

b.)

-There are 7 extreme pathways. The only reaction that produces urea is associated with v_3 , which corresponds to column 3 of the P matrix. You can see that 2 out of the 7 produce Urea.

-The reaction frequency is in red next to each of the 19 reactions below. Reaction frequency is computed by looking at matrix P and using the formula: (number of nonzero values for a reaction column) \div (total number of extreme pathways) for each column. The columns go from 1-19— v_1 is column 1 and b_{14} is column 19.

v_1 ,ATP+L-citrulline+L-Aspartate,AMP+diphosphate+2-(Nomega-L-arginino)succinate,false" 0.286

" v_2 ,2-(Nomega-L-arginino)succinate,L-arginine+fumarate,false" 0.286

" v_3 ,L-arginine+H₂O,Urea+L-ornithine,false" 0.286

" v_4 ,L-ornithine+carbamoylphosphate,L-citrulline+phosphate,false" 0.286

" v_5 ,2*L-arginine+3*NADPH+3*H+4*O₂,2*L-citrulline+2*nitricoxide+3*NADP+4*H₂O,true" 0.143

" B_1 , \emptyset ,carbamoylphosphate,false" 0.286

" b_2 , \emptyset ,L-Aspartate,false" 0.286

" B_3 ,fumarate, \emptyset ,false" 0.286

" b_4 ,Urea, \emptyset ,false" 0.286

" b_5 , \emptyset ,H₂O,true" 0.143

" b_6 ,phosphate, \emptyset , true" 0.286

" b_7 ,diphosphate, \emptyset , true" 0.286

" b_8 ,AMP, \emptyset , false" 0.286

" b_9 , \emptyset , ATP,false" 0.286

" b_{10} ,NADPH, \emptyset , false" 0.143

" b_{11} ,H, \emptyset , false" 0.143

" b_{12} ,O₂, \emptyset , true" 0.143

" b_{13} , \emptyset , NADP,false" 0.143

"b_{14,∅}, nitricoxide,false" 0.143

c.)

To rank the connectivities of metabolites and reactions, I looked at the numbers on the diagonal for each reaction/metabolite—the higher the number, the more reactions a particular metabolite is in/the more metabolites a specific reaction has. The more reactions a metabolite is in, the higher the rank. The more metabolites in a specific reaction, the higher the rank. That is how the rankings below were determined.

RCA:

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julia> show(stdout, "text/plain", reaction_array)
19-element Vector{String}:
"v1,ATP+L-citrulline+L-Aspartate,AMP+diphosphate+2-(Nomega-L-arginino)succinate,false"
"v2,2-(Nomega-L-arginino)succinate,L-arginine+fumarate,false"
"v3,L-arginine+H2O,Urea+L-ornithine,false"
"v4,L-ornithine+carbamoylphosphate,L-citrulline+phosphate,false"
"v5,2*L-arginine+3*NADPH+3*H+4*O2,2*L-citrulline+2*nitricoxide+3*NADP+4*H2O,true"
"b1,∅,carbamoylphosphate,false"
"b2,∅,L-Aspartate,false"
"b3,fumarate,∅,false"
"b4,Urea,∅,false"
"b5,∅,H2O,true"
"b6,phosphate,∅, true"
"b7,diphosphate,∅, true"
"b8,AMP,∅, false"
"b9,∅, ATP,false"
"b10,NADPH,∅, false"
"b11,H,∅, false"
"b12,O2,∅, true"
"b13,∅, NADP,false"
"b14,∅, nitricoxide,false"
julia> show(stdout, "text/plain", RCA)
19×19 Matrix{Int64}:
 6  1  0  1  1  0  1  0  0  0  0  1  1  1  0  0  0  0  0
 1  3  1  0  1  0  0  1  0  0  0  0  0  0  0  0  0  0  0
 0  1  4  1  2  0  0  0  1  1  0  0  0  0  0  0  0  0  0
 1  0  1  4  1  1  0  0  0  0  1  0  0  0  0  0  0  0  0
 1  1  2  1  8  0  0  0  0  1  0  0  0  0  1  1  1  1  1
 0  0  0  1  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0
 1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0
 0  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0
 0  0  1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
 0  0  1  0  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0
 0  0  0  1  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0
 1  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0
 1  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0
 1  0  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0
 0  0  0  0  1  0  0  0  0  0  0  0  0  0  1  0  0  0  0
 0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  1  0  0  0
 0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  1  0  0
 0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  1  0
 0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  1
julia>

```

$v_5 > v_1 > v_3 = v_4 > v_2 > b_1 = b_2 = b_3 = b_4 = b_5 = b_6 = b_7 = b_8 = b_9 = b_{10} = b_{11} = b_{12} = b_{13} = b_{14}$
 MCA:

```

julia> show(stdout, "text/plain", species_array)
18-element Vector{String}:
"2-(Nomega-L-arginino)succinate"
"AMP"
"ATP"
"H"
"H2O"
"L-Aspartate"
"L-arginine"
"L-citrulline"
"L-ornithine"
"NADP"
"NADPH"
"O2"
"Urea"
"carbamoylphosphate"
"diphosphate"
"fumarate"
"nitricoxide"
"phosphate"
julia> show(stdout, "text/plain", MCA)
18x18 Matrix{Int64}:
 2  1  1  0  0  1  1  1  0  0  0  0  0  0  1  1  0  0
 1  2  1  0  0  1  0  1  0  0  0  0  0  0  1  0  0  0
 1  1  2  0  0  1  0  1  0  0  0  0  0  0  1  0  0  0
 0  0  0  2  1  0  1  1  0  1  1  1  1  0  0  0  1  0
 0  0  0  1  3  0  2  1  1  1  1  1  1  0  0  0  1  0
 1  1  1  0  0  2  0  1  0  0  0  0  0  0  1  0  0  0
 1  0  0  1  2  0  3  1  1  1  1  1  1  0  0  1  1  0
 1  1  1  1  1  1  1  3  1  1  1  1  1  0  1  1  0  1
 0  0  0  0  1  0  1  1  2  0  0  0  0  1  1  0  0  0  1
 0  0  0  1  1  0  1  1  0  2  1  1  1  0  0  0  0  1  0
 0  0  0  1  1  0  1  1  0  1  2  1  0  0  0  0  0  1  0
 0  0  0  1  1  0  1  1  0  1  1  2  0  0  0  0  0  1  0
 0  0  0  0  1  0  1  0  1  0  0  0  2  0  0  0  0  0  0
 0  0  0  0  0  0  0  1  1  0  0  0  0  2  0  0  0  0  1
 1  1  1  0  0  1  0  1  0  0  0  0  0  0  2  0  0  0  0
 1  0  0  0  0  0  1  0  0  0  0  0  0  0  0  2  0  0  0
 0  0  0  1  1  0  1  1  0  1  1  1  1  0  0  0  0  2  0
 0  0  0  0  0  0  0  1  1  0  0  0  0  1  0  0  0  0  2
julia>

```

"2-(Nomega-L-arginino)succinate"

"AMP"

"ATP"

"H"

"H2O"

"L-Aspartate"

"L-arginine"

"L-citrulline"

"L-ornithine"

"NADP"

"NADPH"

"O2"

"Urea"

"carbamoylphosphate"

"diphosphate"

"fumarate"

"nitricoxide"

"phosphate"

"H2O"= "L-arginine"= "L-citrulline">every other species (which all are equal in connectivity)

I do not see much of a correlation between extreme pathways and reaction connectivities. The reaction with the most connections (v5) is in the least number of extreme pathways (only 1). Unless that itself is a correlation and points towards that extreme pathway being the most likely of the bunch.