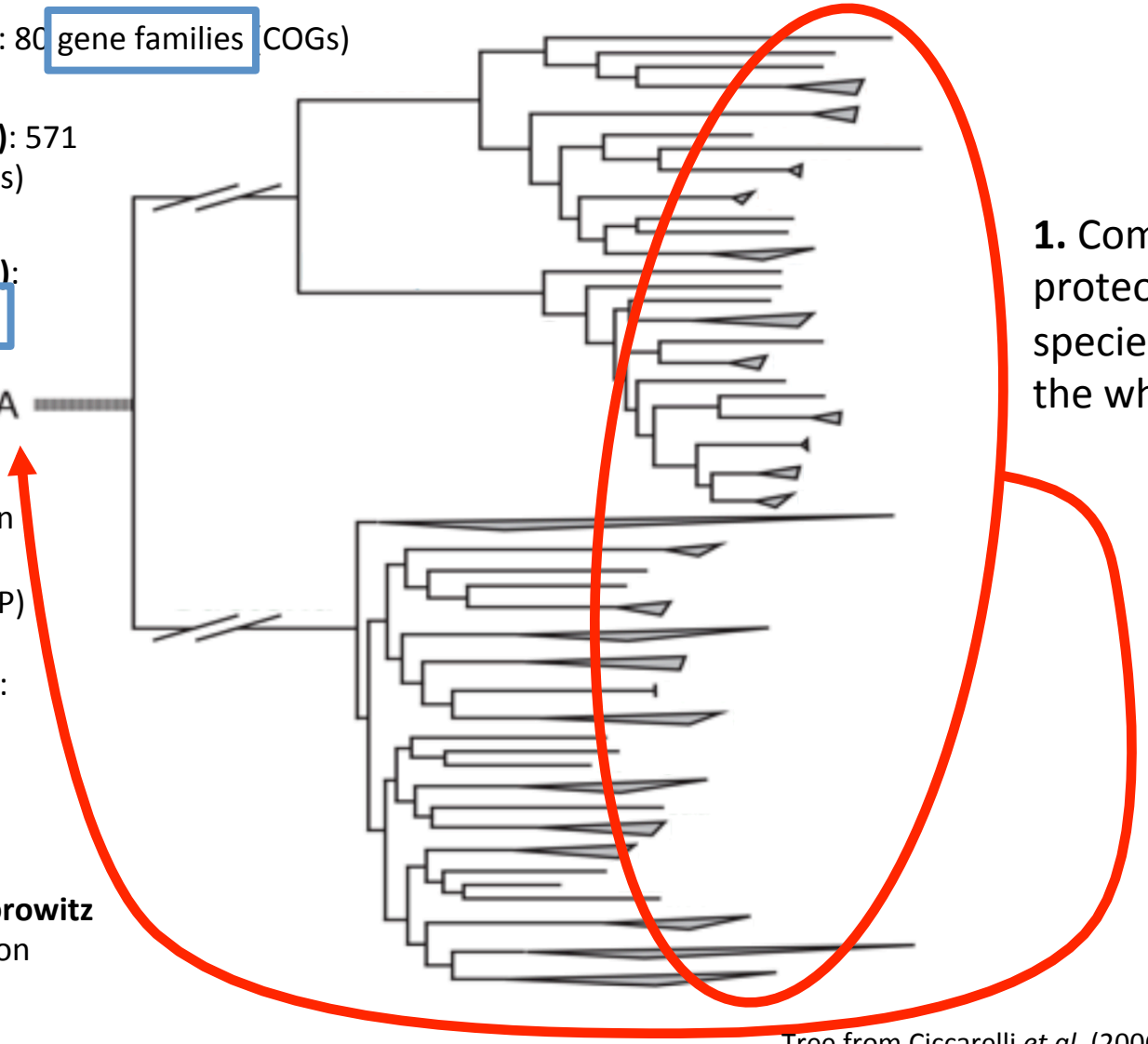

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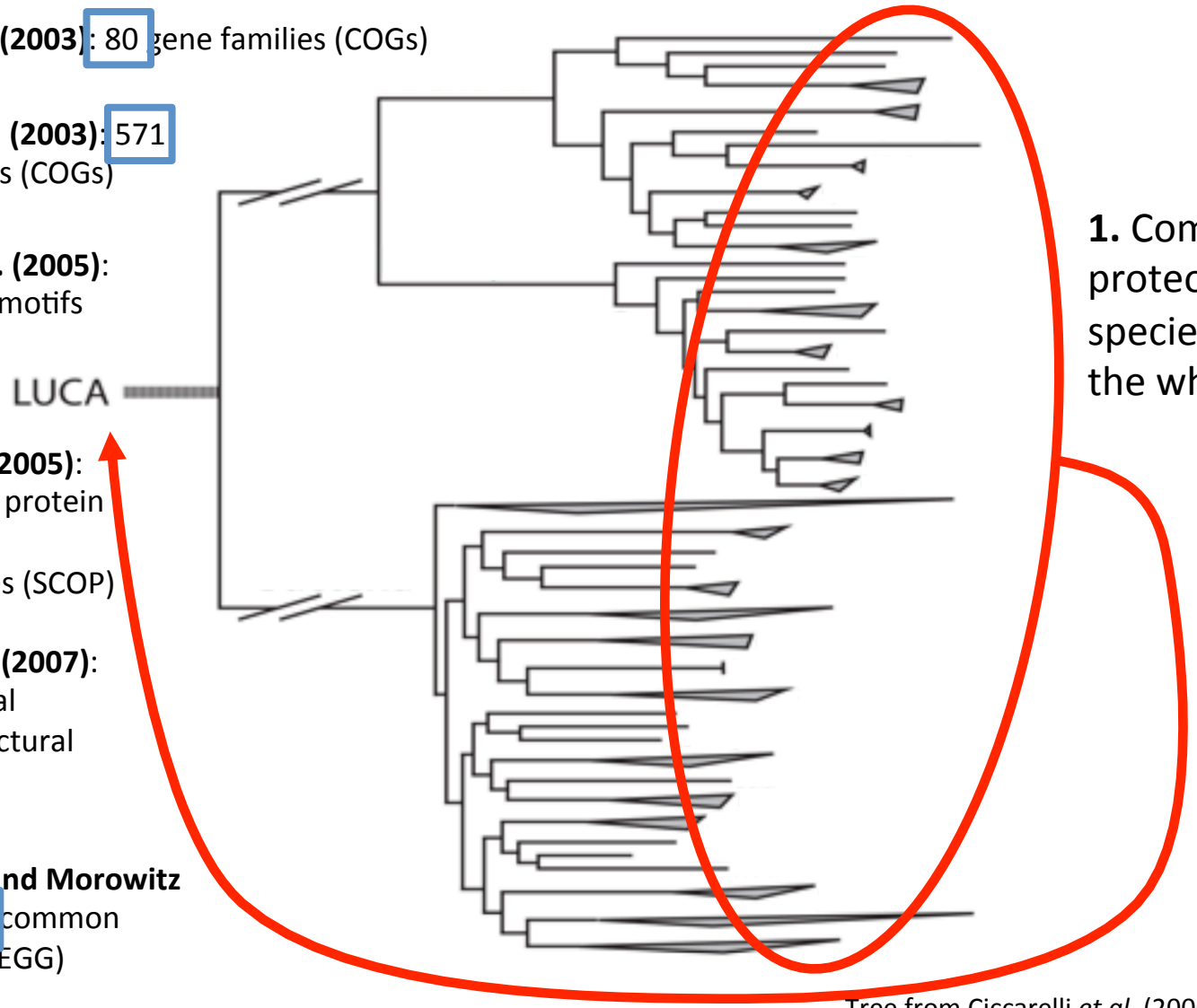

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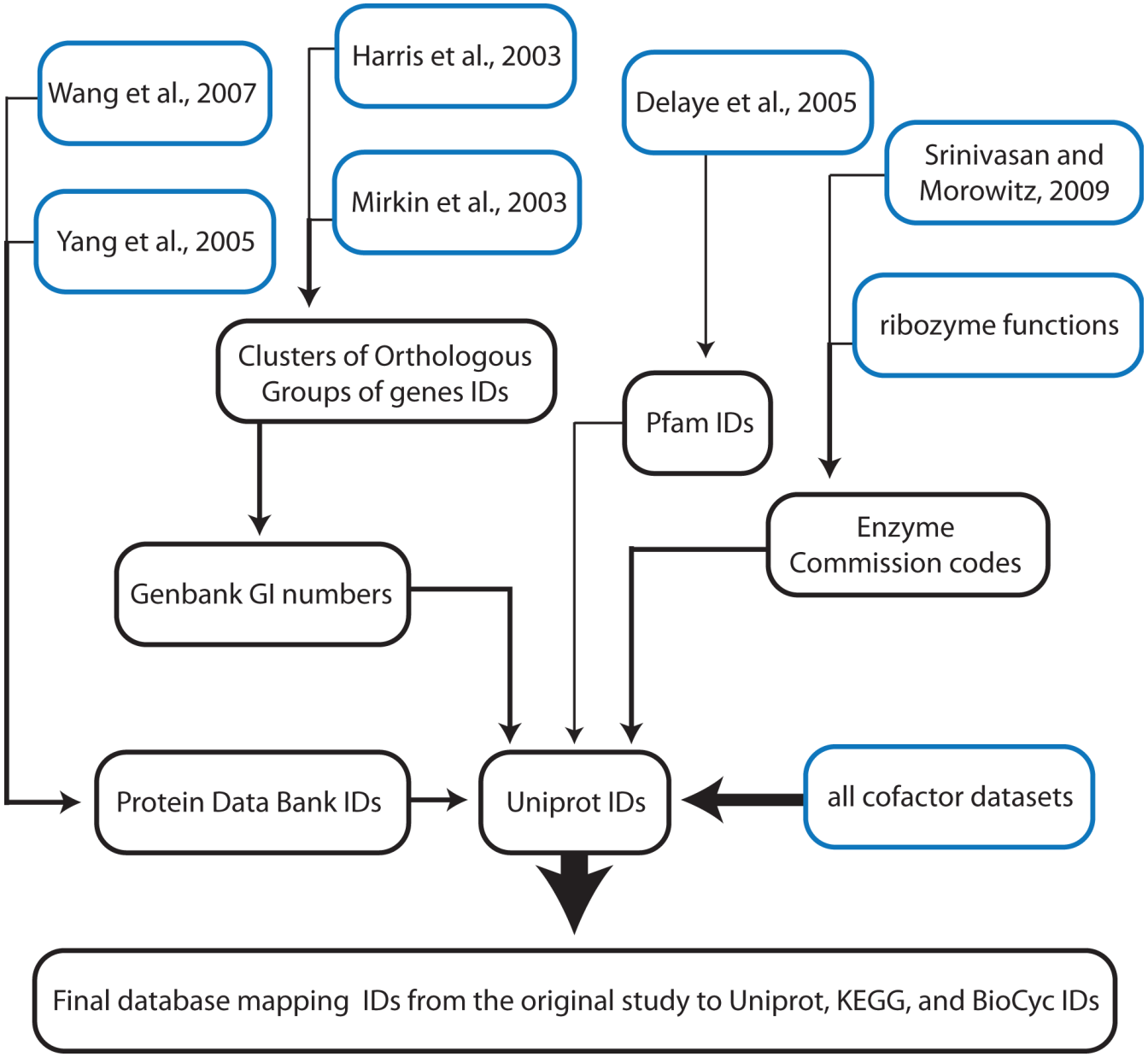
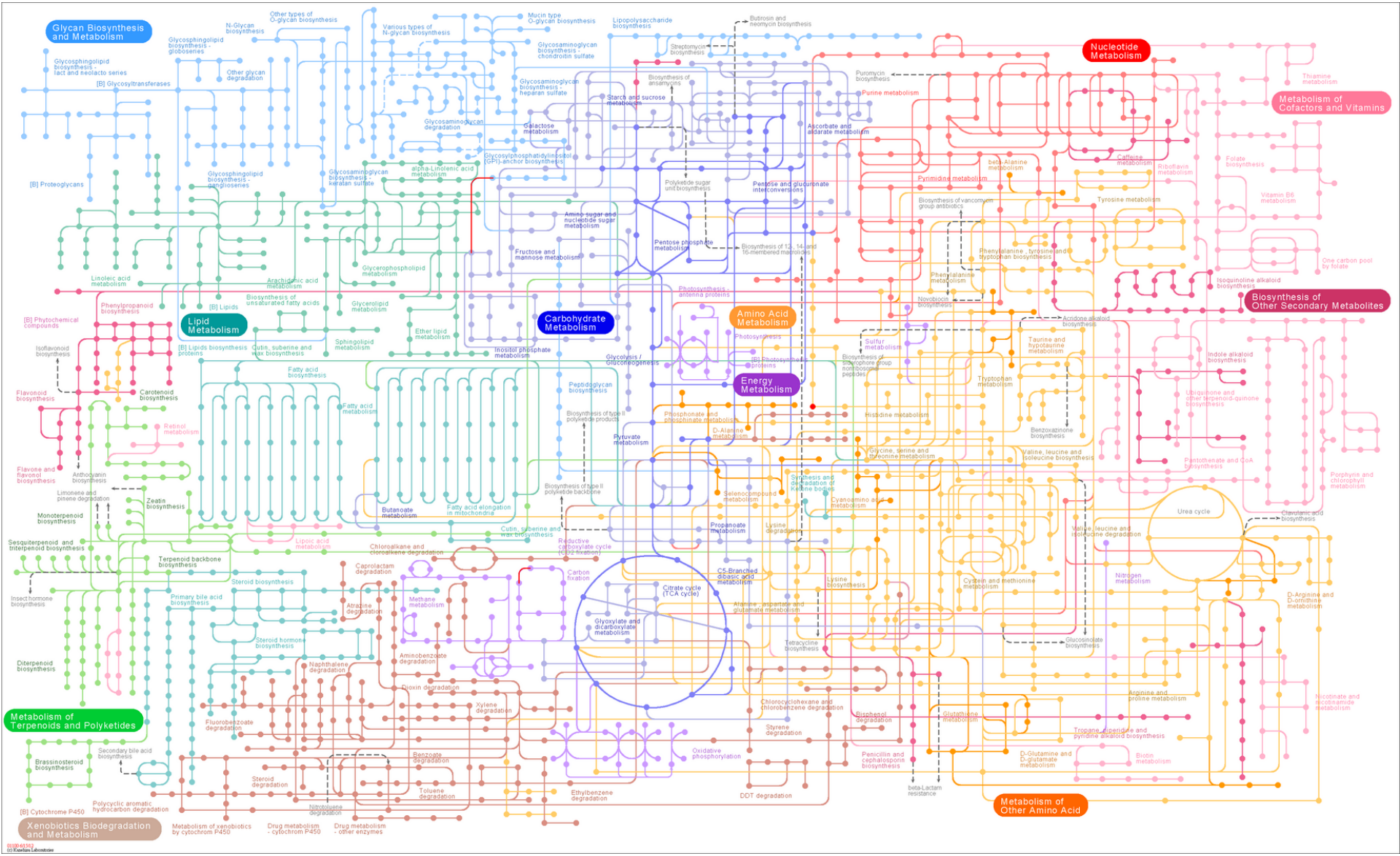


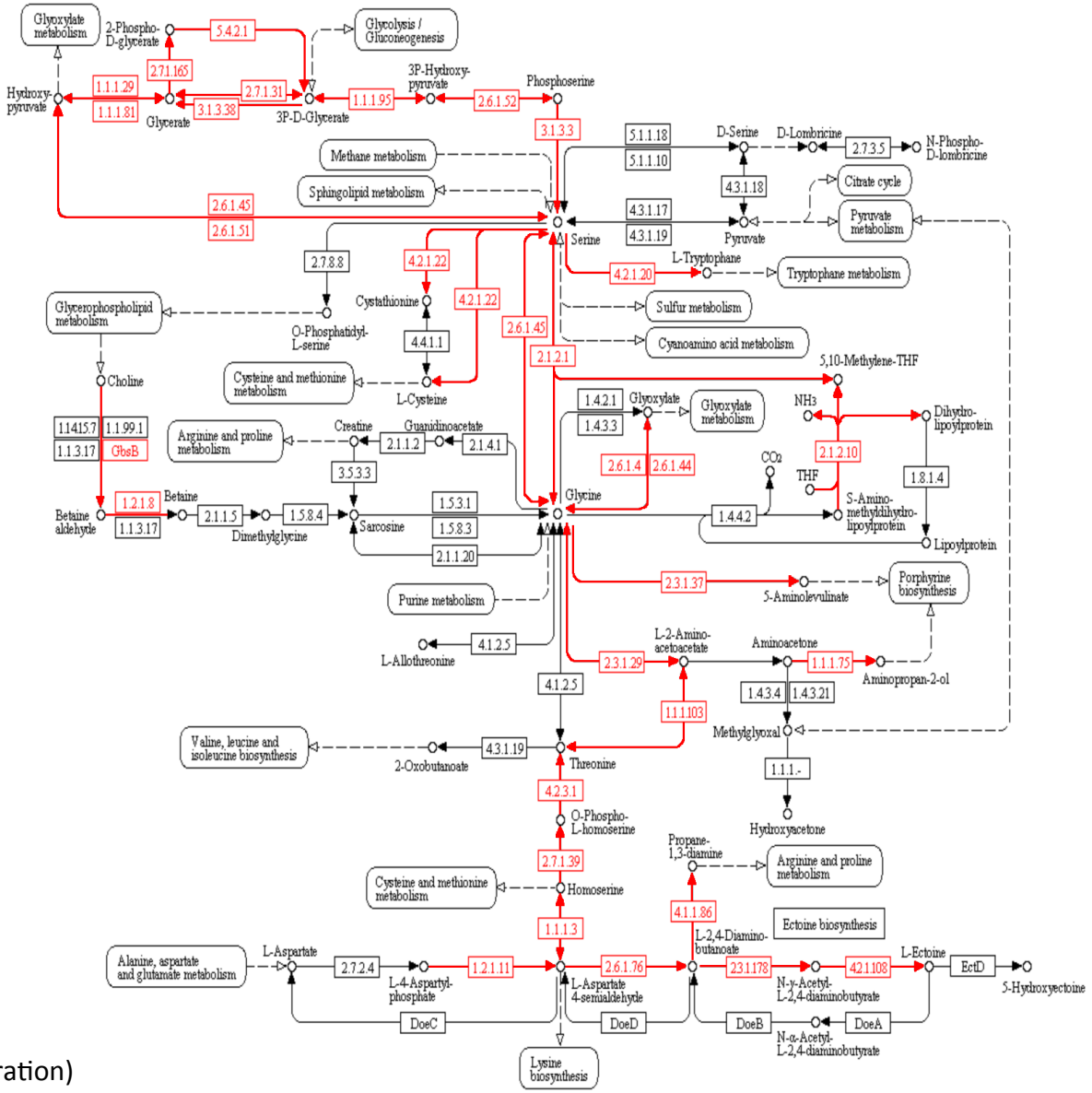
Goldman *et al.* (2013) *Nucleic Acids Res,* 41: D1079-82



KEGG map1100

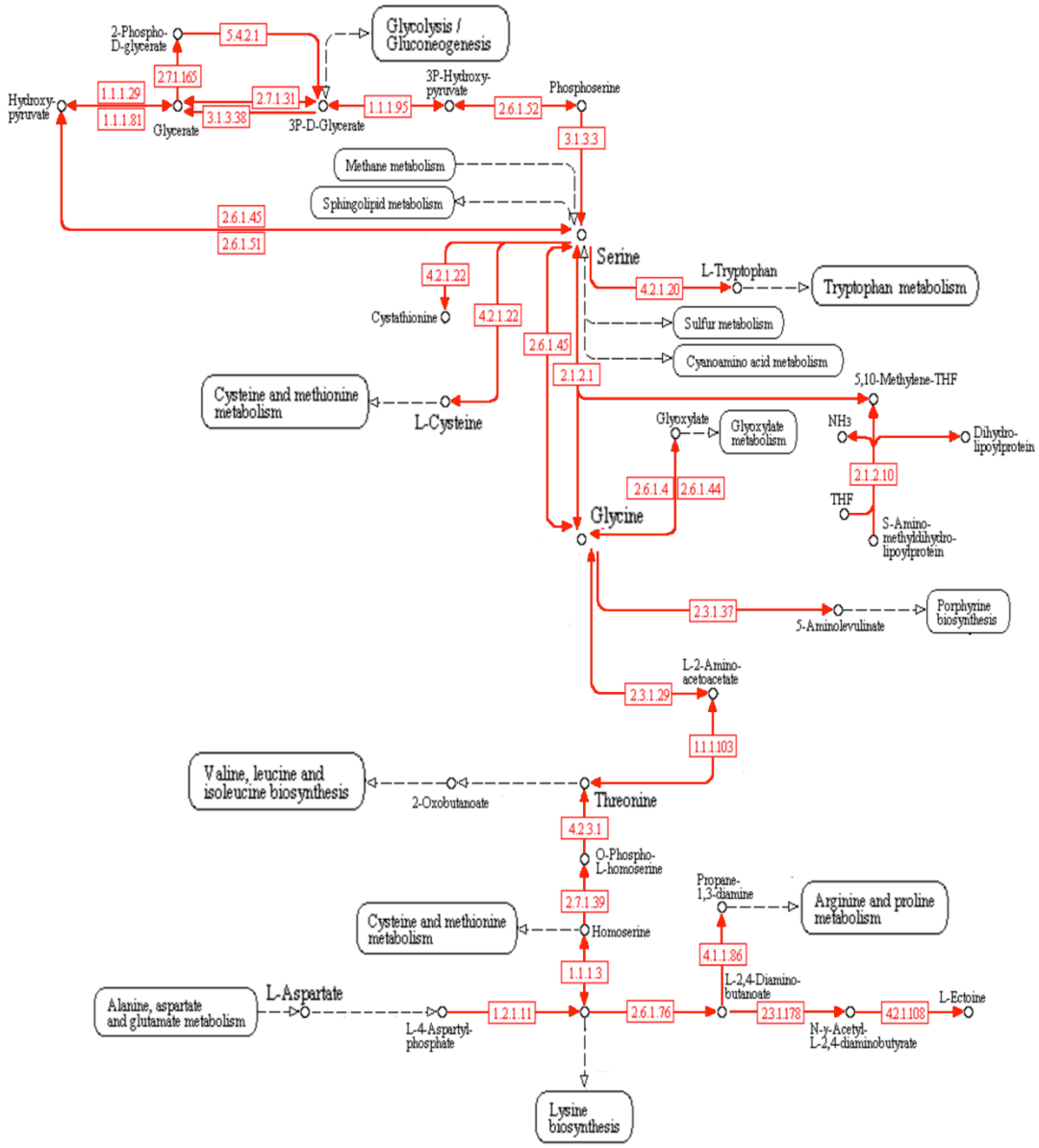
Ancient Enzyme Functions in Metabolic Pathways

Ancient Metabolic Pathways



Matheson *et al*. (in preparation)

Ancient Metabolic Pathways



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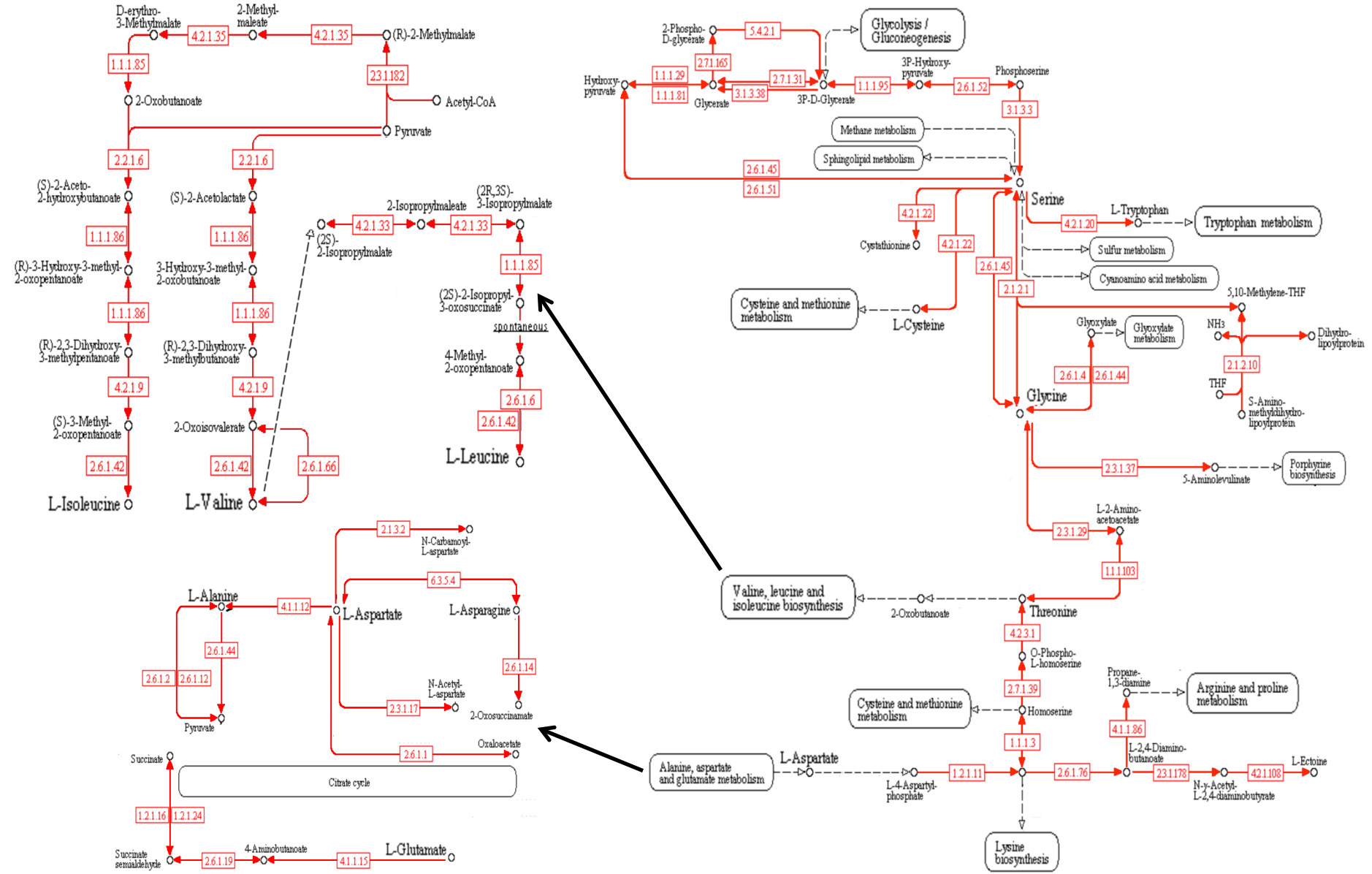


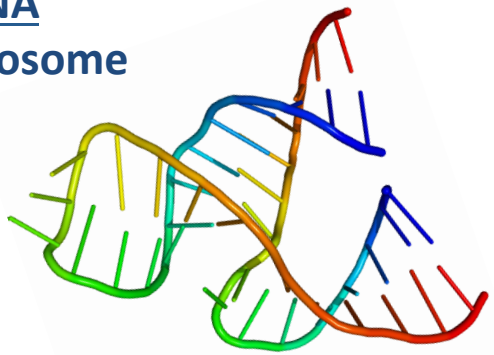
Hypothesis Testing

Ribozymes found in life

Hammerhead ribozyme
self cleavage

RNase P
cleaves RNA

Peptidyl transferase 23S rRNA
is the RNA component of the ribosome



http://reference.findtarget.com/

GIR1 branching ribozyme
mRNA capping

CoTC ribozyme
self cleavage

Hairpin ribozyme
self-cleavage and ligation

Group I and Group II introns
self splicing

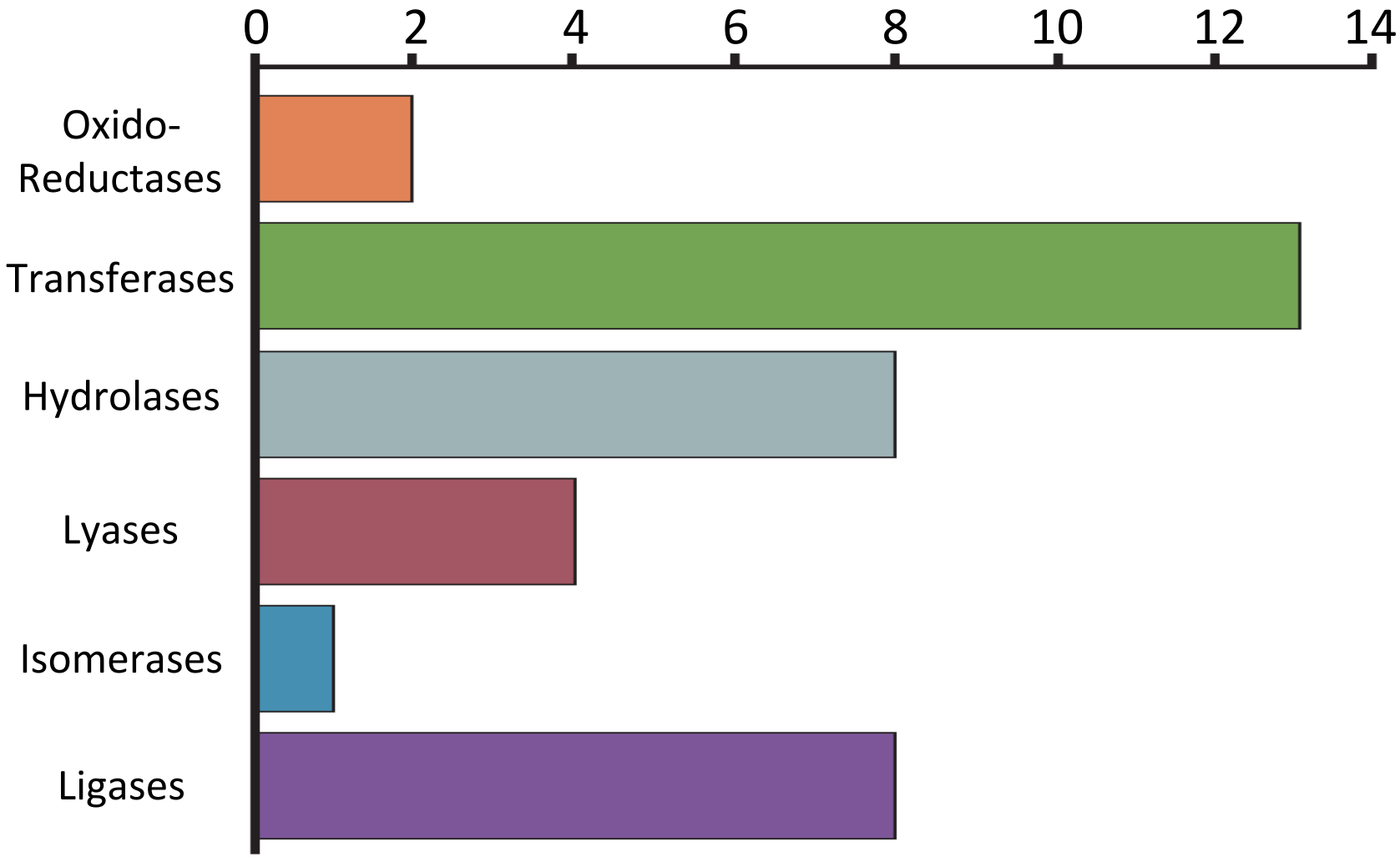
Mammalian CPEB3 ribozyme
self cleavage

HDV ribozyme
process the RNA transcripts to unit lengths

glmS ribozyme
catalyzes the production of glucosamine-6-phosphate

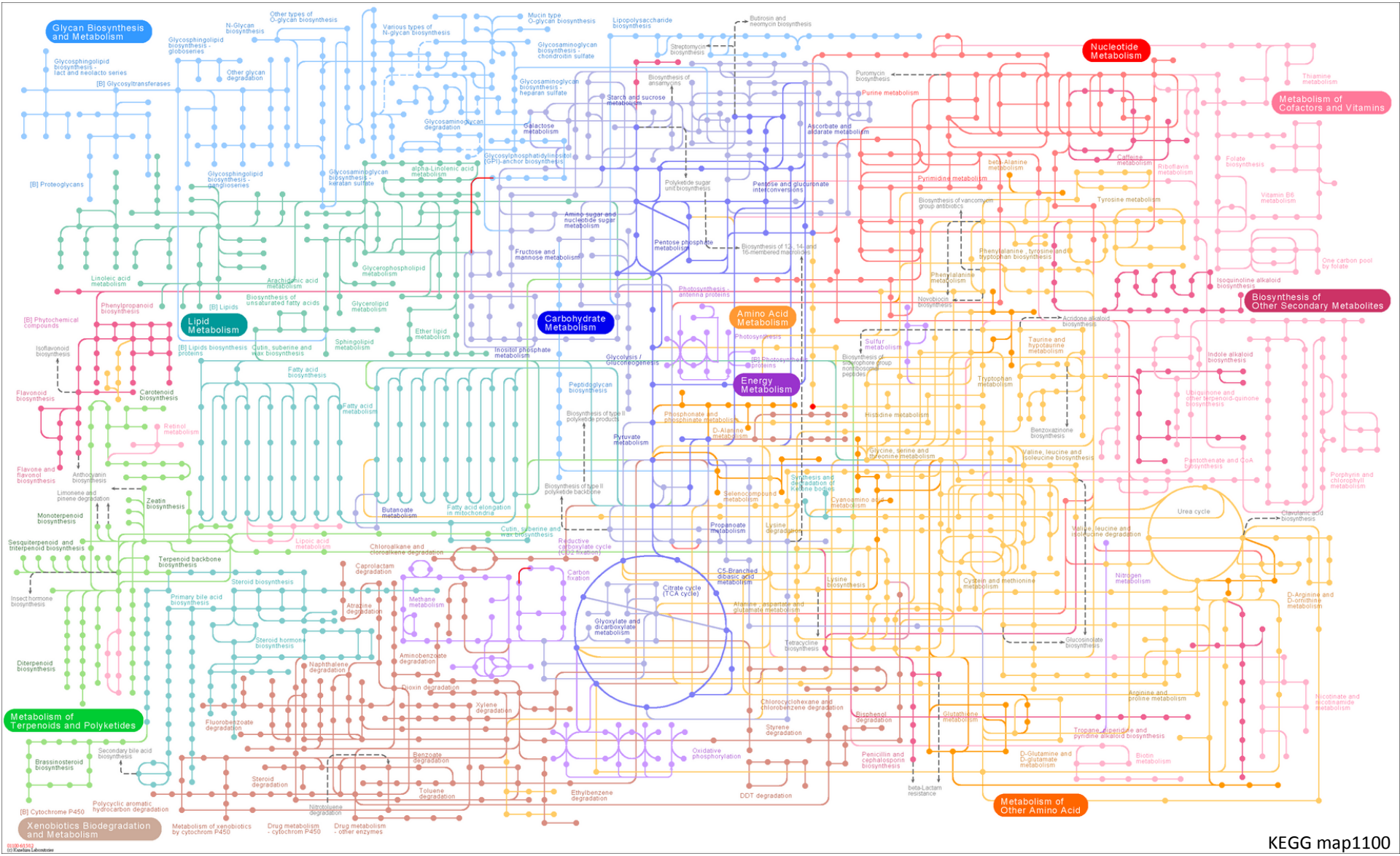
VS ribozyme
cleavage of a phosphodiester bond

Ribozyme Functions



Bernhardt *et al*. (in preparation)

Potential for a Ribozyme Metabolism



KEGG map1100

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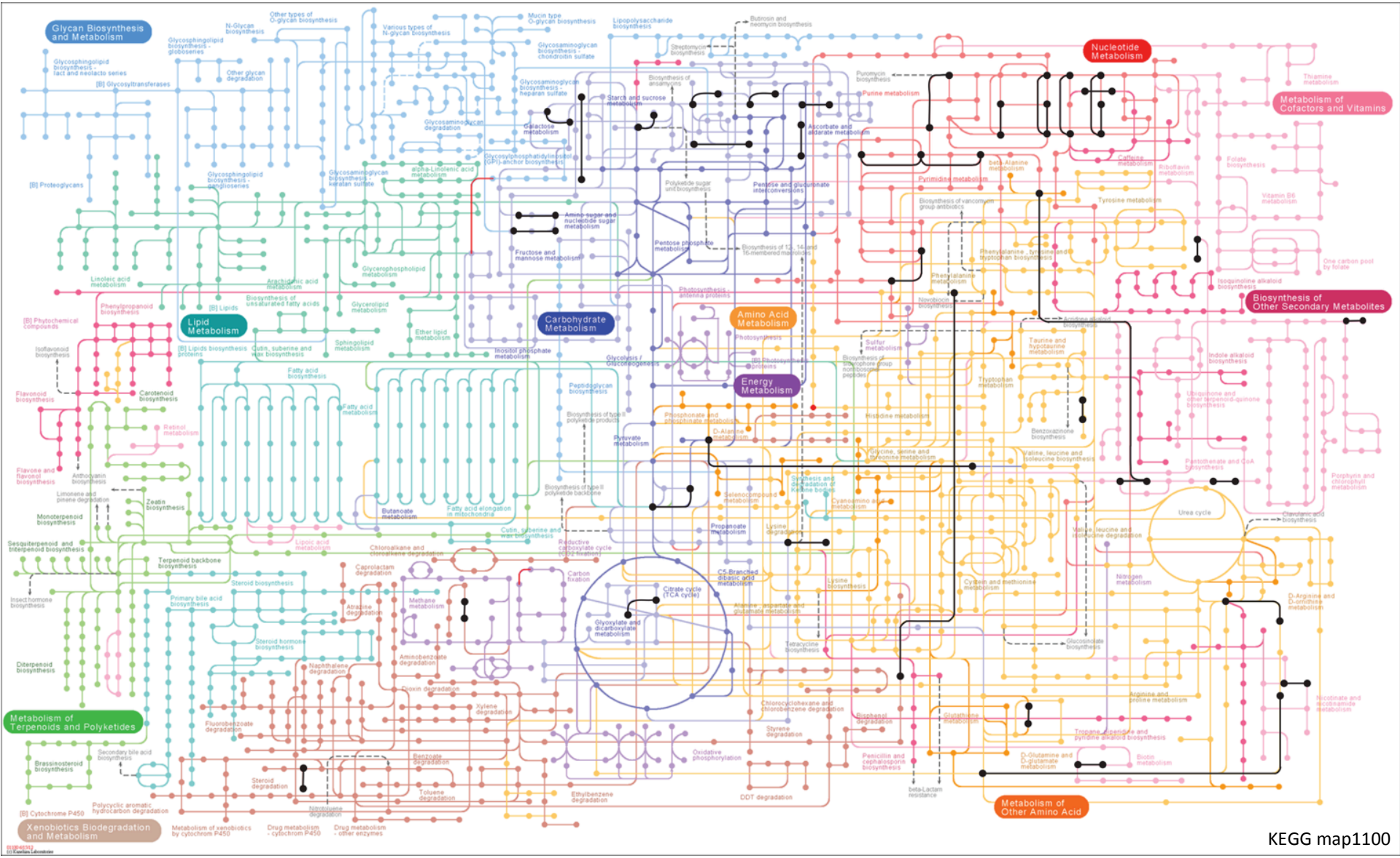
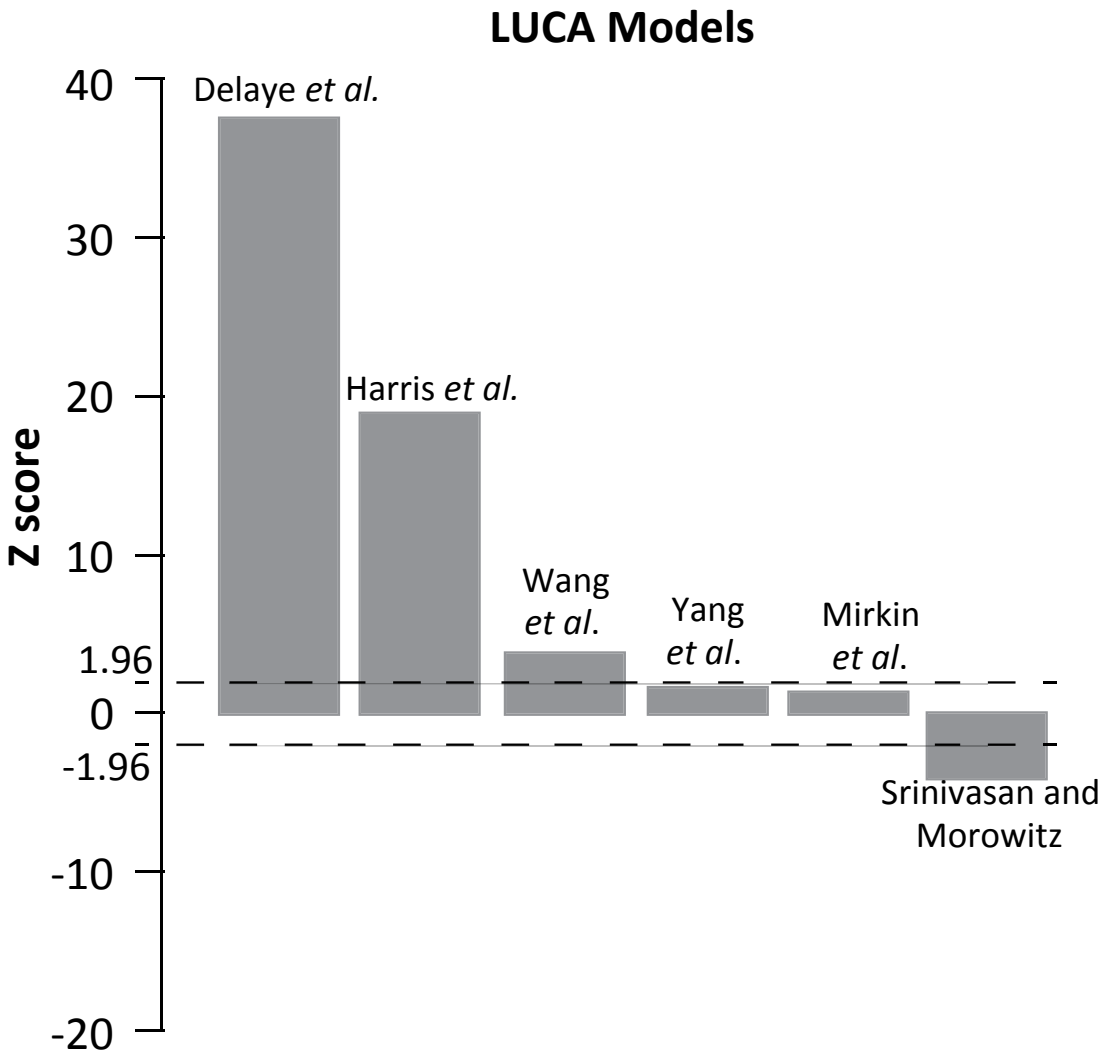
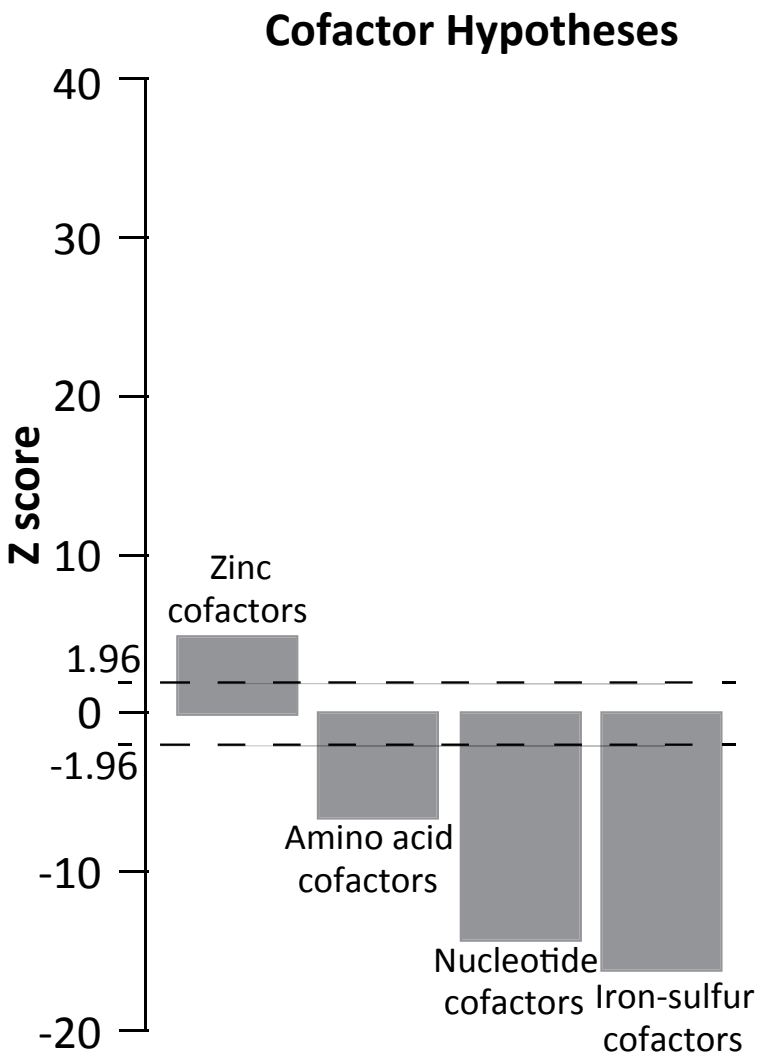


KEGG map1100

Ribozyme Hypothesis Testing





Bernhardt *et al*. (in preparation)

KEGG map1100

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LUCApedia is a unified framework containing multiple datasets related to the Last Universal Common Ancestor (LUCA) and its predecessors. The database can be searched by protein name or Uniprot ID. Text and SQL files are also available on the download page.

Please enter protein name or a Uniprot ID (also called "entry name"):

synthetase Search

exact protein name | partial protein name | Uniprot ID

Next →

displaying first 50 records

protein name	Uniprot IDs[1]	Harris et al., 2003[2] (COG ID[3])	Mirkin et al., 2003[4] (COG ID[3])	Delaye et al., 2005[5] (Pfam ID[6])	Yang et al., 2005[7] (SCOP superfamily ID[8])	Wang et al., 2007[9] (SCOP fold ID[8])	Srinivasan and Morowitz, 2009[10] (Enzyme commission code[11])	Ribozyme function (Enzyme commission code[11])	Nucleotide cofactor usage	Amino acid cofactor usage	Iron sulfur cofactor usage	Zinc cofactor usage
Threonyl-tRNA synthetase	SYT_STAAW	-	-	tRNA-synt_2b, HGTP_anticodon	d.67.1, d.104.1, c.51.1	d.67, d.15, d.104, c.51	-	-	-	-	-	zinc (By similarity)
Threonyl-tRNA synthetase	SYT_ECOLI	-	-	tRNA-synt_2b, HGTP_anticodon	d.67.1, d.104.1, c.51.1	d.67, d.15, d.104, c.51	-	-	-	-	-	zinc
Methionyl-tRNA synthetase	SYM_PYRAB	-	-	-	c.26.1, b.40.4, a.27.1	c.26, b.40, a.27	-	6.1.1.10	-	-	-	zinc (By similarity)
Prolyl-tRNA synthetase	SYP_METJA	COG0442	COG0442	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.68, d.104, c.51	-	-	-	-	-	-
Prolyl-tRNA synthetase	SYP_METTH	COG0442	COG0442	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.68, d.104, c.51	-	-	-	-	-	-
Arginyl-tRNA synthetase	SYRC_YEAST	COG0018	COG0018	tRNA-synt_1d, Arg_tRNA_synt_N	c.26.1, a.27.1	d.67, c.26, a.27	-	-	-	-	-	-
Glycyl-tRNA synthetase	SYG_THET8	-	-	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.104, c.51	6.1.1.14	-	-	-	-	-
Phenylalanyl-tRNA synthetase alpha subunit	SYFA_THET8	-	-	tRNA-synt_2d	d.104.1, b.40.4	d.58, d.104, b.40, a.6, a.2	-	6.1.1.20	-	-	-	-

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synthetase [Search]

exact protein name | partial protein name | Uniprot ID

Next →

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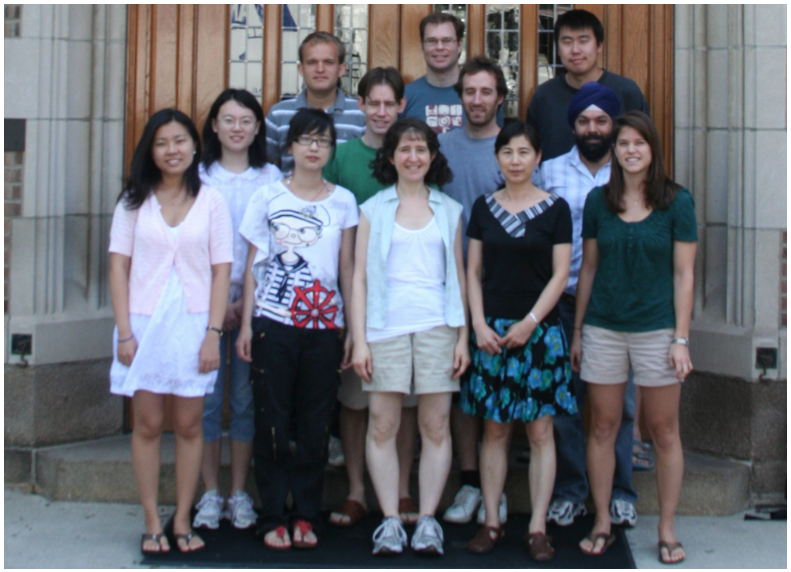
Threonyl-tRNA synthetase	SYT_ECOLI	-	-	tRNA-synt_2b, HGTP_anticodon	d.67.1, d.104.1, c.51.1	d.67, d.15, d.104, c.51	-	-	-	-	-	zinc
Methionyl-tRNA synthetase	SYM_PYRAB	-	-	-	c.26.1, b.40.4, a.27.1	c.26, b.40, a.27	-	6.1.1.10	-	-	-	zinc (By similarity)
Prolyl-tRNA synthetase	SYP_METJA	COG0442	COG0442	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.68, d.104, c.51	-	-	-	-	-	-
Prolyl-tRNA synthetase	SYP_METTH	COG0442	COG0442	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.68, d.104, c.51	-	-	-	-	-	-
Arginyl-tRNA synthetase	SYRC_YEAST	COG0018	COG0018	tRNA-synt_1d, Arg_tRNA_synt_N	c.26.1, a.27.1	d.67, c.26, a.27	-	-	-	-	-	-
Glycyl-tRNA synthetase	SYG_THET8	-	-	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.104, c.51	6.1.1.14	-	-	-	-	-
Phenylalanyl-tRNA synthetase alpha subunit	SYFA_THET8	-	-	tRNA-synt_2d	d.104.1, b.40.4	d.58, d.104, b.40, a.6, a.2	-	6.1.1.20	-	-	-	-

Goldman *et al.* (2013) *Nucleic Acids Res,* 41: D1079-82

http://eeb.princeton.edu/lucapedia

Thanks to…

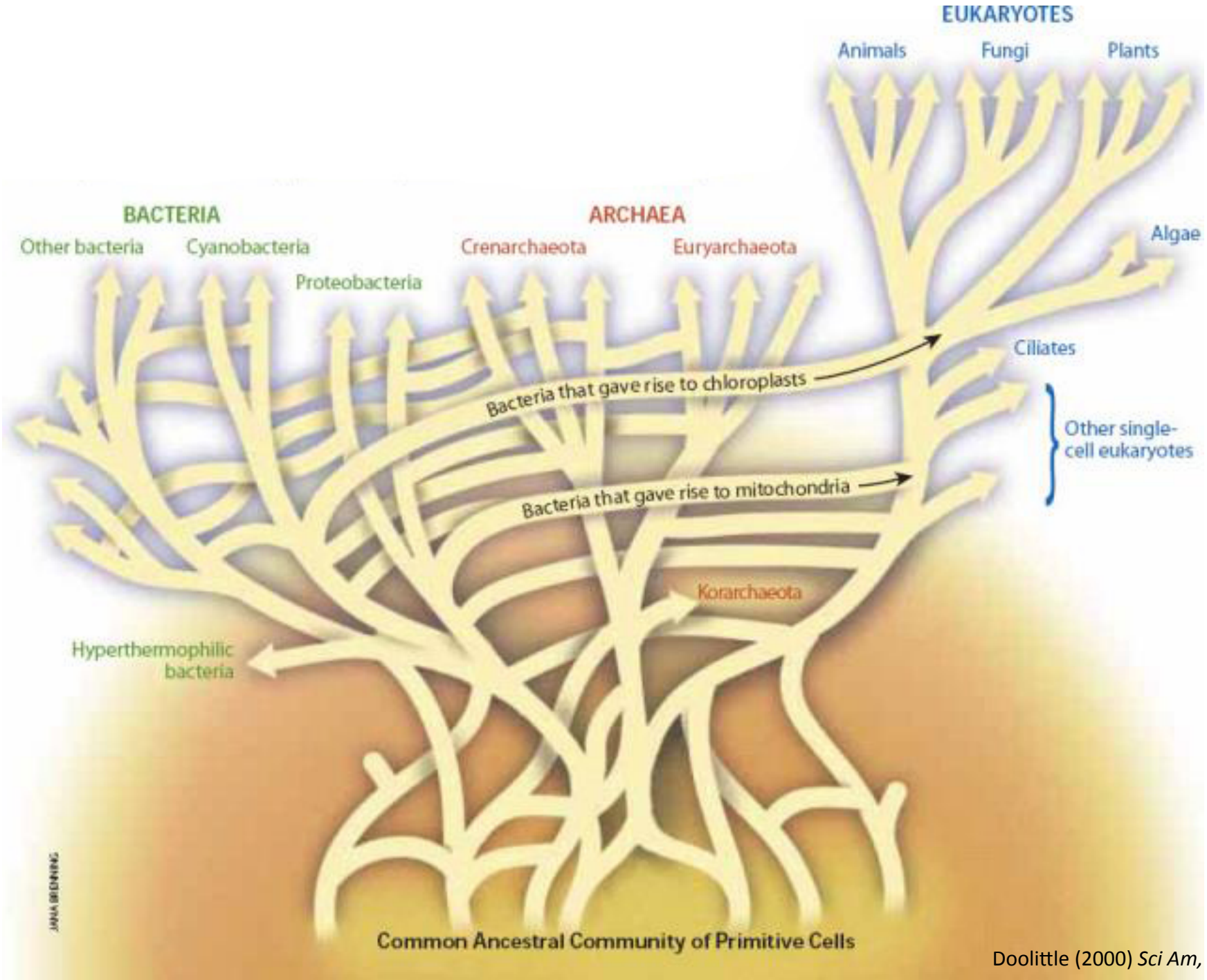
Laura Landweber and the lab



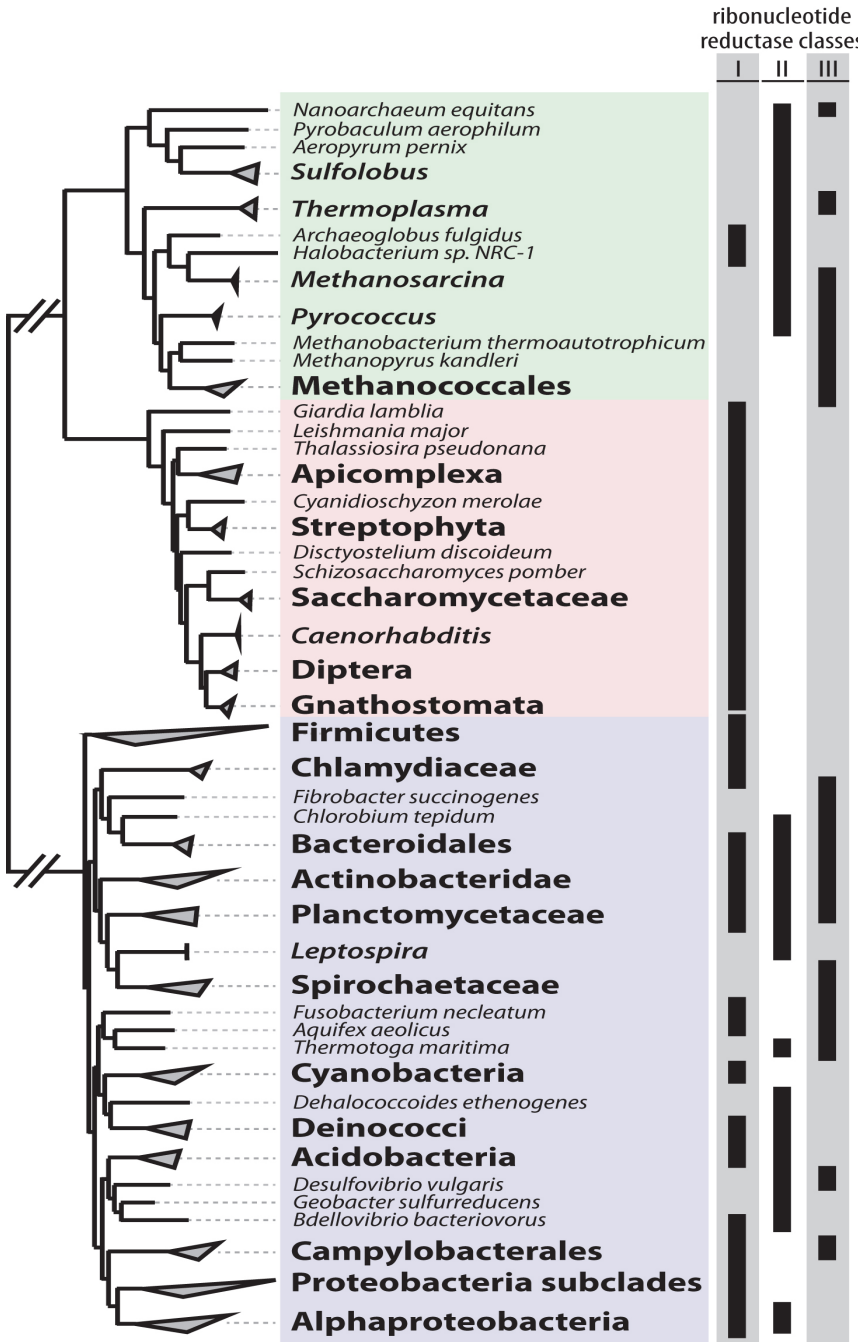
LUCApedia TEAM

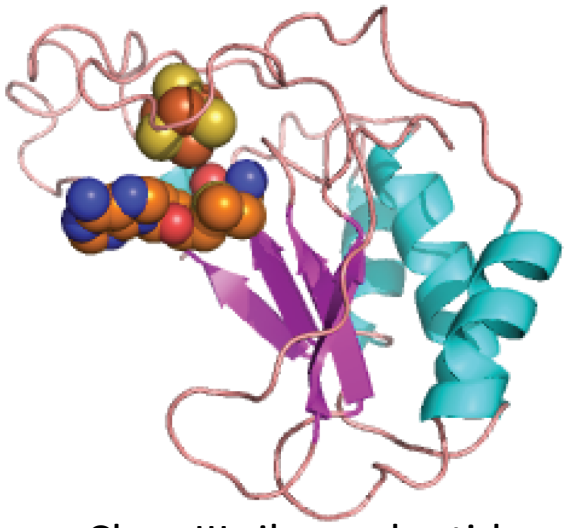
Funding

NASA Postdoctoral Fellowship



Doolittle (2000) *Sci Am,* 2:90



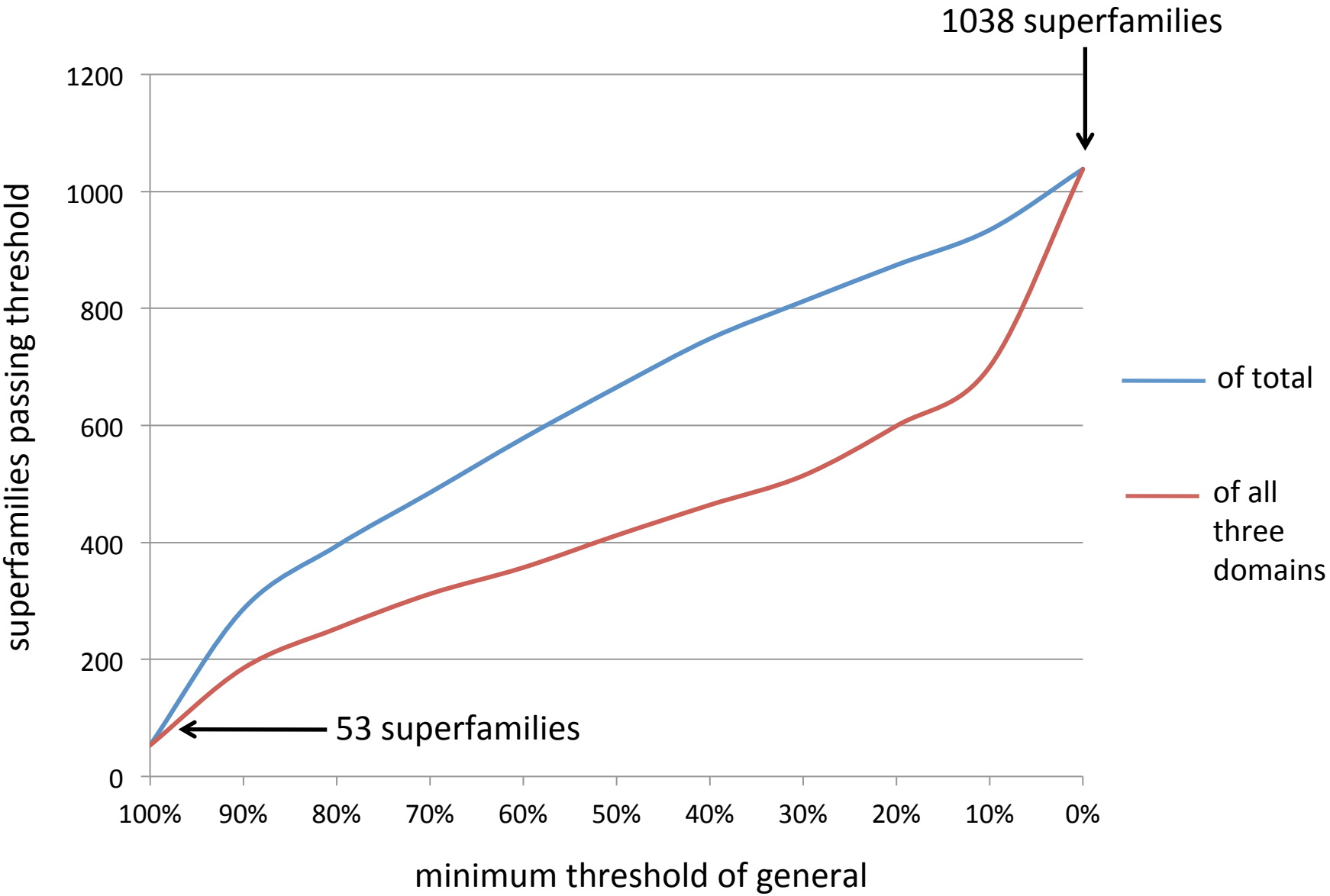


Class III ribonucleotide reductase activating protein

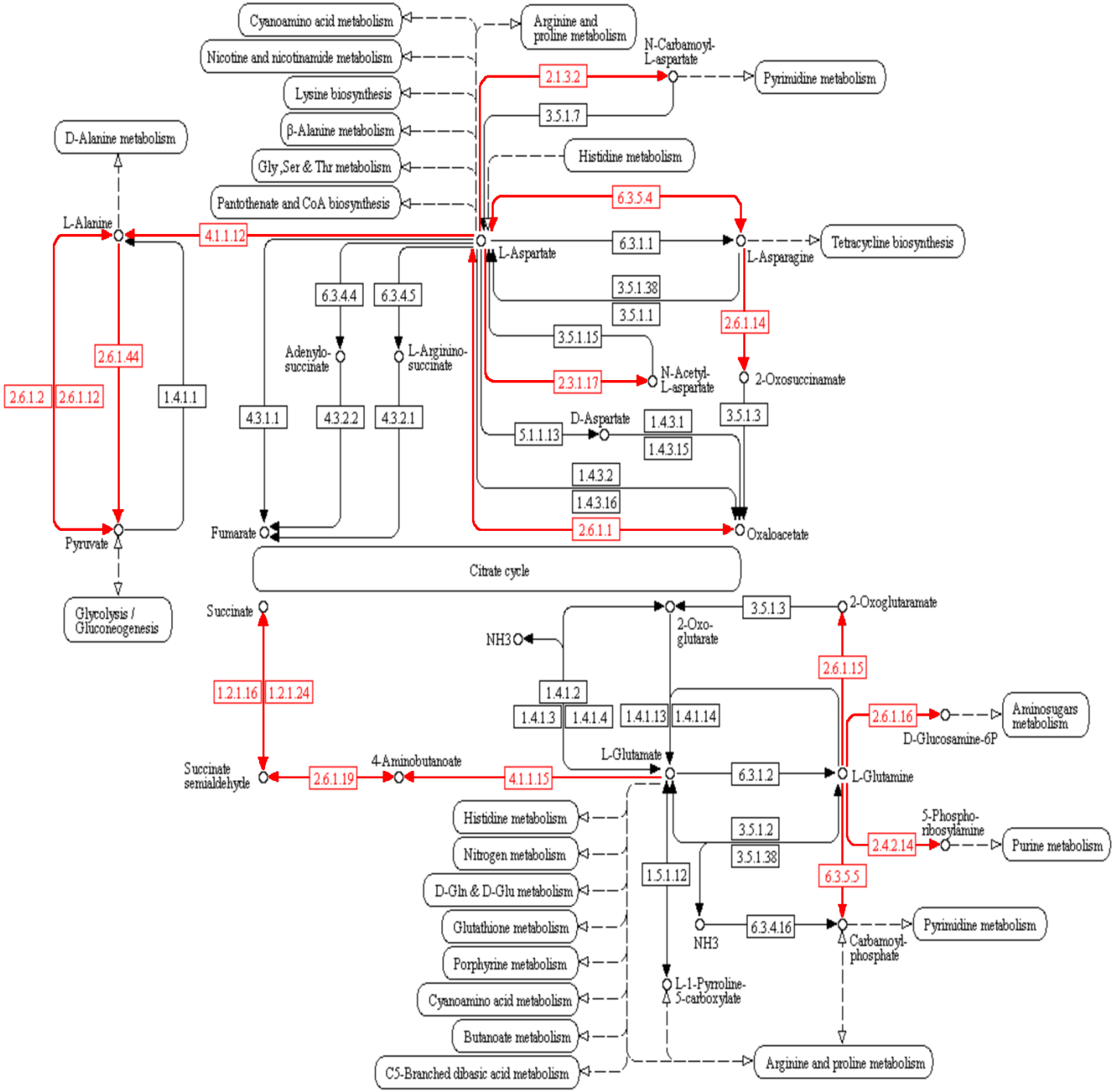
Goldman and Landweber (2012) *Trends Genet* **28**: 382-388

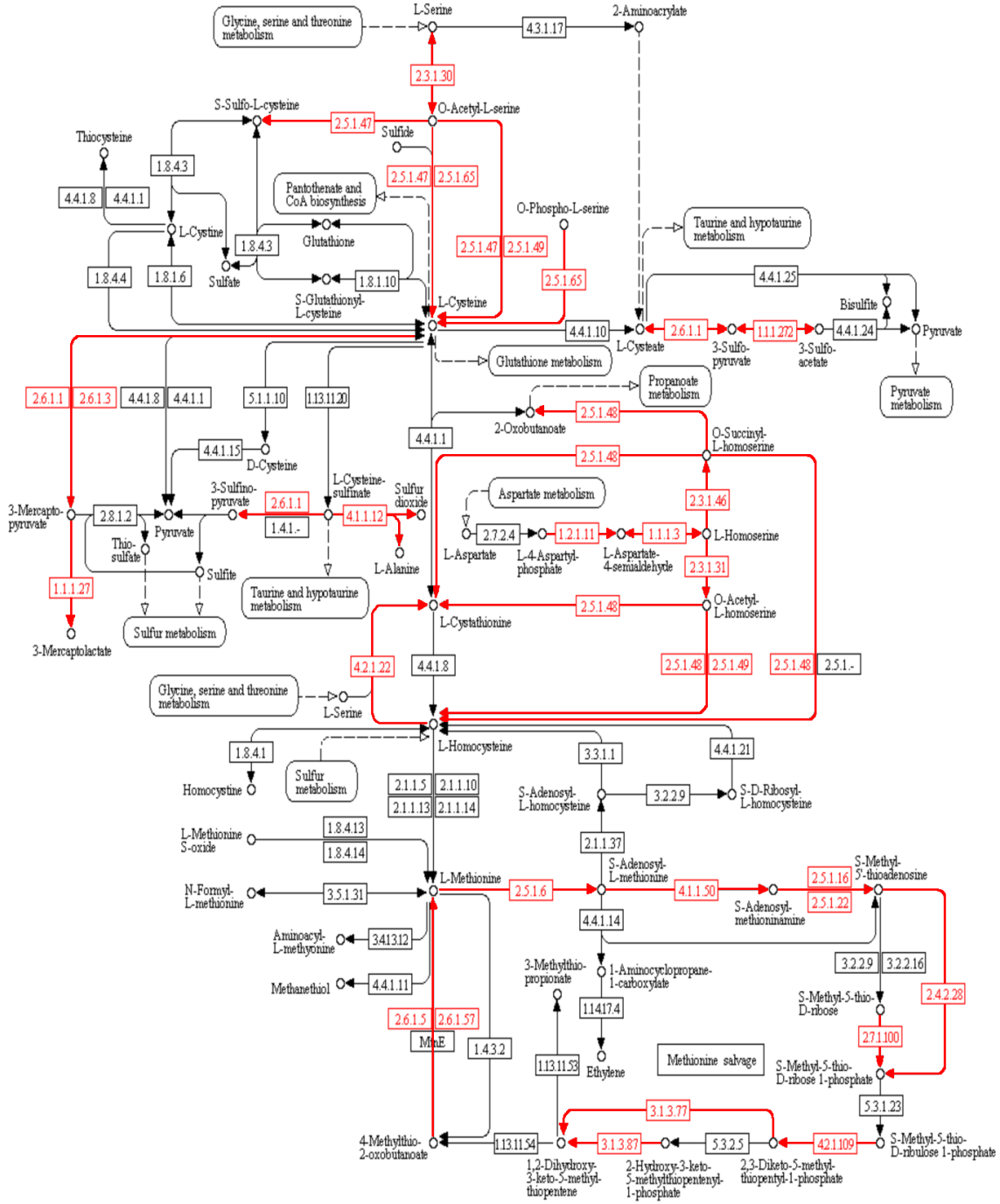
RNR structure from Goldman and Landweber (submitted)

Tree from Ciccarelli *et al.* (2006) Science 311:1283–1287



Data from www.supfam.org


Cyanoamino acid metabolism
Arginine and proline metabolism
Nicotine and nicotinamide metabolism
N-Carbamoyl-L-aspartate
Pyrimidine metabolism
2.1.3.2
Lysine biosynthesis
3.5.1.7
β-Alanine metabolism
D-Alanine metabolism
Histidine metabolism
Gly ,Ser & Thr metabolism
6.3.5.4
Pantothenate and CoA biosynthesis
L-Alanine
4.1.1.12
L-Aspartate
6.3.1.1
L-Asparagine
Tetracycline biosynthesis
6.3.4.4
6.3.4.5
3.5.1.38
3.5.1.1
3.5.1.15
2.6.1.14
Adenylo-succinate
L-Arginino-succinate
2.6.1.44
2.3.1.17
N-Acetyl-L-aspartate
2-Oxosuccinamate
2.6.1.2
2.6.1.12
1.4.1.1
4.3.1.1
4.3.2.2
4.3.2.1
3.5.1.3
D-Aspartate
5.1.1.13
1.4.3.1
1.4.3.15
1.4.3.2
1.4.3.16
Fumarate
2.6.1.1
Oxaloacetate
Pyruvate
Citrate cycle
Glycolysis / Gluconeogenesis
Succinate
2-Oxoglutaramate
3.5.1.3
NH3
2-Oxo-glutarate
2.6.1.15
1.4.1.2
1.2.1.16
1.2.1.24
1.4.1.3
1.4.1.4
1.4.1.13
1.4.1.14
2.6.1.16
Aminosugars metabolism
D-Glucosamine-6P
L-Glutamate
Succinate semialdehyde
2.6.1.19
4-Aminobutanoate
4.1.1.15
6.3.1.2
L-Glutamine
Histidine metabolism
3.5.1.2
5-Phospho-ribosylamine
Nitrogen metabolism
3.5.1.38
2.4.2.14
Purine metabolism
D-Gln & D-Glu metabolism
1.5.1.12
6.3.5.5
Glutathione metabolism
NH3
6.3.4.16
Pyrimidine metabolism
Porphyrine metabolism
Carbamoyl-phosphate
L-1-Pyrroline-5-carboxylate
Cyanoamino acid metabolism
Butanoate metabolism
Arginine and proline metabolism
C5-Branched dibasic acid metabolism


Glycine, serine and threonine metabolism
L-Serine
2-Aminoacrylate
4.3.1.17
2.3.1.30
O-Acetyl-L-serine
S-Sulfo-L-cysteine
2.5.1.47
Sulfide
Thiocysteine
1.8.4.3
4.4.1.8
4.4.1.1
2.5.1.47
2.5.1.65
Pantothenate and CoA biosynthesis
L-Cystine
1.8.4.3
Glutathione
O-Phospho-L-serine
Taurine and hypotaurine metabolism
2.5.1.47
2.5.1.49
2.5.1.65
4.4.1.25
1.8.4.4
1.8.1.6
Sulfate
1.8.1.10
S-Glutathionyl-L-cysteine
L-Cysteine
Bisulfite
4.4.1.10
L-Cysteate
2.6.1.1
1.1.1.272
4.4.1.24
Pyruvate
3-Sulfo-pyruvate
3-Sulfo-acetate
Glutathione metabolism
Propanoate metabolism
Pyruvate metabolism
2.6.1.1
2.6.1.3
4.4.1.8
4.4.1.1
5.1.1.10
1.13.11.20
2.5.1.48
2-Oxobutanoate
4.4.1.1
O-Succinyl-L-homoserine
4.4.1.15
D-Cysteine
2.5.1.48
3-Sulfino-pyruvate
2.6.1.1
L-Cysteine-sulfinate
Sulfur dioxide
Aspartate metabolism
2.3.1.46
3-Mercapto-pyruvate
2.8.1.2
Pyruvate
1.4.1.-
4.1.1.12
2.7.2.4
1.2.1.11
1.1.1.3
L-Homoserine
L-Aspartate
L-4-Aspartyl-phosphate
L-Aspartate-4-semialdehyde
2.3.1.31
Thio-sulfate
Sulfite
L-Alanine
1.1.1.27
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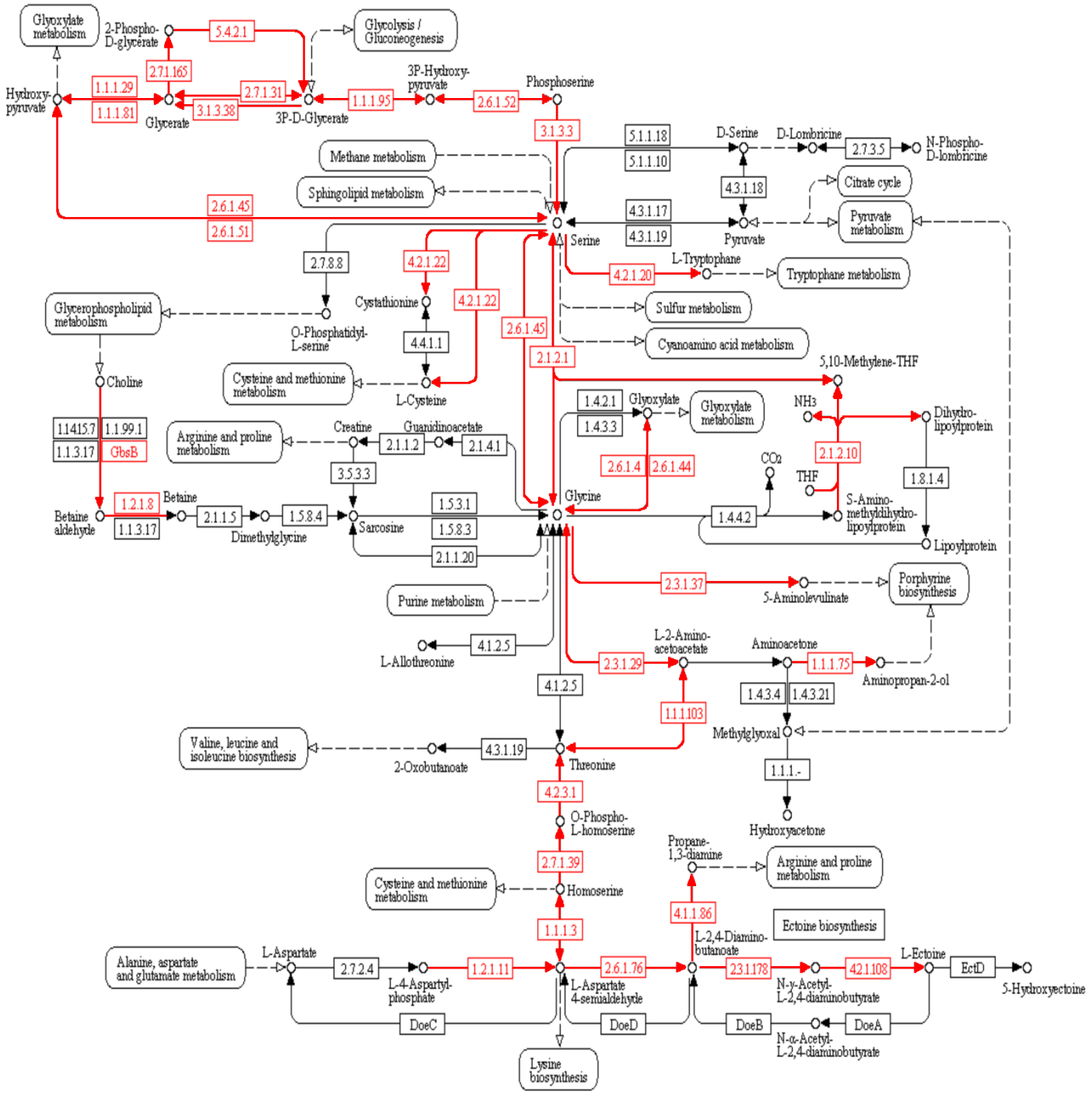
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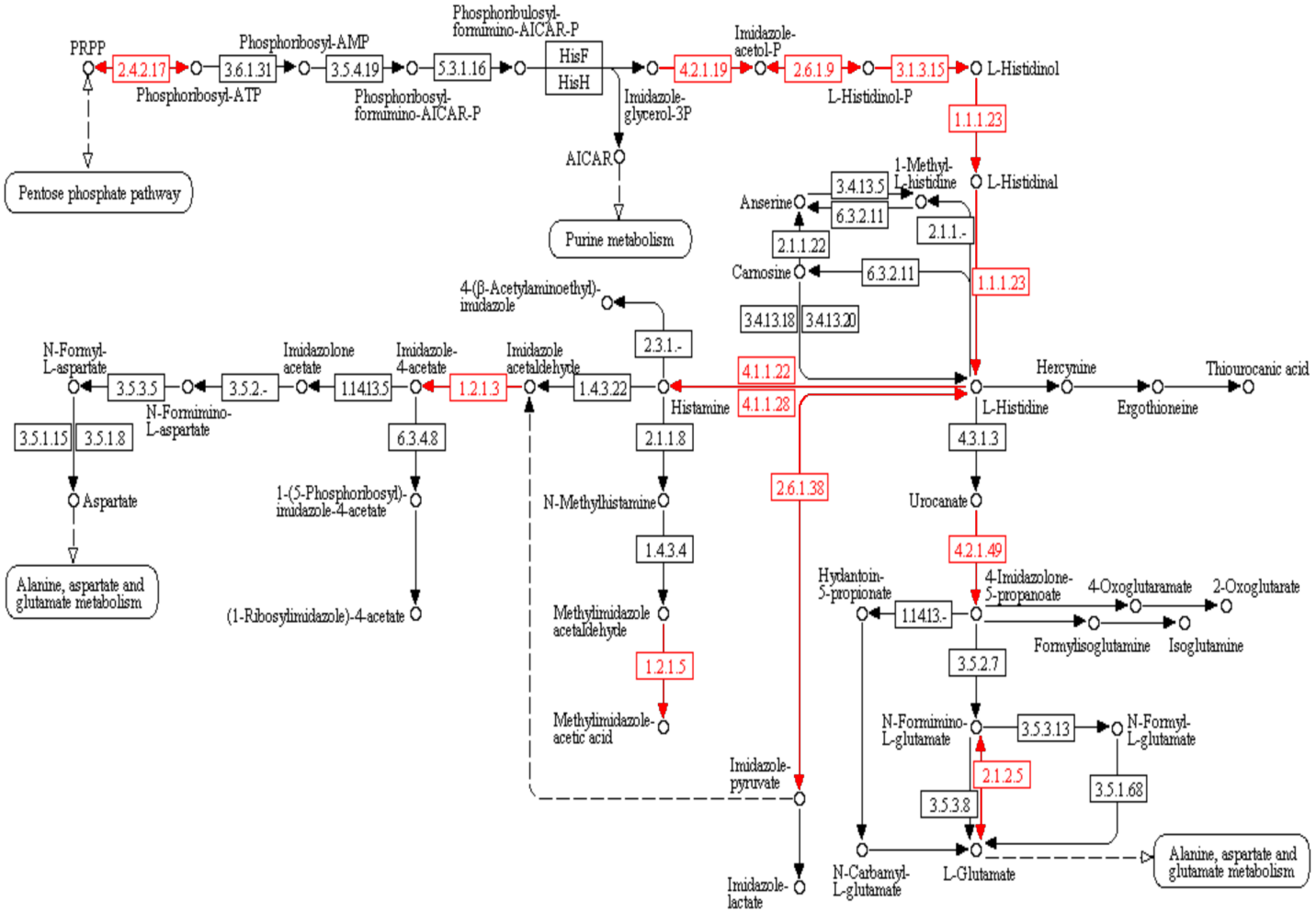
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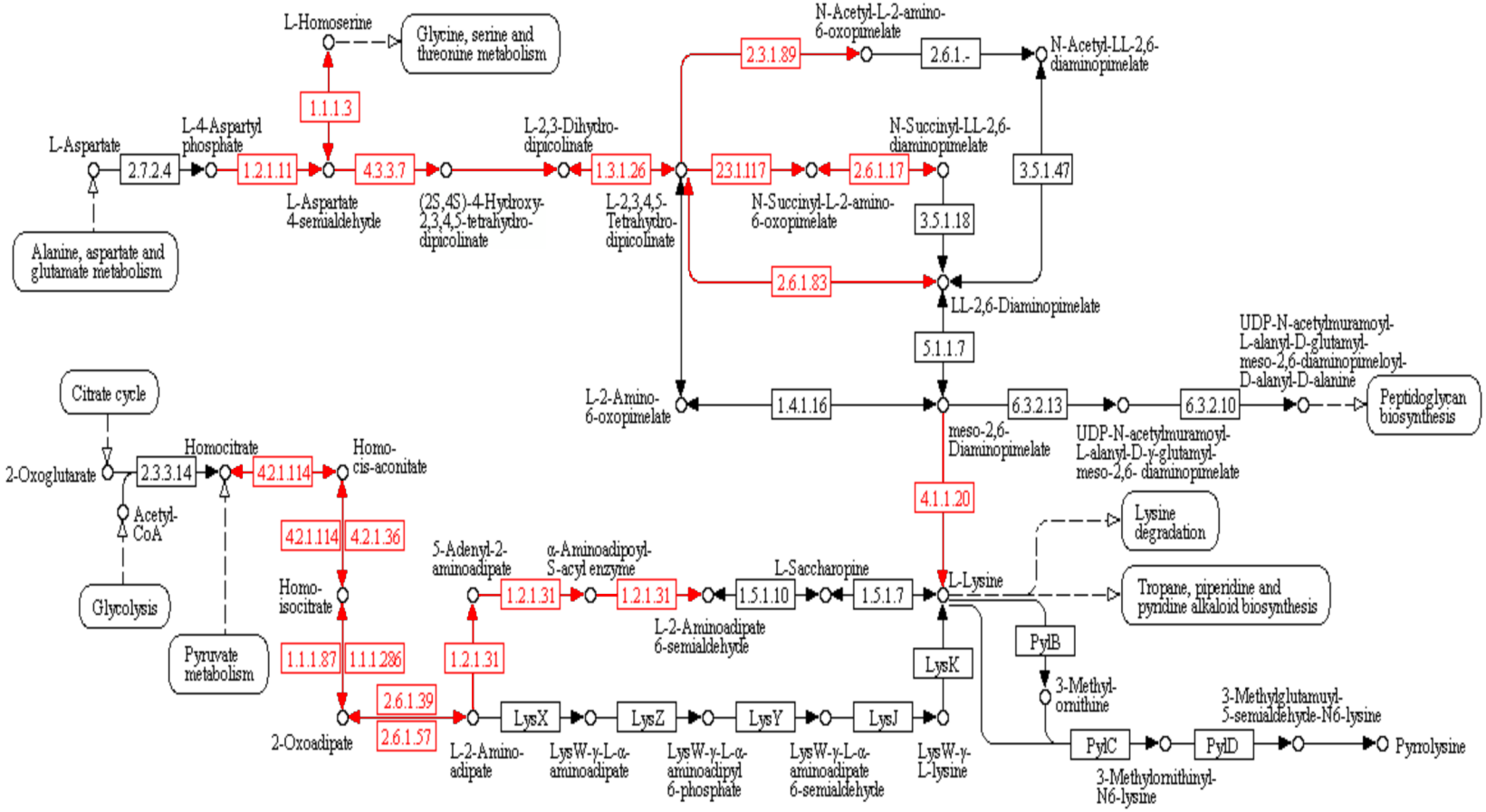
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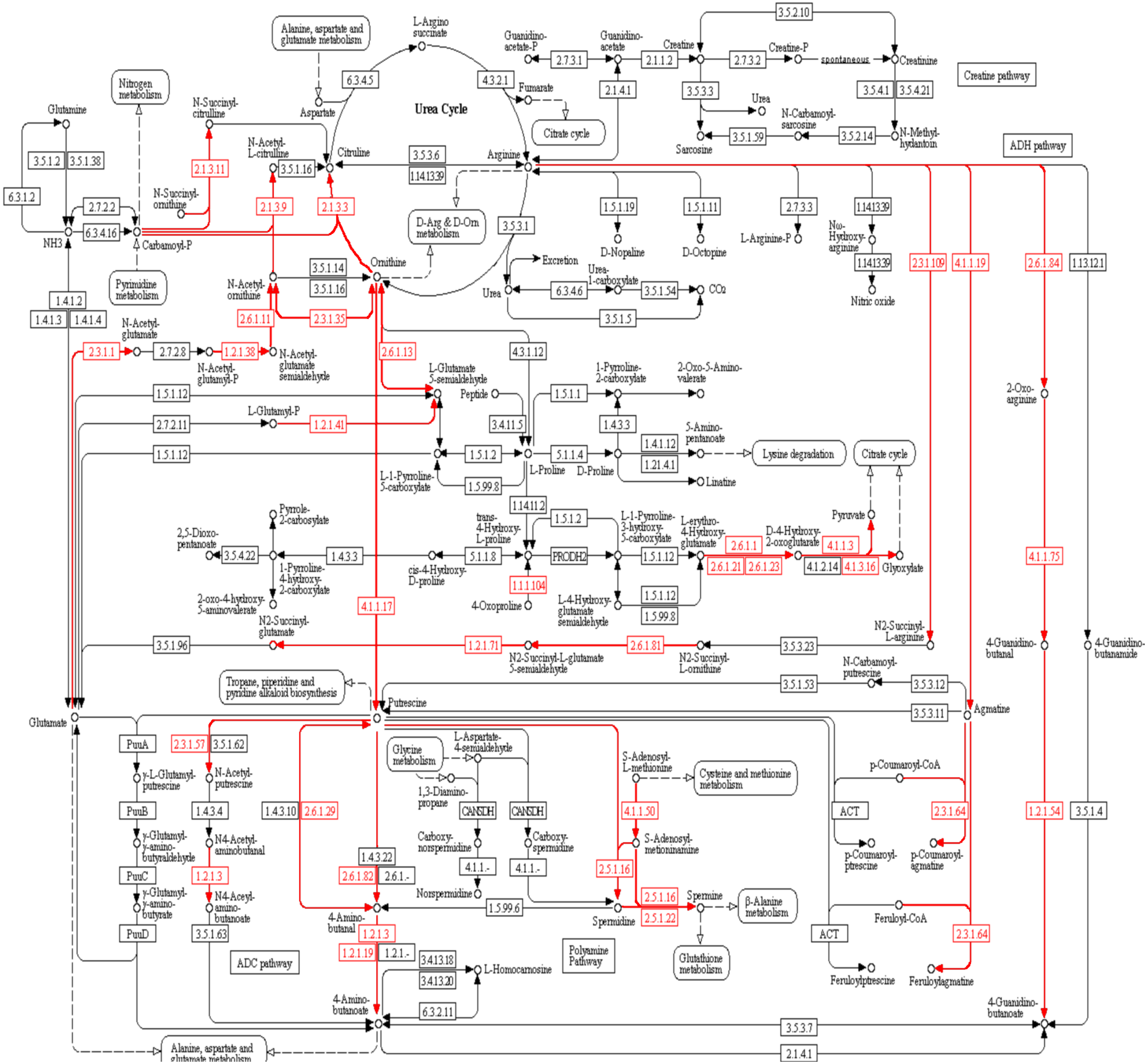

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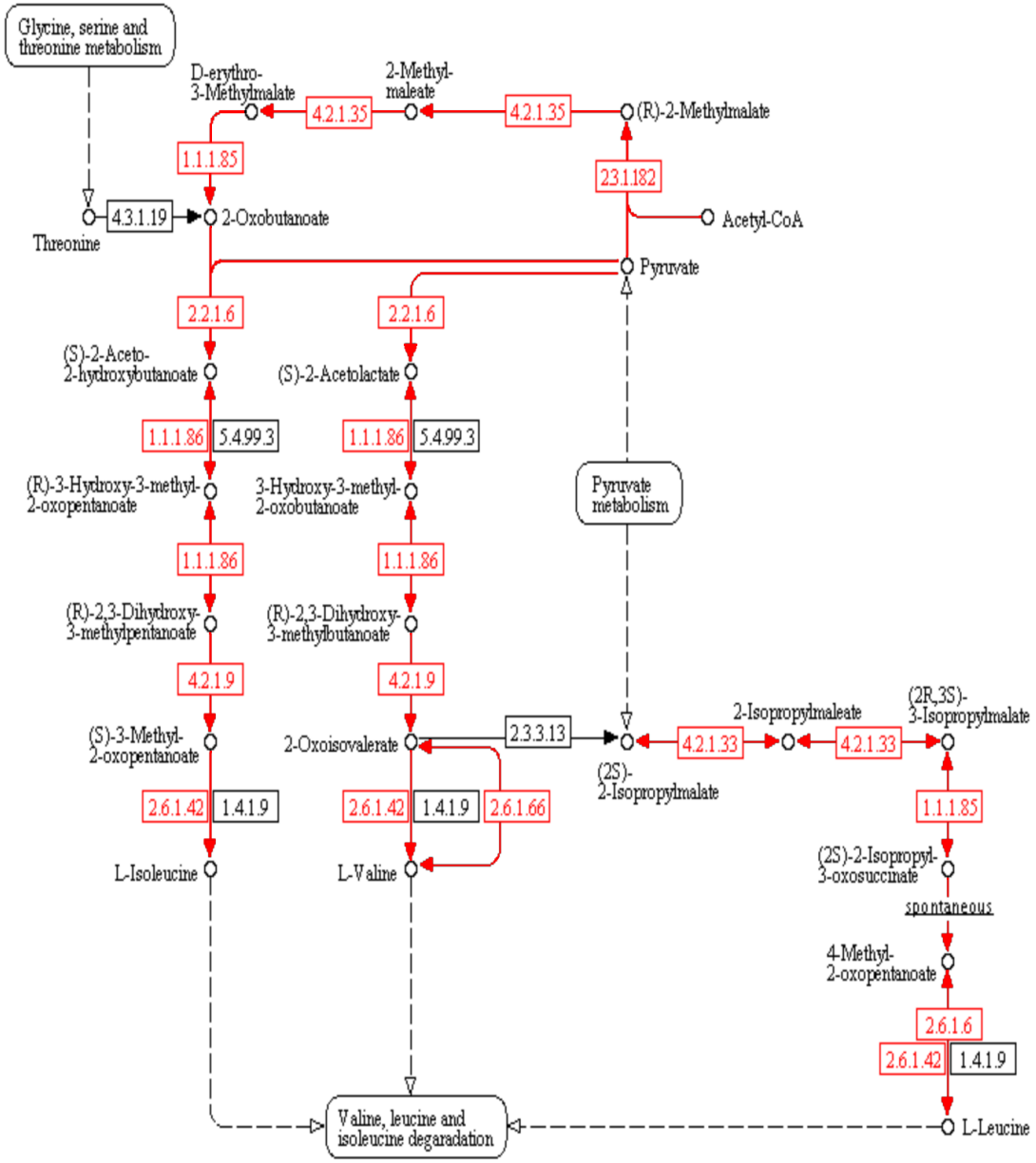
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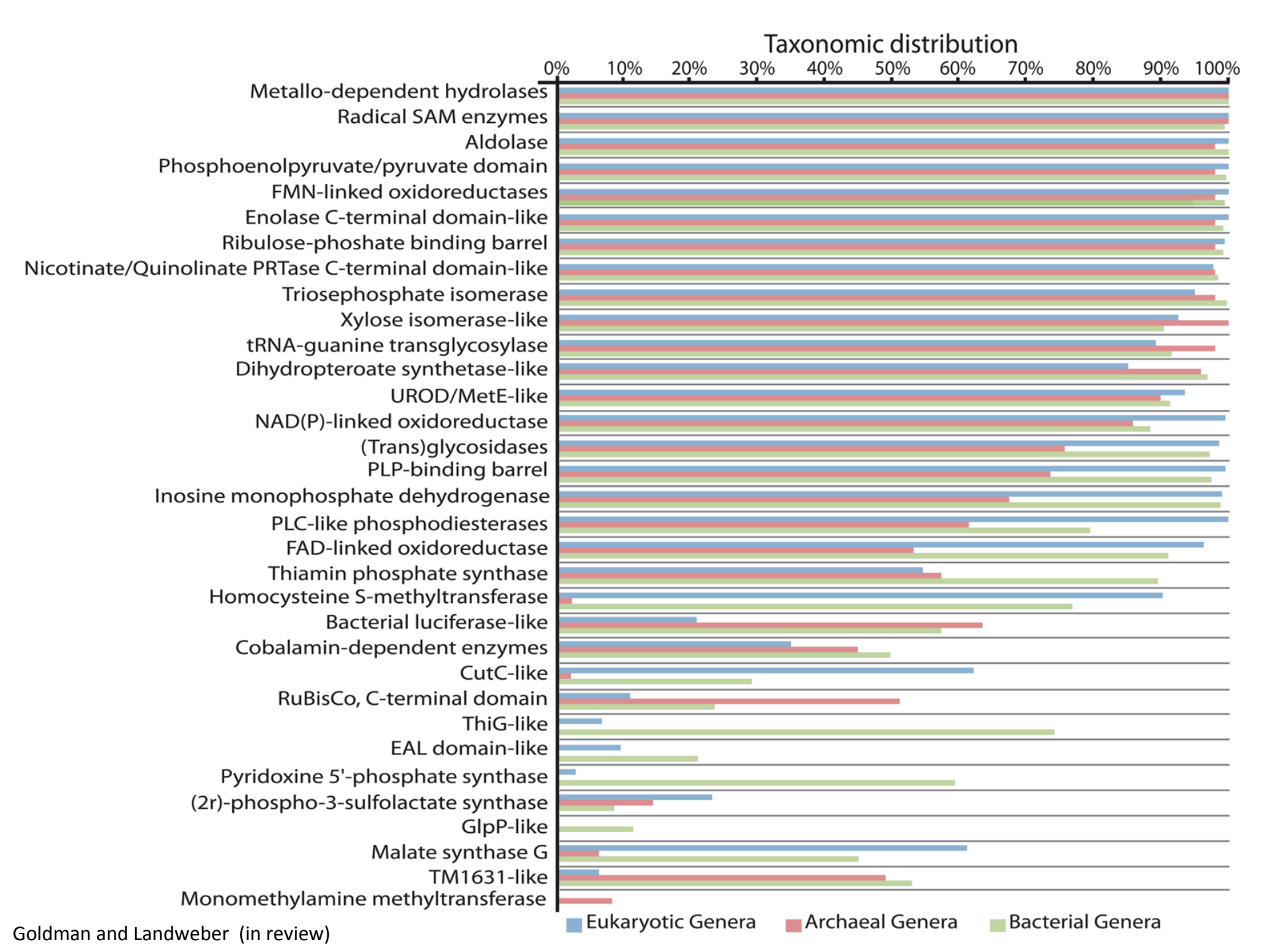

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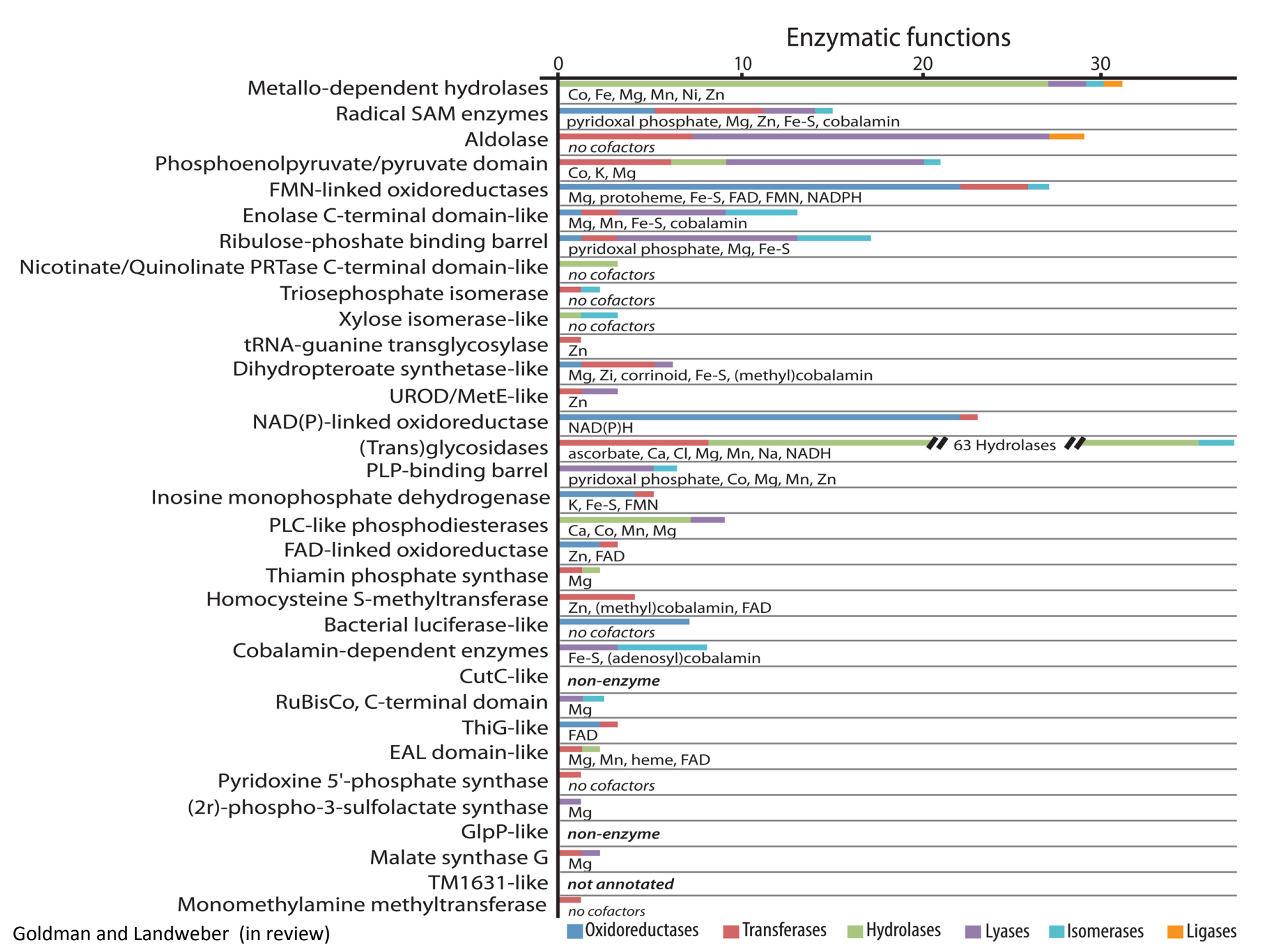

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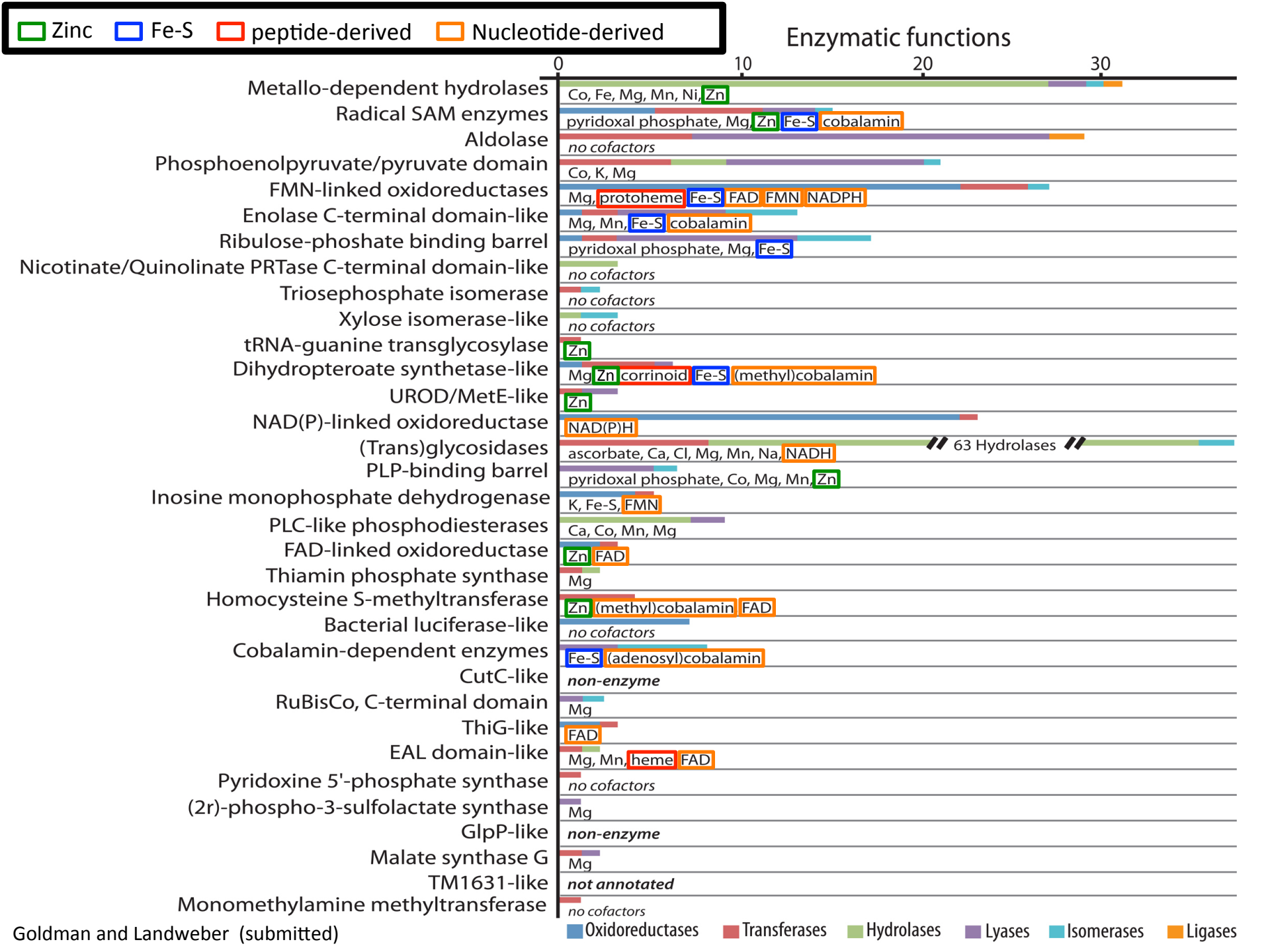

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protein name	Uniprot IDs[1]	Harris et al., 2003[2] (COG ID[3])	Mirkin et al., 2003[4] (COG ID[3])	Delaye et al., 2005[5] (Pfam ID[6])	Yang et al., 2005[7] (SCOP superfamily ID[8])	Wang et al., 2007[9] (SCOP fold ID[8])	Srinivasan and Morowitz, 2009[10] (Enzyme commission code[11])	Ribozyme function (Enzyme commission code[11])	Nucleotide cofactor usage	Amino acid cofactor usage	Iron sulfur cofactor usage	Zinc cofactor usage
Threonyl-tRNA synthetase	SYT_STAAW	-	-	tRNA-synt_2b, HGTP_anticodon	d.67.1, d.104.1, c.51.1	d.67, d.15, d.104, c.51	-	-	-	-	-	zinc (By similarity)
Threonyl-tRNA synthetase	SYT_ECOLI	-	-	tRNA-synt_2b, HGTP_anticodon	d.67.1, d.104.1, c.51.1	d.67, d.15, d.104, c.51	-	-	-	-	-	zinc
Methionyl-tRNA synthetase	SYM_PYRAB	-	-	-	c.26.1, b.40.4, a.27.1	c.26, b.40, a.27	-	6.1.1.10	-	-	-	zinc (By similarity)
Prolyl-tRNA synthetase	SYP_METJA	COG0442	COG0442	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.68, d.104, c.51	-	-	-	-	-	-
Prolyl-tRNA synthetase	SYP_METTH	COG0442	COG0442	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.68, d.104, c.51	-	-	-	-	-	-
Arginyl-tRNA synthetase	SYRC_YEAST	COG0018	COG0018	tRNA-synt_1d, Arg_tRNA_synt_N	c.26.1, a.27.1	d.67, c.26, a.27	-	-	-	-	-	-
Glycyl-tRNA synthetase	SYG_THET8	-	-	tRNA-synt_2b, HGTP_anticodon	d.104.1, c.51.1	d.104, c.51	6.1.1.14	-	-	-	-	-
Phenylalanyl-tRNA synthetase alpha subunit	SYFA_THET8	-	-	tRNA-synt_2d	d.104.1, b.40.4	d.58, d.104, b.40, a.6, a.2	-	6.1.1.20	-	-	-	-

Goldman *et al.* (2013) *Nucleic Acids Res,* 41: D1079-82

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