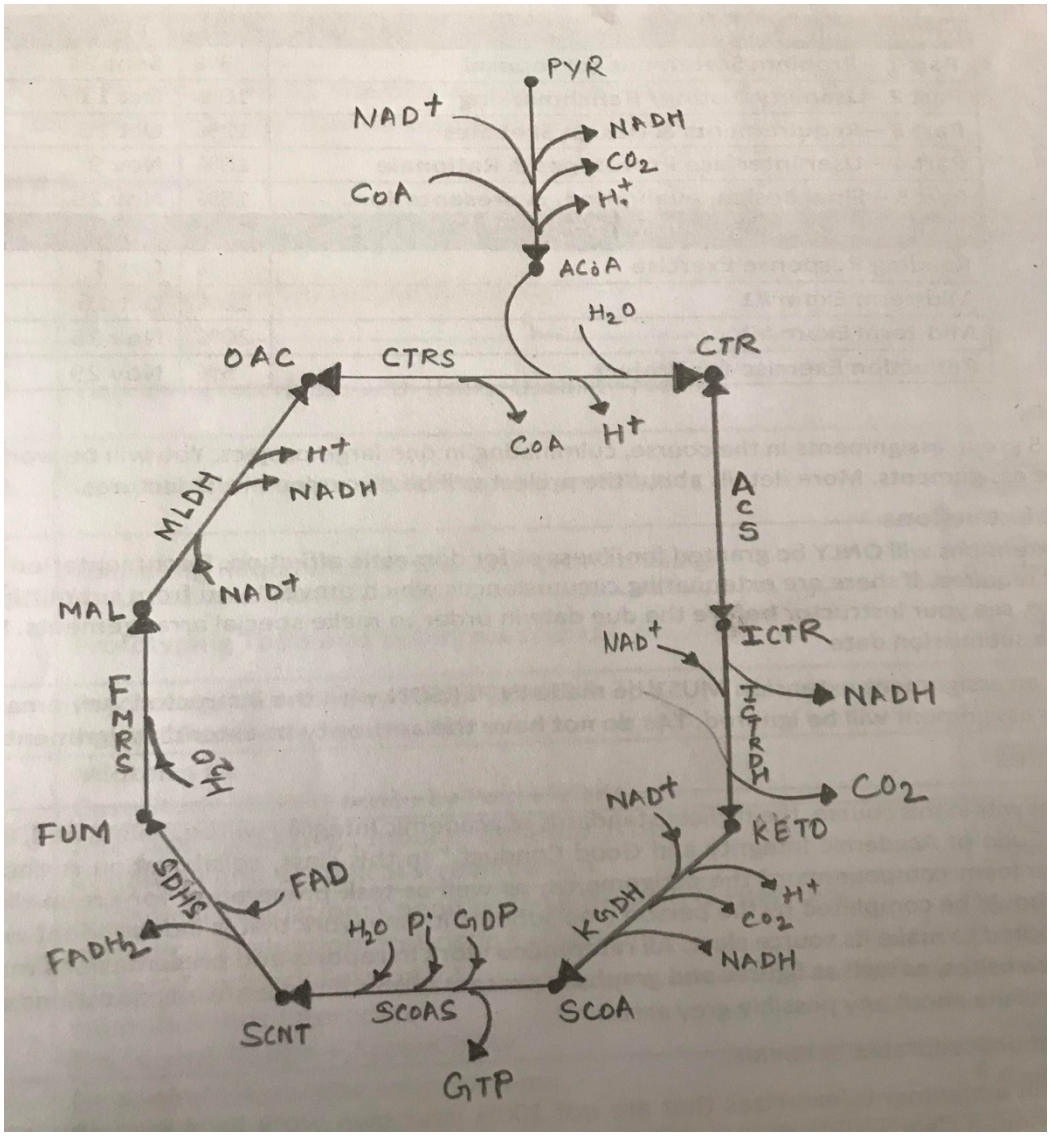
MBB440/839
Assignment #2
September 16 2015
Student name : Akshay Nanda
Student number: 301215514
Due date September 16 2015 12am
Total marks : /20

Reconstruct the TCA cycle pathway for E.coli, (limit the reconstruction from citrate to succinate) including , the S matrix (connectivity matrix, stoichiometric matrix). Make a network representation of the TCA cycle + three tables (20 marks)

i) Make a network representation of the TCA cycle (connectivity graph)



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ii) Make the table containing enzyme name Abbreviation with intermediates and cofactor (for the column) (order the compounds in three groups intermediate, cofactors, inorganic compounds for the rows).

Compounds and abbreviation table (table 2.1)

#	abbreviation	intermediates and cofactors
intermediates		
ex:1	Gluc	Glucose
	pyr	Pyruvate
	A-CoA	Acetyl CoA
	OAC	Oxaloacetae
	CTR	Citrate
	I - CTR	Isocitrate
	KETO	a-ketoglutarate
	SCOA	succinyl CoA
	FUM	Fumerate
	MAL	Malate
	COA	Co Enzyme A
co-factors		
	NAD	Nicotinamide Adenosine Dinulceotide (reduced)
	NADH	Nicotinamide Adenosine Dinulceotide (oxidized)
	GDP	Guanosine Di Phosphate
	GTP	Guanosine Tri Phosphate
	FAD	Flavin Adenine Dinulceotide (Reduced)
	FADH2	Flavin Adenine Dinulceotide (oxidized)
inorganic components		
	H2O	water
	H+	Hydrogn Ion (+)
	Pi	Inorganic Phosphate

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iii) Make the table enzyme abbreviation with elemental balanced reactions (for the column).

Enzyme/transporters -abbreviations and chemical reactions (Table 2.2)			
#	Abbreviation	Enzymes/transporters/load	Elementally balanced reactions
reactions			
ex:1	*ex:HK*	ex:Hexokinase	ex: gluc + ATP -> G6P + ADP + H+
	CtrSyn	Citrate Synthase	A-CoA + O- Ace -> Ctr + HS-CoA + H+
	ACS	Aconitase	Ctr -> i-Ctr
	ICTRDH	isocitrate Dehydrogenase	i-Ctr+ NAD+ + H+ -> CO2 + NADH + a-KtGlu
	KGDH	a-Ketoglutarate Dehydrogenase Complex	HS-CoA + NAD+ -> CO2 + suc-CoA + NADH + H+
	SCoAS	Succinyl - CoA Synthtase	-CoA + H2O + Pi + GDP -> GTP +Suc + HS-CoA
	SDHS	Succinate Dehydrogenase	SucN + FAD -> FADH2 + Fmrt
	FMRS	Fumerase	FumRt + H2O -> Mal
	MLDH	Malate Dehydrgenase	Mal + NaD+ -> NaDH + H+ + OxaAc
primary input			
	Pyr	Pyruvate	-> pyr
	A-CoA	Acetyl CoA	->ACOA
primary output/export			
	CO2	Carbon Dioxide	CO2 -->
Phosphate Nucleotide Metabolism			
	NAD	otinamide Adenosine Dinulceotide (reduced)	NADH -> NAD+ + H+
	FAD	Flavin Adenine Dinulceotide (Reduced)	FADH2 -> FAD + 2 H+
	NADH	otinamide Adenosine Dinulceotide (oxidixed)	NAD+ -> NADH + H+
	FADH2	Flavin Adenine Dinulceotide (Reduced)	FAD + 2H+ -> FADH
Cofactors			
	GTP	Adenosine Tri-Phosphate	GDP + Pi + H+ -> GTP + H2O
	GDP	Adenosine DI-Phosphate	GTP + H2O -> GDP + Pi + H +
inorganic			
	H+	Hydrogen Cation	<--> H+
	Pi	Inorganic Phosphate	-> Pi
	H2O	Water	<--> H20

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iv) make the connectivity matrix (Stoichiometry matrix) with the columns (reaction, nucleotide metabolism, primary export, co-factors, primary inputs, inorganic compounds IF NECESSARY (similar to figure 2.2 textbook). on the left draw the network wih input output, on the right the stoichiometry matrix refer to figure 2.2 as example

	CtrSyn	ACS	*ICTRDH*	KGDH	SCoAS	*SDHS*	FMRS	MLDH		Pyr	A-CoA		CO2	NADH	FADH2	GTP		H+	H2O
pyr	0	0	0	0	0	0	0	0		1	0		0	0	0	0		0	0
A-CoA	-1	0	0	0	0	0	0	0		0	1		0	0	0	0		0	0
CTR	1	-1	0	0	0	0	0	0		0	0		0	0	0	0		0	0
OAC	-1	0	0	0	0	0	0	1		0	0		0	0	0	0		0	0
I - CTR	0	1	-1	0	0	0	0	0		0	0		0	0	0	0		0	0
KETO	0	0	1	-1	0	0	0	0		0	0		0	0	0	0		0	0
SCOA	0	0	0	1	-1	0	0	0		0	0		0	0	0	0		0	0
SCNT	0	0	0	0	1	-1	0	0		0	0		0	0	0	0		0	0
FUM	0	0	0	0	0	1	-1	0		0	0		0	0	0	0		0	0
MAL	0	0	0	0	0	0	1	0		0	0		0	0	0	0		0	0
COA	1	0	0	0	0	0	0	0		0	0		0	0	0	0		0	0
CO2	0	0	1	0	0	0	0	0		0	0		-1	0	0	0		0	0
NAD	0	0	-1	-1	0	0	0	-1		0	0		0	-1	0	0		0	0
NADH	0	0	1	1	0	0	0	1		0	0		0	1	0	0		0	0
GDP	0	0	0	0	-1	0	0	0		0	0		0	0	0	-1		0	0
GTP	0	0	0	0	1	0	0	0		0	0		0	0	0	1		0	0
FAD	0	0	0	0	0	-1	0	0		0	0		0	0	-1	0		0	0
FADH2	0	0	0	0	0	1	0	0		0	0		0	0	1	0		0	0
H2O	-1	0	0	0	-1	0	-1	0		0	0		0	0	0	1		0	0
H+	1	0	0	1	0	0	0	1		0	0		0	-1	-1	-1		-1	1
Pi	0	0	0	0	-1	0	0	0		0	0		0	0	0	-1		0	0

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