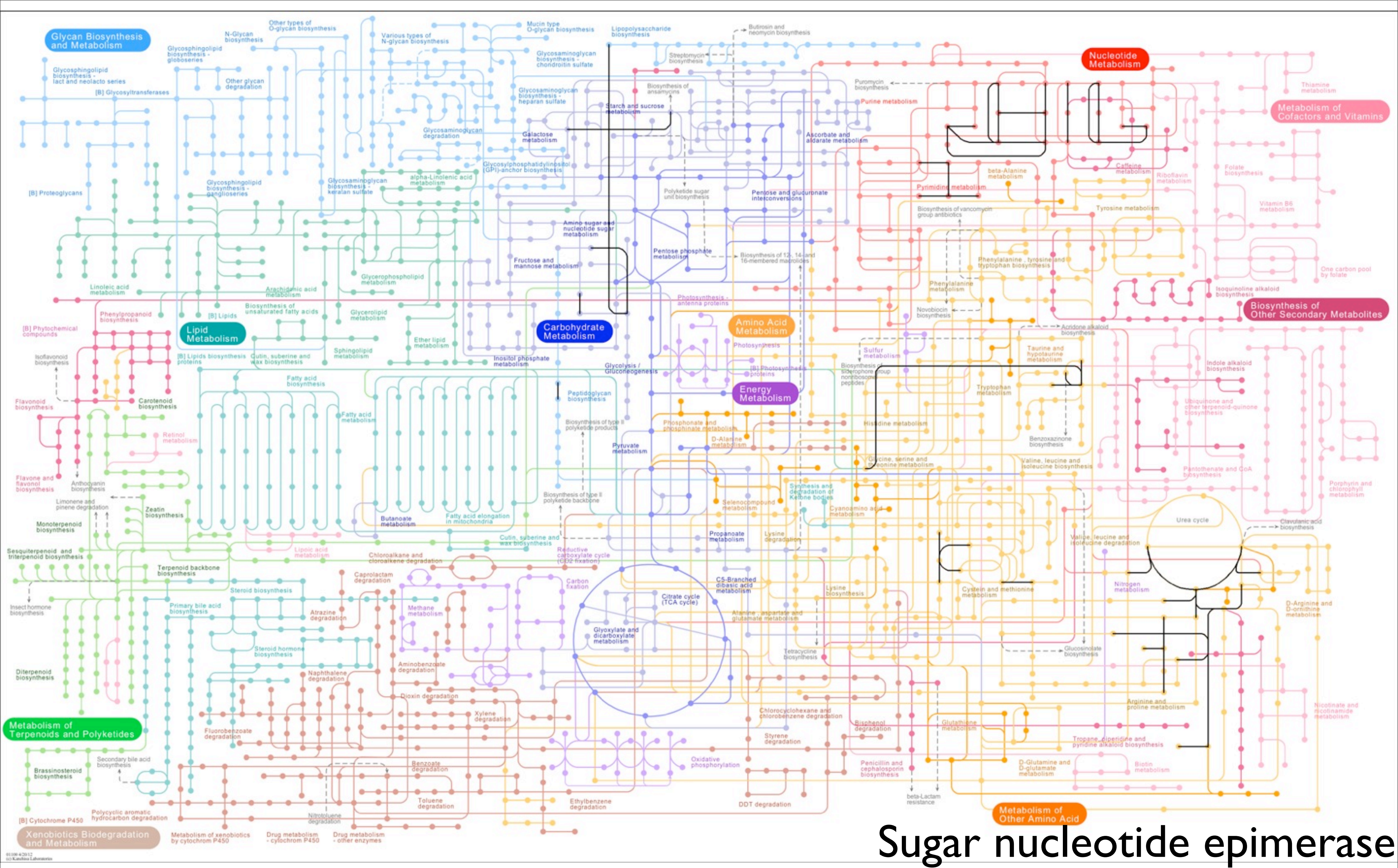# Dimensions 05-03-12 Update
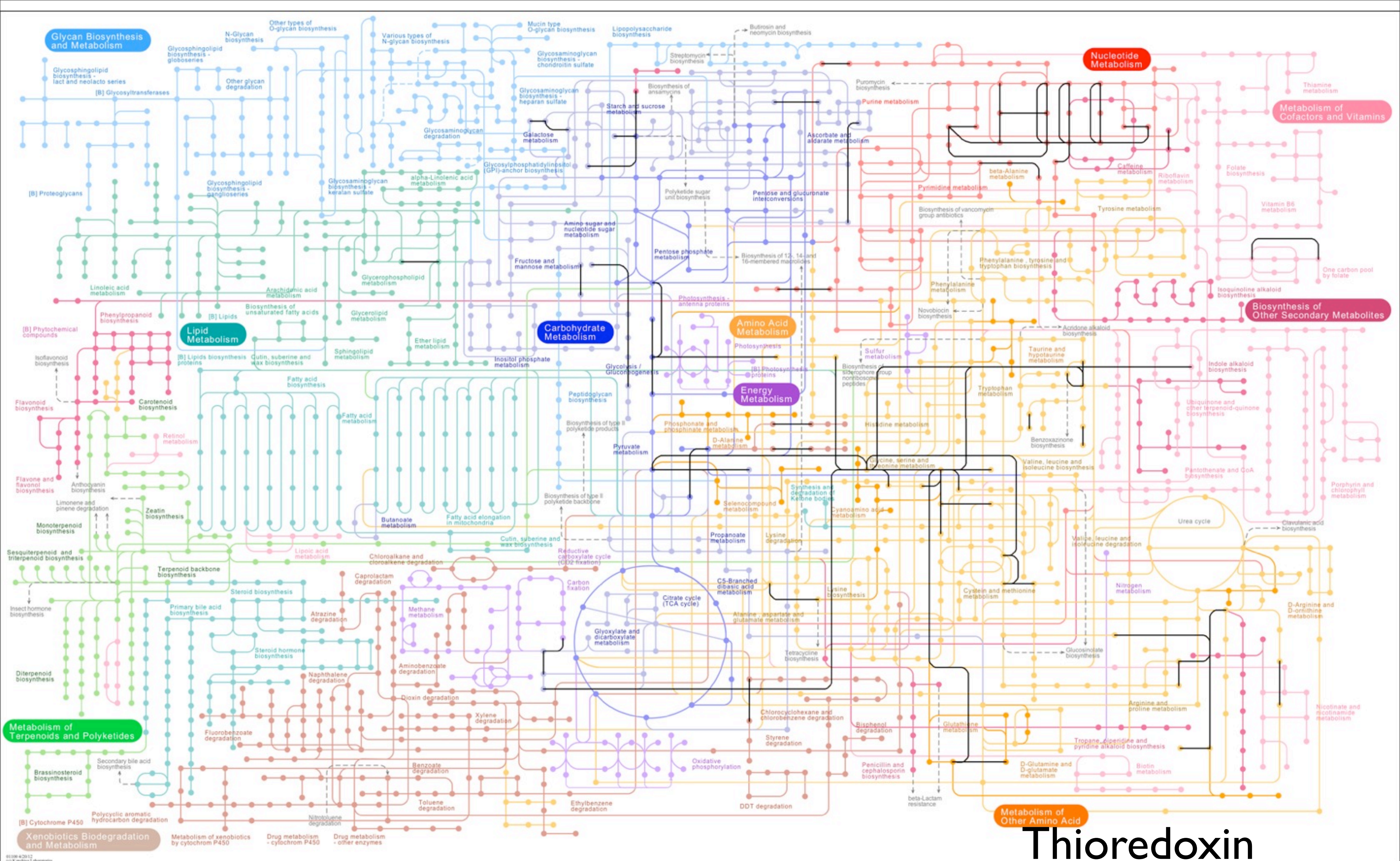
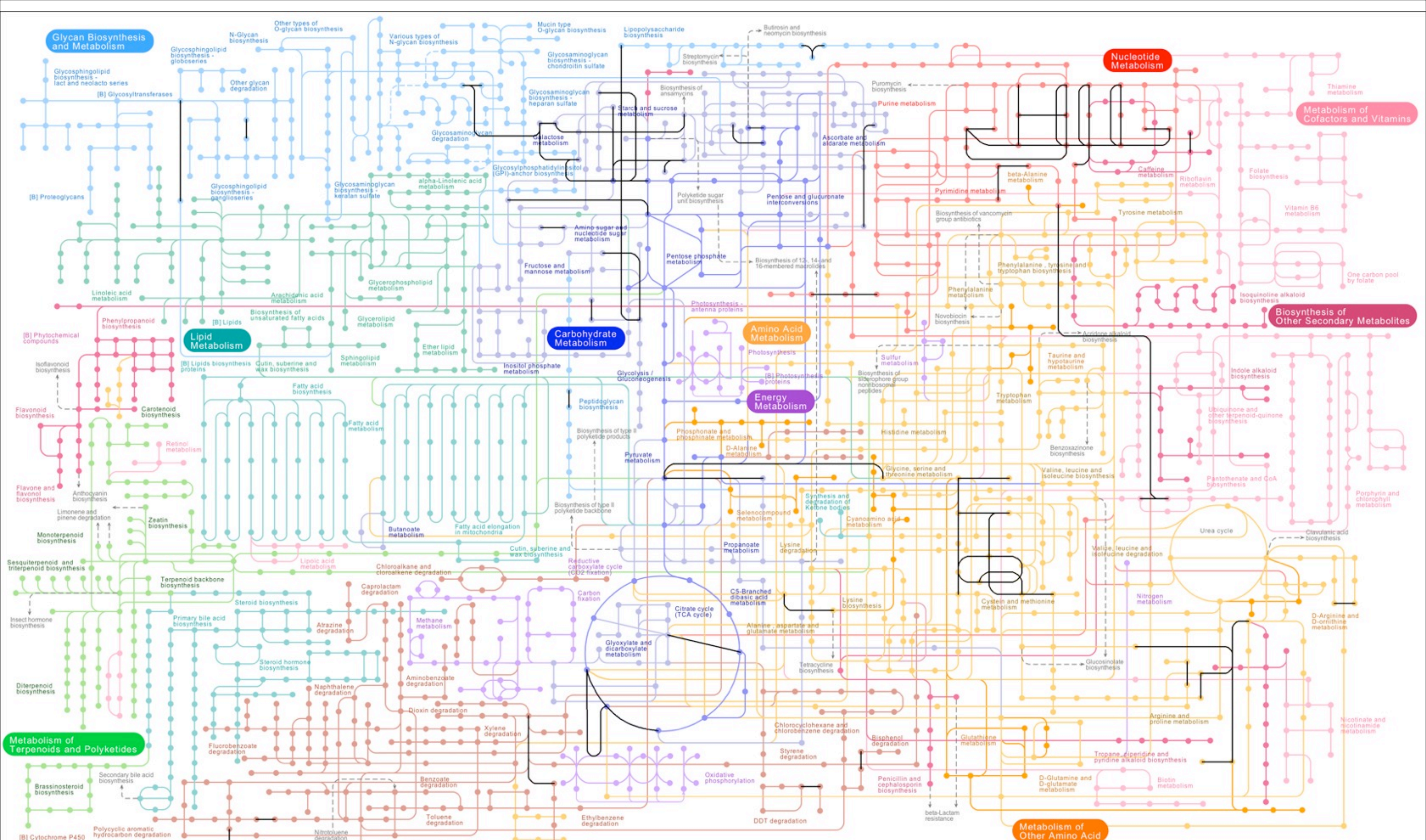Jeremy Frank

Dimensions Physiology Data

- Evaluated all metabolomics data (clone vs empty vector pairwise comparisons)

- Some compounds/subsystems come up all the time

- Will compare all comparisons to identify which pathways are always hit (= less informative)

- Do subtraction and evaluate left over data

- Starting the code for converting significant reactions to colored metabolic maps

- Need to identify which maps are most informative

- Will still have a list of 10s of maps

- Need to generate "longest affected pathways" to show linkage between maps...have the code, need to edit it to increase efficiency
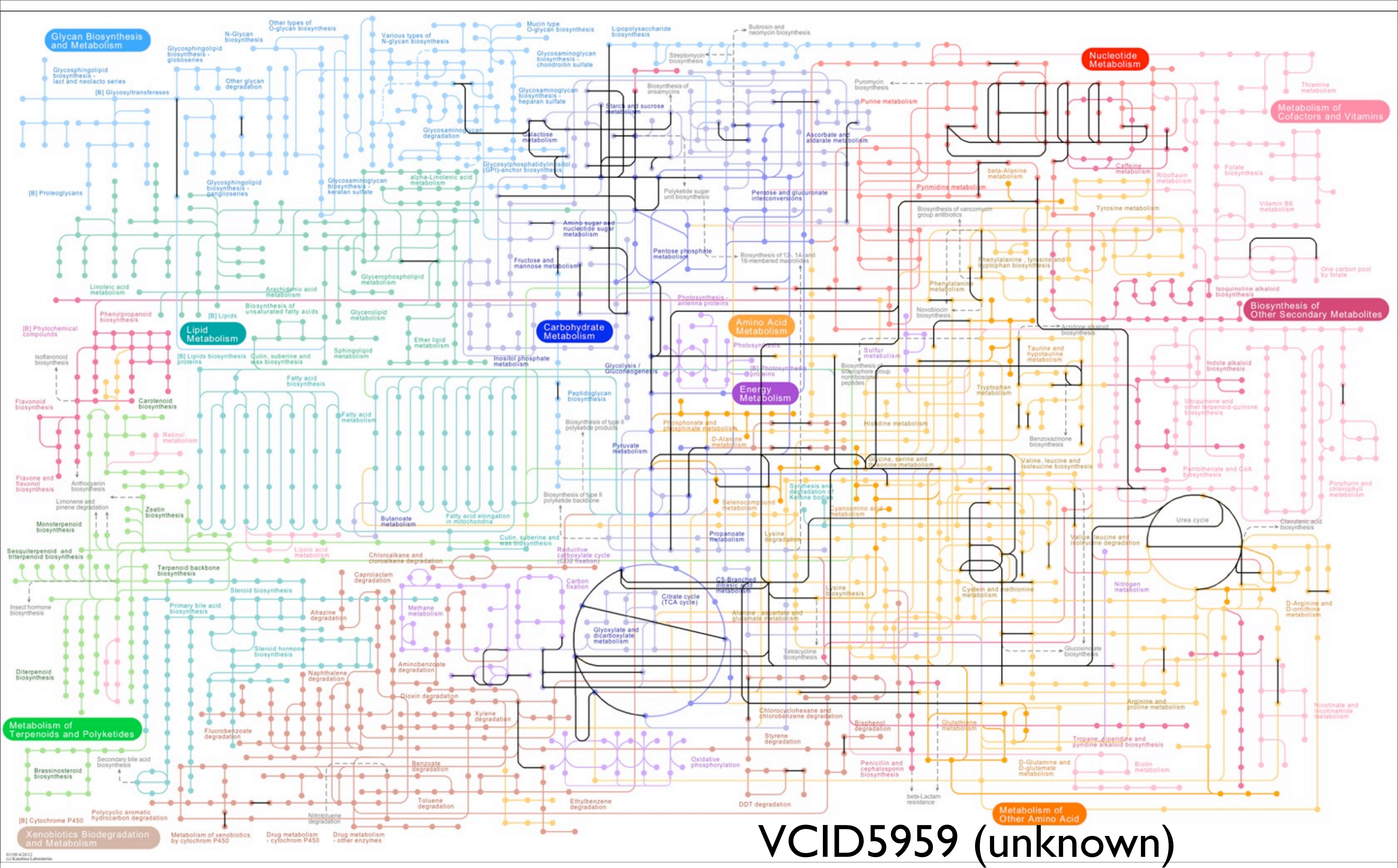
Sugar nucleotide epimerase

Thioredoxin

Glycan Biosynthesis and Metabolism

Nucleotide Metabolism

Metabolism of Cofactors and Vitamins

Carbohydrate Metabolism

Amino Acid Metabolism

Lipid Metabolism

Energy Metabolism

Biosynthesis of Other Secondary Metabolites

Metabolism of Terpenoids and Polyketides

Metabolism of Other Amino Acid

Xenobiotics Biodegradation and Metabolism

Phosphoribosylglycinamide formyltransferase

VCID5959 (unknown)

Glycan Biosynthesis and Metabolism

Nucleotide Metabolism

Metabolism of Cofactors and Vitamins

Carbohydrate Metabolism

Amino Acid Metabolism

Energy Metabolism

Lipid Metabolism

Biosynthesis of Other Secondary Metabolites

Metabolism of Terpenoids and Polyketides

Metabolism of Other Amino Acid

Xenobiotics Biodegradation and Metabolism
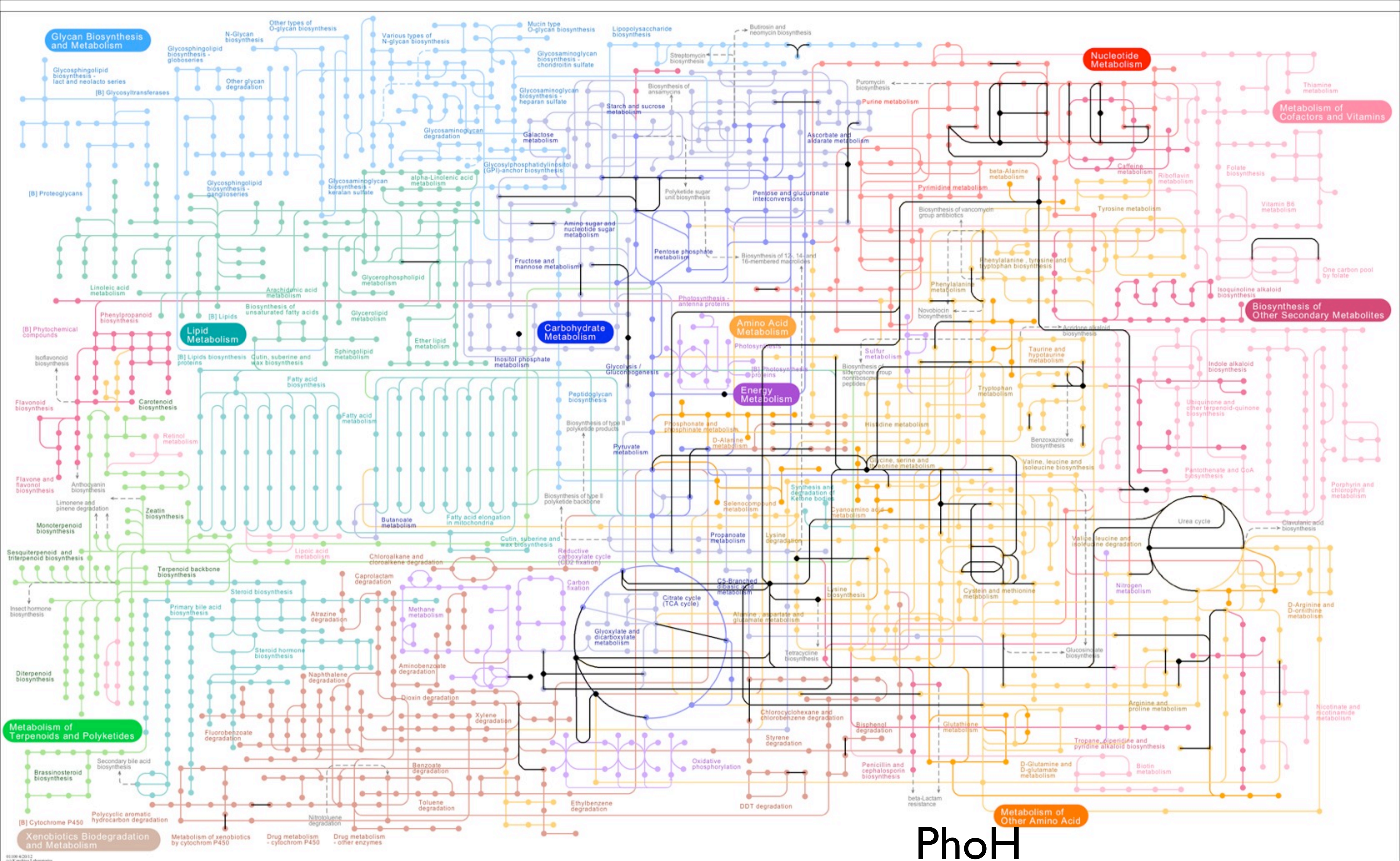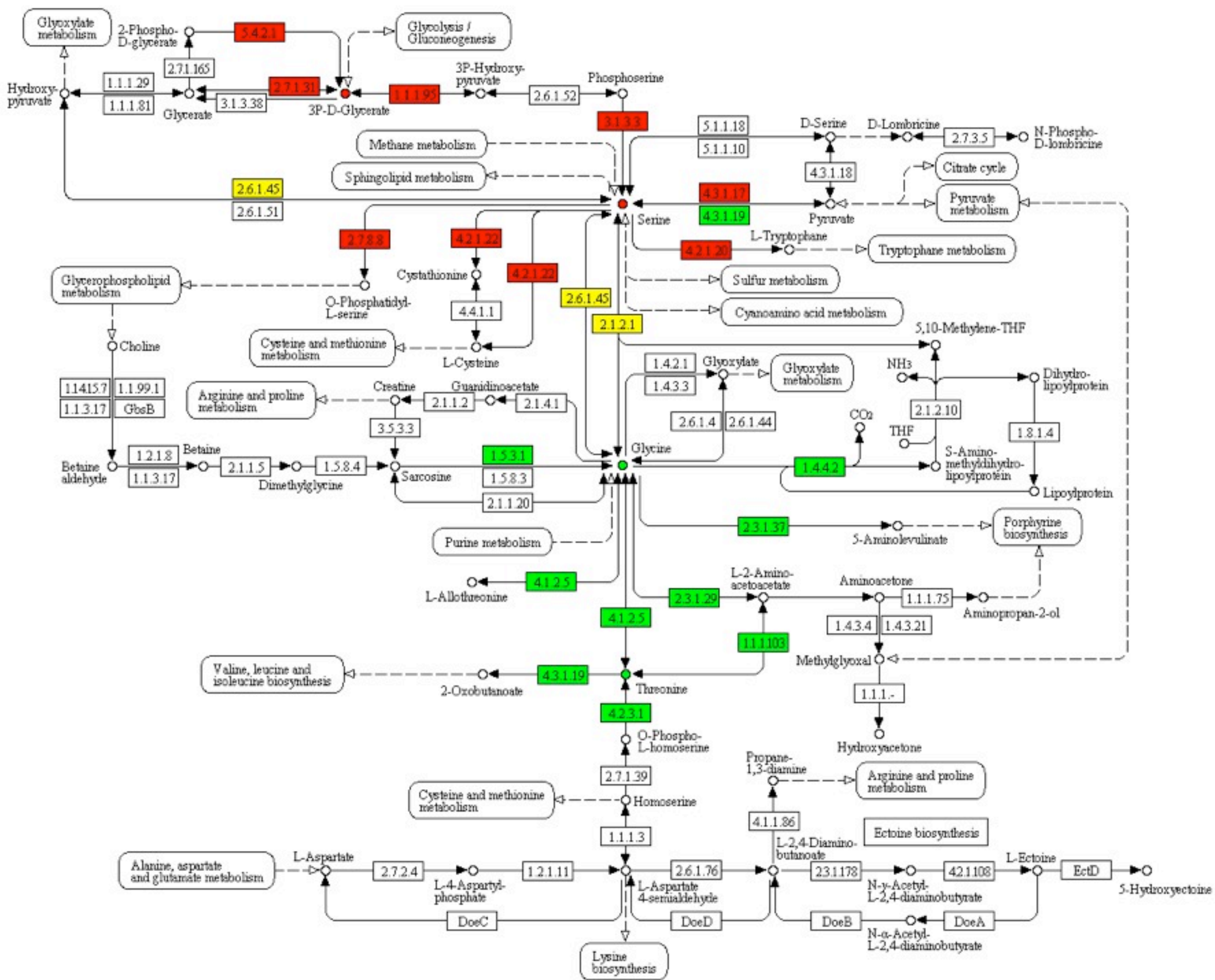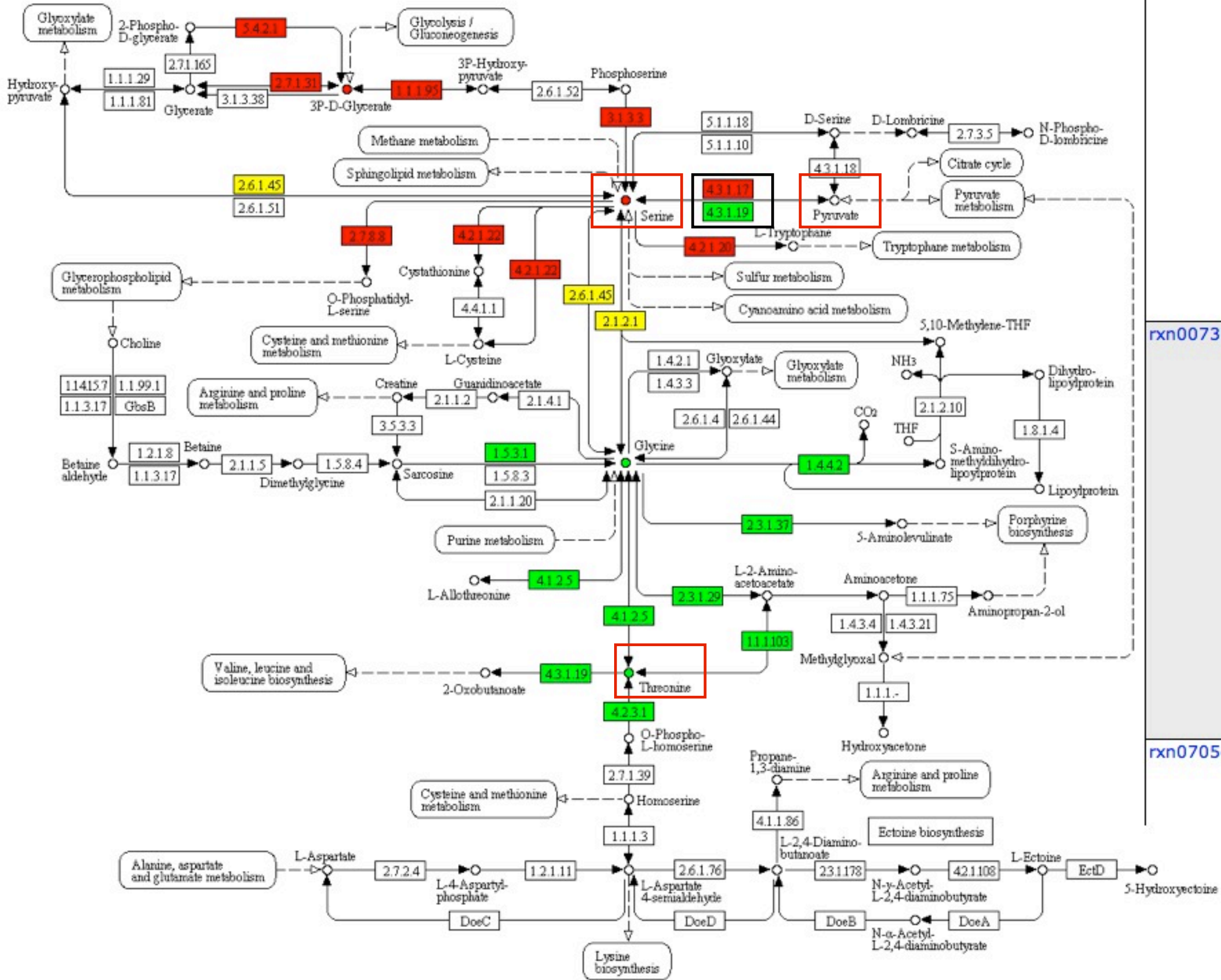
PhoH

GLYCINE, SERINE AND THREONINE METABOLISM

- Thioredoxin

- Changed the coloring scheme for reactions to green, red, yellow

- Colored in significant compounds

- Need to change map ranking to significant compounds from significant reactions (map looks more important than it is)
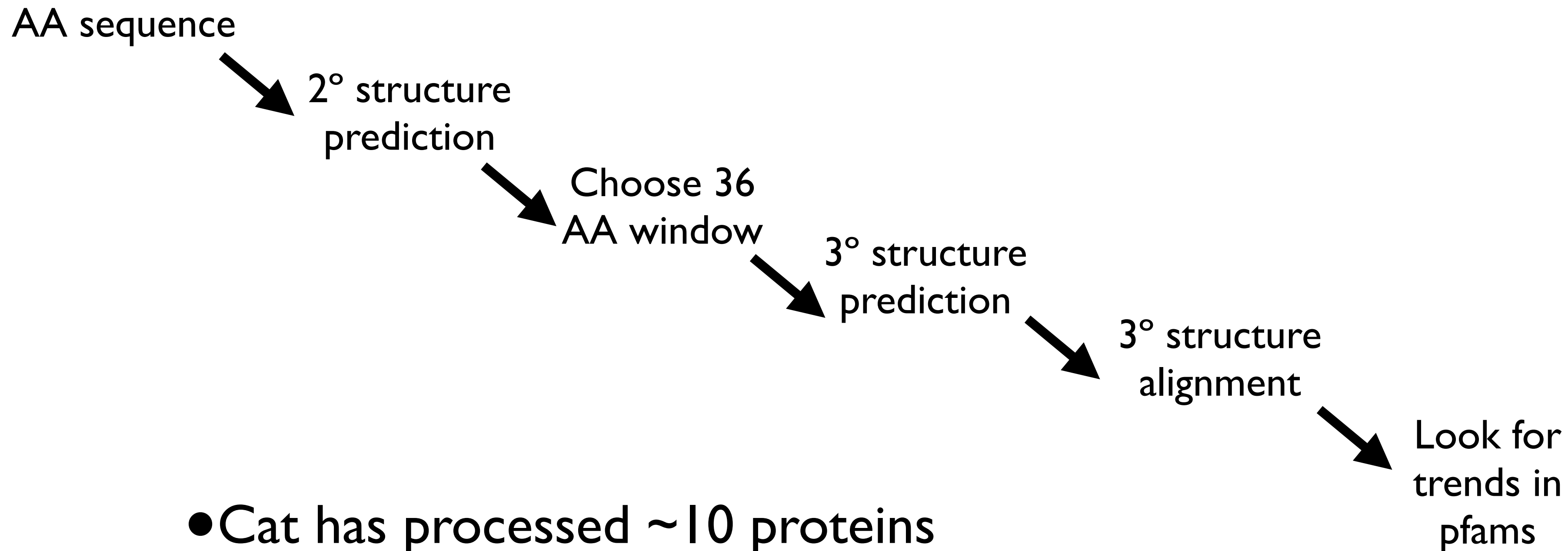
- Issue with coloring reactions

Reaction	Name	Equation	Roles	Subsystems	KEGG maps	Enzyme	KEGG RID
						4.3.1.19	
rxn00165	L-serine ammonia-lyase	L-Serine => NH3 + Pyruvate	L-serine dehydratase (EC 4.3.1.17) L-serine dehydratase, beta subunit (EC 4.3.1.17) L-serine dehydratase 1 (EC 4.3.1.17) L-serine dehydratase, alpha subunit (EC 4.3.1.17)	Glycine and Serine Utilization Pyruvate Alanine Serine Interconversions	Glycine, serine and threonine metabolism	4.2.1.13 4.3.1.15 4.3.1.17 4.3.1.19	R00220 R00223
rxn00737	L-threonine ammonia-lyase	L-Threonine => NH3 + 2-Oxobutyrate	Threonine dehydratase, catabolic (EC 4.3.1.19) L-serine dehydratase 1 (EC 4.3.1.17) Threonine dehydratase (EC 4.3.1.19) Threonine dehydratase biosynthetic (EC 4.3.1.19)	Branched-Chain Amino Acid Biosynthesis	Valine, leucine and isoleucine biosynthesis Glycine, serine and threonine metabolism	4.3.1.19	R00996
rxn07054	rxn07054	alpha-Amino acid => NH3 + 2-Oxo acid	None	None	Nitrogen metabolism	4.3.1.17 4.3.1.18 4.3.1.19 4.3.1.20	R06131

displaying 1 - 3 of 3

Significant (and not found on this part of map)

- Will change to: only color reactions only if reactants are found on map

Dimensions Physiology

- Protein sequence analysis
  - Developed a pipeline that seems to work

AA sequence → 2° structure prediction → Choose 36 AA window → 3° structure prediction → 3° structure alignment → Look for trends in pfams

- Cat has processed ~10 proteins
- Tried two different window choosing criteria for one protein
- In depth evaluation of pfams for one protein