Barituziga Banuna
CHEME 7770
4/12/2020

PROBLEM SET 3

PART A

Based on the reactions found on KEGG a stoichiometric matrix was formed using all the species contained in the reactions as well as boundary transport species. The fifth reaction EC# 1.14.13.39 was composed of a multi-step reaction with an intermediate that is completely consumed. The step reactions are RN R00558 & RN R00111. Based on what was provided the reaction is not balanced, to balance it we simply need two R00558 reactions for each R00111. Adding the reaction steps together then recovers the accurate RN 00557 described in EC 1.14.13.39. The full STOIC matrix is shown below along with the corrected matrix that does not include the intermediate species.

		R01954	R01086	R00551	R01398	R00557	R00557	R00558	R00558	R00111	*Carbamoyl Phosphate*	*Aspartate*	*Fumarate*	*Urea*	*ATP*	*AMP*	*Diphosphate*	*Orthophosphate*	*O2*	*NADPH*	*H+*	*NO*	NADP+	*H2O*	*H2O*
		v1	v2	v3	v4	v5_for	v5_rev	v5_1_for	v5_1_for_adj	v5_2_for	b1	b2	b3	b4	b5	b6	b7	b8	b9	b10	b11	b12	b13	b14_for	b14_rev
1	Carbamoyl Phosphate	0	0	0	-1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	Citrulline	-1	0	0	1	2	-2	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	Aspartate	-1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
4	Arginosuccinate	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	Fumarate	0	1	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0
6	Arginine	0	1	-1	0	-2	2	-1	-2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	Orinithine	0	0	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	ATP	-1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
9	Urea	0	0	1	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
10	Orthophosphate	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0
11	AMP	1	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0
12	Diphosphate	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0
13	NO	0	0	0	0	2	-2	0	0	2	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0
14	O2	0	0	0	0	-4	4	-1	-2	-2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
15	H+	0	0	0	0	-3	3	-1	-2	-1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
16	NADPH	0	0	0	0	-3	3	-1	-2	-1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
17	NADP+	0	0	0	0	3	-3	1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0
18	H2O	0	0	-1	0	4	-4	1	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	1
19	Hydroxyarginine	0	0	0	0	0	0	1	2	-2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

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		R01954	R01086	R00551	R01398	R00557	R00557	*Carbamoyl Phosphate*	*Aspartate*	*Fumarate*	*Urea*	*ATP*	*AMP*	*Diphosphate*	*Orthophosphate*	*O2*	*NADPH*	*H+*	*NO*	NADP+	*H2O*	*H2O*
		v1	v2	v3	v4	v5_for	v5_rev	b1	b2	b3	b4	b5	b6	b7	b8	b9	b10	b11	b12	b13	b14_for	b14_rev
1	Carbamoyl Phosphate	0	0	0	-1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	Citrulline	-1	0	0	1	2	-2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	Aspartate	-1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
4	Arginosuccinate	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	Fumarate	0	1	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0
6	Arginine	0	1	-1	0	-2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	Orinithine	0	0	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	ATP	-1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
9	Urea	0	0	1	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
10	Orthophosphate	0	0	0	1	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0
11	AMP	1	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0
12	Diphosphate	1	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0
13	NO	0	0	0	0	2	-2	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0
14	O2	0	0	0	0	-4	4	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
15	H+	0	0	0	0	-3	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
16	NADPH	0	0	0	0	-3	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
17	NADP+	0	0	0	0	3	-3	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0
18	H2O	0	0	-1	0	4	-4	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	1

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PART B

To check to see the reactions are balanced we need to perform an atom balance of the metabolites. The table for constructing the ATOM matrix is below.

		C	H	N	O	P	S
1	**Carbamoyl Phosphate**	1	4	1	5	1	0
2	**Citrulline**	6	13	3	3	0	0
3	**Aspartate**	4	7	1	4	0	0
4	**Arginosuccinate**	10	18	4	6	0	0
5	**Fumarate**	4	4	0	4	0	0
6	**Arginine**	6	14	4	2	0	0
7	**Orinithine**	5	12	2	2	0	0
8	**ATP**	10	16	5	13	3	0
9	**Urea**	1	4	2	1	0	0
10	**Orthophosphate**	0	3	0	4	1	0
11	**AMP**	10	14	5	7	1	0
12	**Diphosphate**	0	4	0	7	2	0
13	**NO**	0	0	1	1	0	0
14	**O2**	0	0	0	2	0	0
15	**H+**	0	1	0	0	0	0
16	**NADPH**	21	30	7	17	3	0
17	**NADP+**	21	29	7	17	3	0
18	**H2O**	0	2	0	1	0	0

This is crossed with the STOIC matrix in the equation E = transpose(ATOM) X STOIC. If the values for the E are 0 then they are balanced. If not, they need to be adjusted. When running the matrix through my Julia program the resultant E was:

Reaction Set

[0 0 0 0 0 0; 0 0 0 0 0 0; 0 0 0 0 0 0; 0 0 0 0 0 0; 0 0 0 0 0 0; 0 0 0 0 0 0]

Transport Set

[1 4 -4 -1 10 -10 0 0 0 21 0 0 -21 0 0; 4 7 -4 -4 16 -14 -4 -3 0 30 1 0 -29 -2 2; 1 1 0 -2 5 -5 0 0 0 7 0 -1 -7 0 0; 5 4 -4 -1 13 -7 -7 -4 2 17 0 -1 -17 -1 1; 1 0 0 0 3 -1 -2 -1 0 3 0 0 -3 0 0; 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]

Stoichiometric Matrix

[0 0 0 0 0 0 1 4 -4 -1 10 -10 0 0 0 21 0 0 -21 0 0; 0 0 0 0 0 0 4 7 -4 -4 16 -14 -4 -3

0 30 1 0 -29 -2 2; 0 0 0 0 0 0 1 1 0 -2 5 -5 0 0 0 7 0 -1 -7 0 0; 0 0 0 0 0 0 5 4 -4 -1 13 -7 -7 -4 2 17 0 -1 -17 -1 1; 0 0 0 0 0 0 1 0 0 0 3 -1 -2 -1 0 3 0 0 -3 0 0; 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]

The values for the reaction set are 0 indicating that they are balanced. The transport values are no not though.

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PART C

The optimization of the Urea flux was completed using a Julia code that references the Flux.jl code provided by the Varner lab which was then modified to solve the problem in our conditions. The output of the Solve.jl script is below. The max flux of Urea was 1.242 mmol/gDW-hr.

(-1.242, [1.242, 1.242, 1.242, 1.242, 0.0, 0.0, 1.242, 1.242, 1.242, 1.242 … 1.242, 1.242, 1.242, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.242], [0.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0 … 0.0, 0.0, 0.0, 0.5, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0], 0, 5)