

Some applications of Elementary Modes

Sudip kundu

Department of Biophysics, Molecular Biology &
Bioinformatics

University of Calcutta
skbmbg@caluniv.ac.in

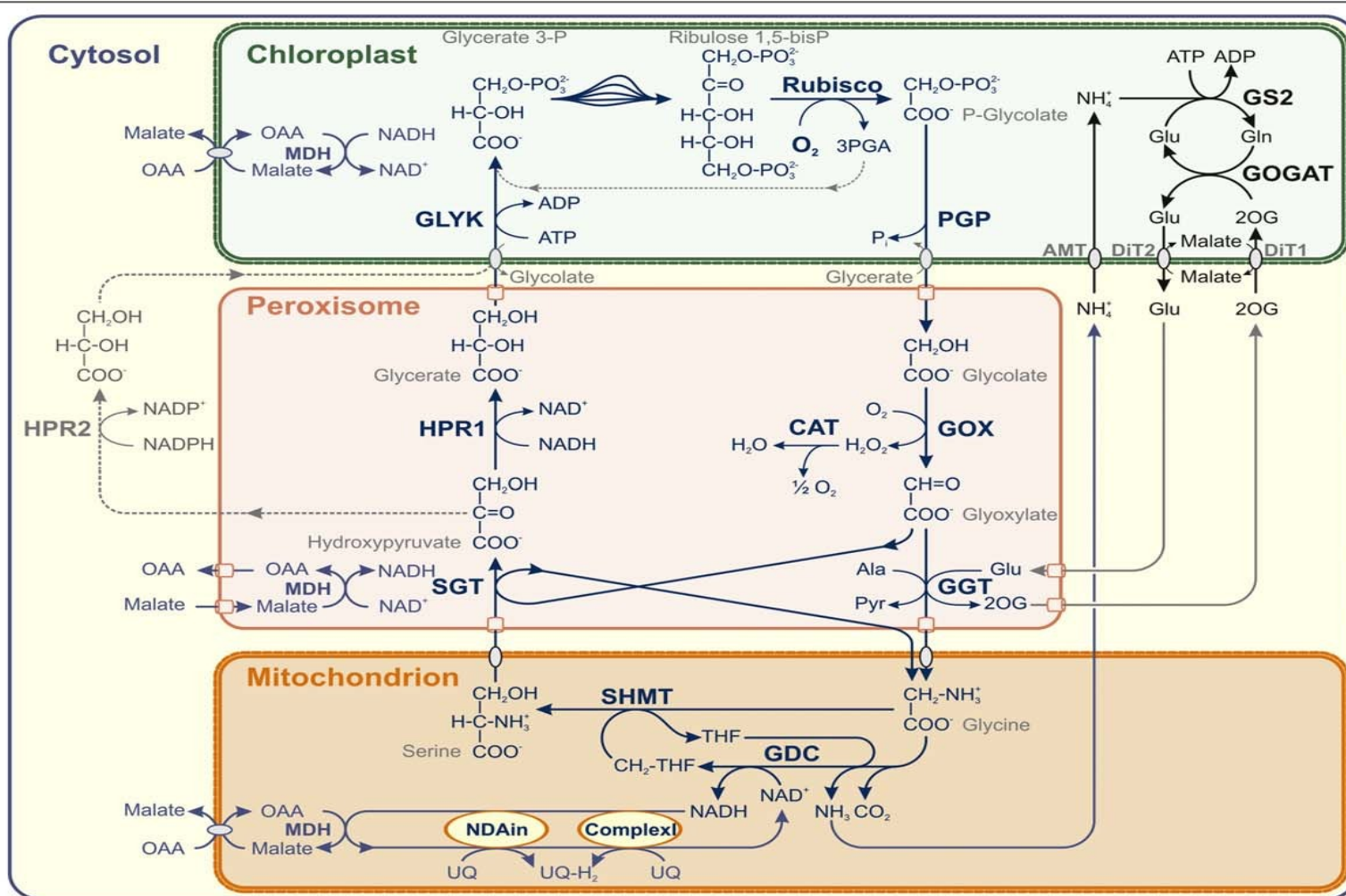
Just to remind you...

An elementary mode can be described as a minimal set of reactions that, at steady-state, catalyse some net reaction between input(s) and output(s) with a characteristic stoichiometry.

An elementary mode can be thought of as a minimal biochemical pathway, capable of operating independently from the rest of the system.

The complete metabolic capability of a given system is thus encapsulated by its elementary modes.

Photorespiration



per_RXN969:
 1/1 per_GLYCOLLATE + 1/1 "per_OXYGEN-MOLECULE"
 -> 1/1 "per_HYDROGEN-PEROXIDE" + 1/1 per_GLYOX

per_CATRXN: #####(added) (Water ignored)
 2/1 "per_HYDROGEN-PEROXIDE" -> 1/1 "per_OXYGEN-MOLECULE"

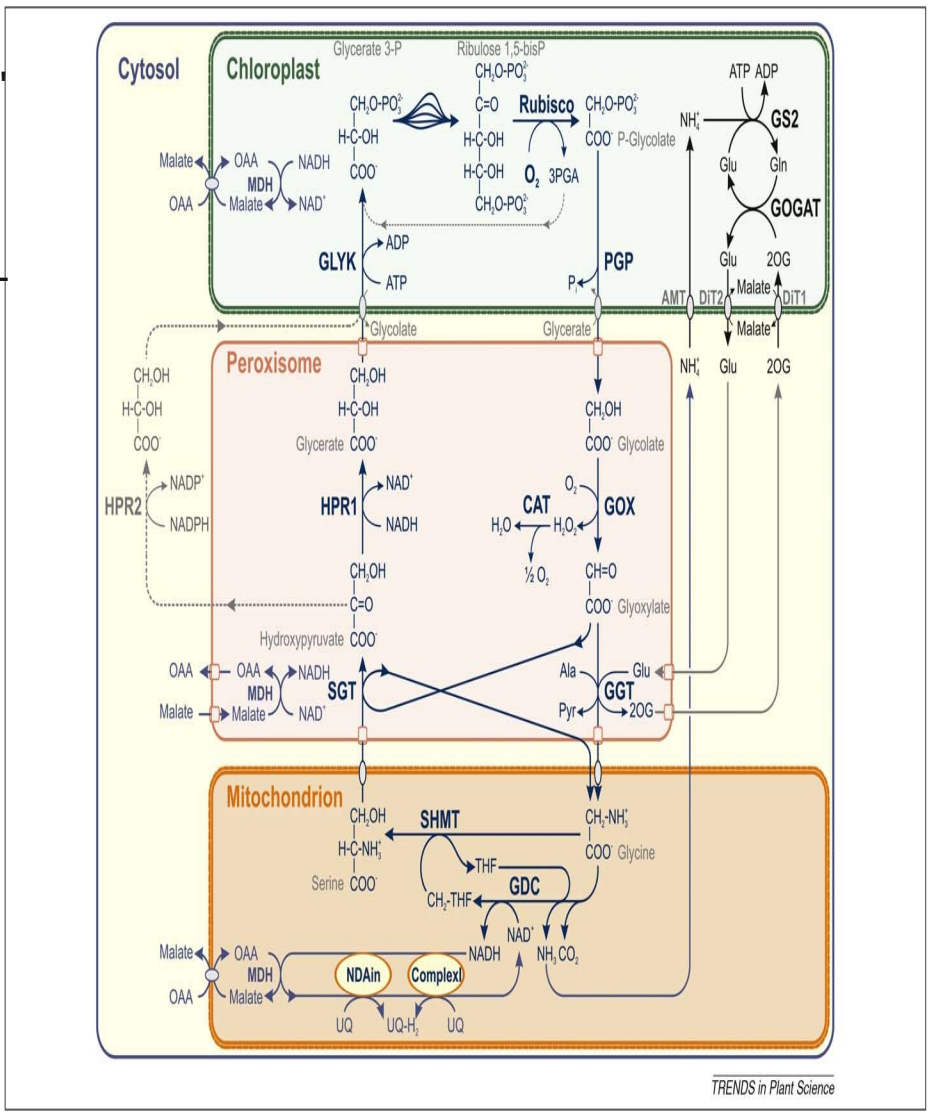
per_ALANINEGLYOXYLATEAMINOTRANSFERASERXN:
 1/1 "per_L-ALPHA-ALANINE" + 1/1 per_GLYOX -> 1/1
 per_PYRUVATE + 1/1 per_GLY

per_GLYCINEAMINOTRANSFERASERXN:
 1/1 per_GLT + 1/1 per_GLYOX -> 1/1 "per_2-KETOGLUTARATE" + 1/1 per_GLY

per_SERINEGLYOXYLATEAMINOTRANSFERASERXN:
 1/1 per_SER + 1/1 per_GLYOX -> 1/1 per_GLY + 1/1
 "per_OH-PYR"

per_GLYCERATEDEHYDROGENASERXN:
 1/1 per_NADH + 1/1 "per_OH-PYR" -> 1/1 per_NAD + 1/1
 per_GLYCERATE

per_MALATEDEHRXN:
 1/1 per_NAD + 1/1 per_MAL <> 1/1 per_NADH + 1/1
 per_OAA



#####

peroxisome_transporters

#####

per_OAA_tx:

per_OAA <> "OXALACETIC_ACID"

per_Mal_tx:

per_MAL <> "MAL"

per_OHPYR_tx:

"per_OH-PYR" -> "OH-PYR"

per_GLT_tx:

per_GLT <> "GLT"

per_2KETOGLUTARATE_tx:

"per_2-KETOGLUTARATE" <> "2-KETOGLUTARATE"

per_LALPHAALANINE_tx:

"per_L-ALPHA-ALANINE" <> "L-ALPHA-ALANINE"

per_PYRUVATE_tx:

per_PYRUVATE <> "PYRUVATE"

per_GLY_tx:

per_GLY <> "GLY"

per_SER_tx:

per_SER <> "SER"

per_OXYGENMOLECULE_tx:

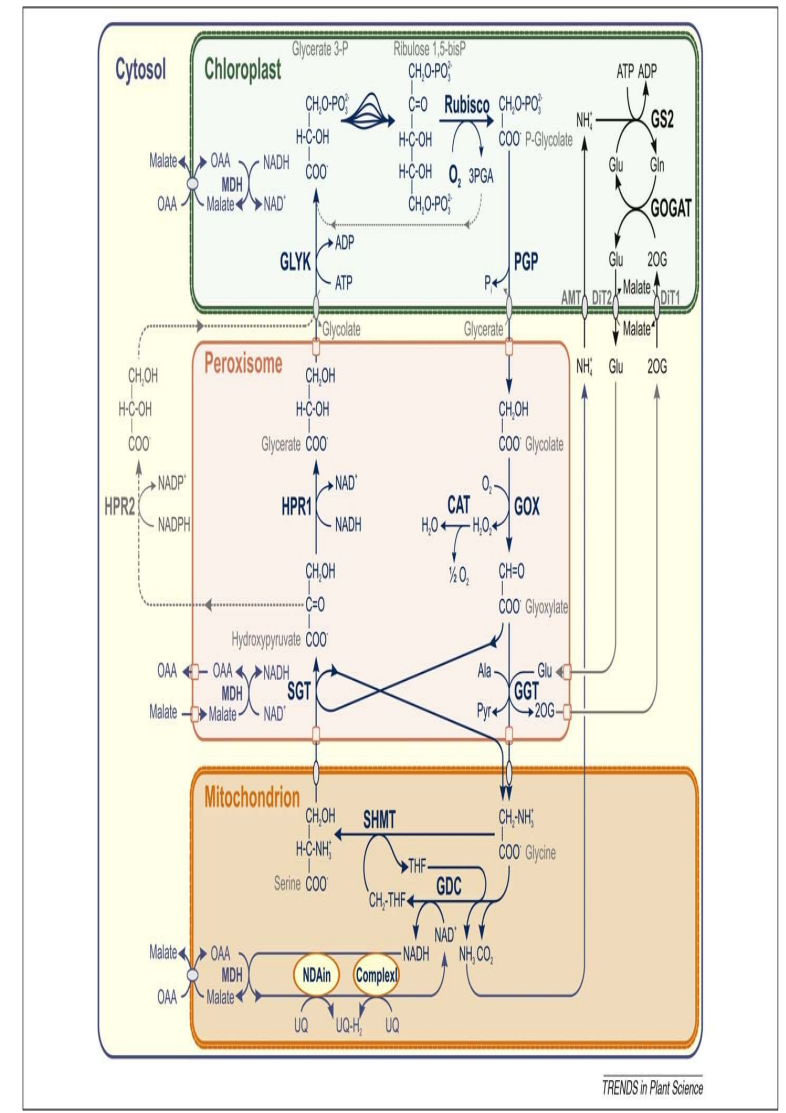
"per_OXYGEN-MOLECULE" <> "OXYGEN-MOLECULE"

per_GLYCOLLATE_tx:

per_GLYCOLLATE <> "GLYCOLLATE"

per_GLYCERATE_tx:

per_GLYCERATE <> "GLYCERATE"



Structural()

External("OXALACETIC_ACID","MAL","OH-PYR","GLT","2-KETOGLUTARATE","L-ALPHA-ALANINE","PYRUVATE","GLY","SER","OXYGEN-MOLECULE","GLYCOLLATE","GLYCERATE")

per_RXN969:

1/1 per_GLYCOLLATE + 1/1 "per_OXYGEN-MOLECULE" -> 1/1 "per_HYDROGEN-PEROXIDE" + 1/1 per_GLYOX

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per_CATRXN: #####(added) (Water ignored)

2/1 "per_HYDROGEN-PEROXIDE" -> 1/1 "per_OXYGEN-MOLECULE"

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per_ALANINEGLYOXYLATEAMINOTRANSFERASERXN:

1/1 "per_L-ALPHA-ALANINE" + 1/1 per_GLYOX -> 1/1 per_PYRUVATE + 1/1 per_GLY

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per_GLYCINEAMINOTRANSFERASERXN:

1/1 per_GLT + 1/1 per_GLYOX -> 1/1 "per_2-KETOGLUTARATE" + 1/1 per_GLY

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#####

Transport reactions

#

Elementary mode: 1/1 "MAL" + 1/1 "GLYCOLLATE" + 1/2 "OXYGEN-MOLECULE" + 1/1 "SER"
 -> 1/1 "GLYCERATE" + 1/1 "GLY" + 1/1 "OXALACETIC_ACID"

er_RXN969:

1/1 per_GLYCOLLATE + 1/1 "per_OXYGEN-MOLECULE" -> 1/1 "per_HYDROGEN-PEROXIDE"
 + 1/1 per_GLYOX

per_CATRXN: (Water ignored)

2/1 "per_HYDROGEN-PEROXIDE" -> 1/1 "per_OXYGEN-MOLECULE"

per_SERINEGLYOXYLATEAMINOTRANSFERASERXN

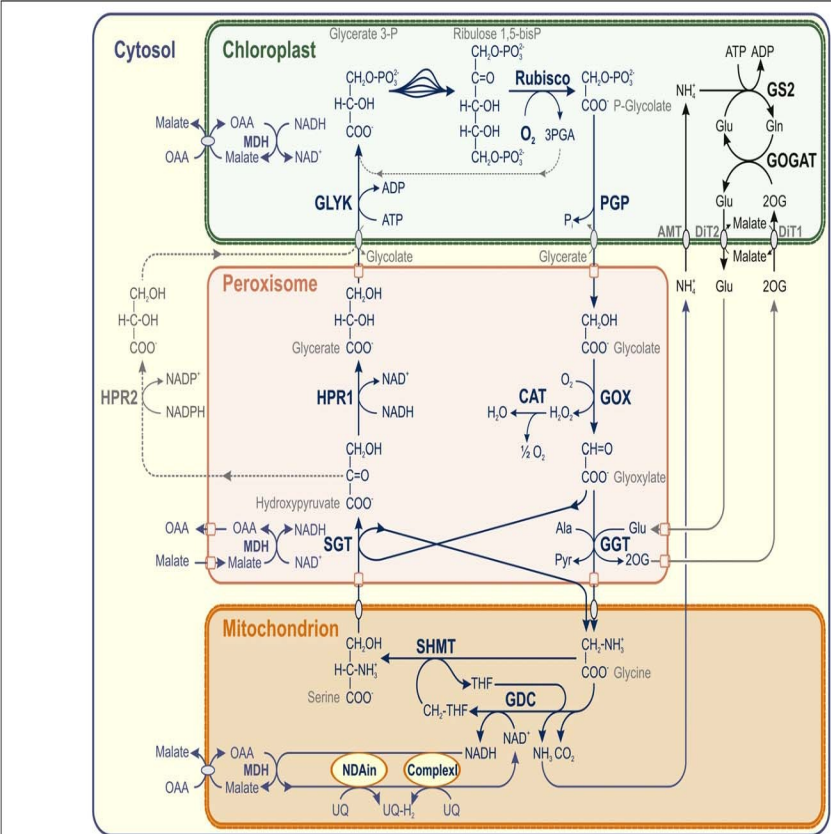
1/1 per_SER + 1/1 per_GLYOX -> 1/1 per_GLY + 1/1
 "per_OH-PYR"

per_GLYCERATEDEHYDROGENASERXN:

1/1 per_NADH + 1/1 "per_OH-PYR" -> 1/1 per_NAD
 + 1/1 per_GLYCERATE

per_MALATEDEHRXN:

1/1 per_NAD + 1/1 per_MAL <> 1/1 per_NADH + 1/1
 per_OAA



1/1 "GLYCOLLATE" + 1/1 "GLT" + 1/2 "OXYGEN-MOLECULE" -> 1/1 "2-KETOGLUTARATE" + 1/1 "GLY"

per_RXN969:

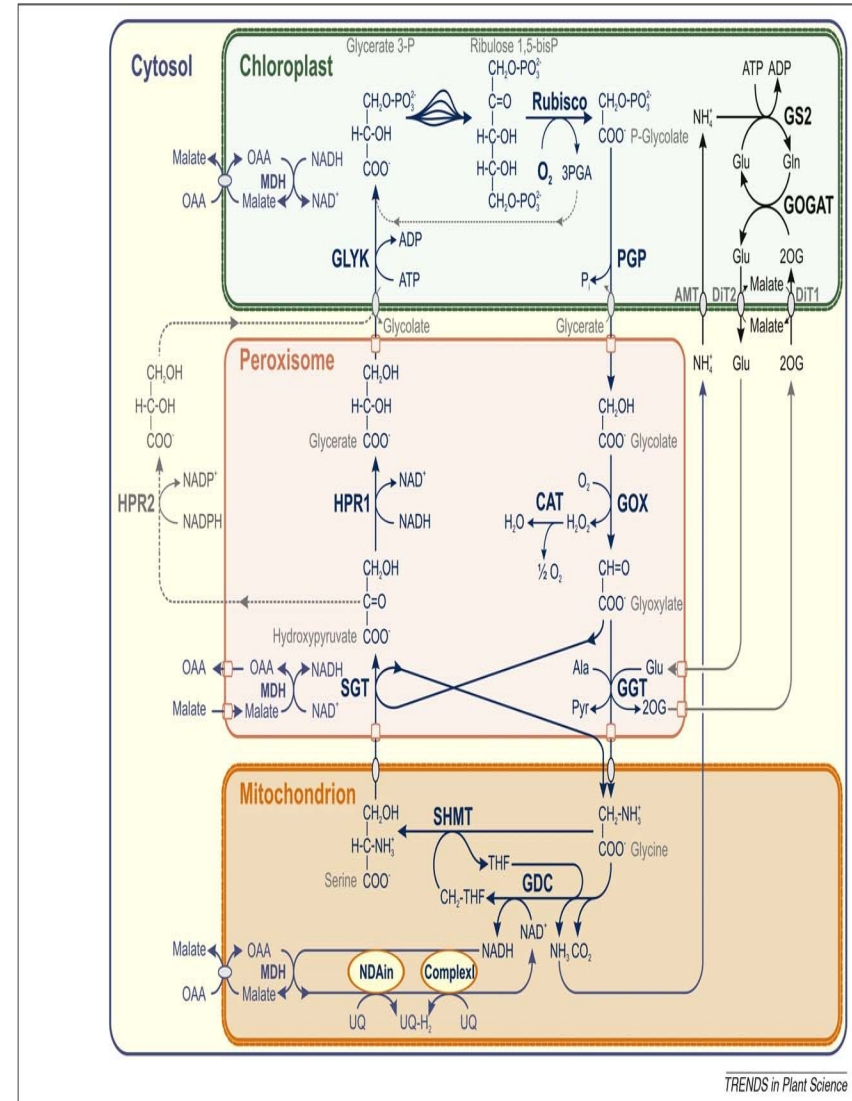
1/1 per_GLYCOLLATE + 1/1 "per_OXYGEN-MOLECULE" -> 1/1 "per_HYDROGEN-PEROXIDE" + 1/1 per_GLYOX

per_CATRNXN: (Water ignored)

2/1 "per_HYDROGEN-PEROXIDE" -> 1/1 "per_OXYGEN-MOLECULE"

per_GLYCINEAMINOTRANSFERASERXN:

1/1 per_GLT + 1/1 per_GLYOX -> 1/1 "per_2-KETOGLUTARATE" + 1/1 per_GLY



1/1 "SER" + 1/1 "GLYCOLLATE" + 1/2 "OXYGEN-MOLECULE" -> 1/1 "GLY" + 1/1 "OH-PYR"

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per_RXN969:

1/1 per_GLYCOLLATE + 1/1 "per_OXYGEN-MOLECULE" -> 1/1 "per_HYDROGEN-PEROXIDE" + 1/1 per_GLYOX

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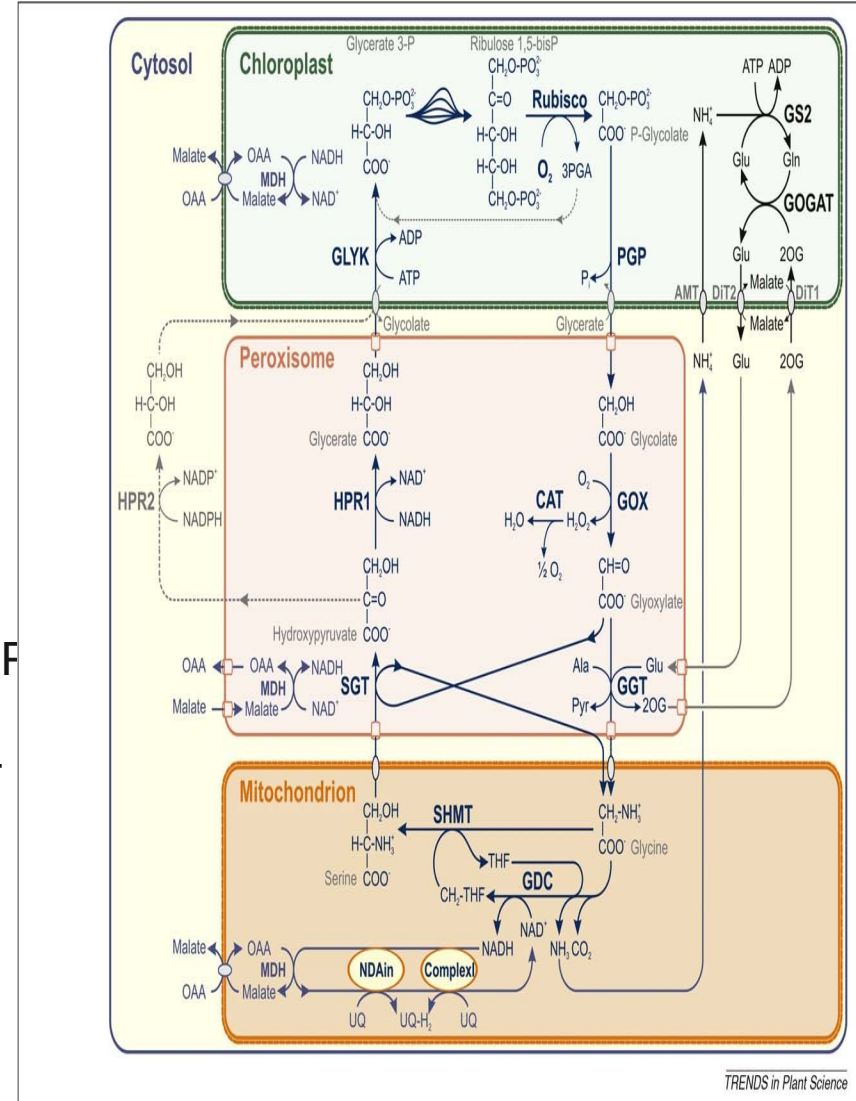
per_CATRXN: (Water ignored)

2/1 "per_HYDROGEN-PEROXIDE" -> 1/1 "per_OXYGEN-MOLECULE"

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per_SERINEGLYOXYLATEAMINOTRANSFERASEFXN:

1/1 per_SER + 1/1 per_GLYOX -> 1/1 per_GLY + 1/1 "per_OH-PYR"

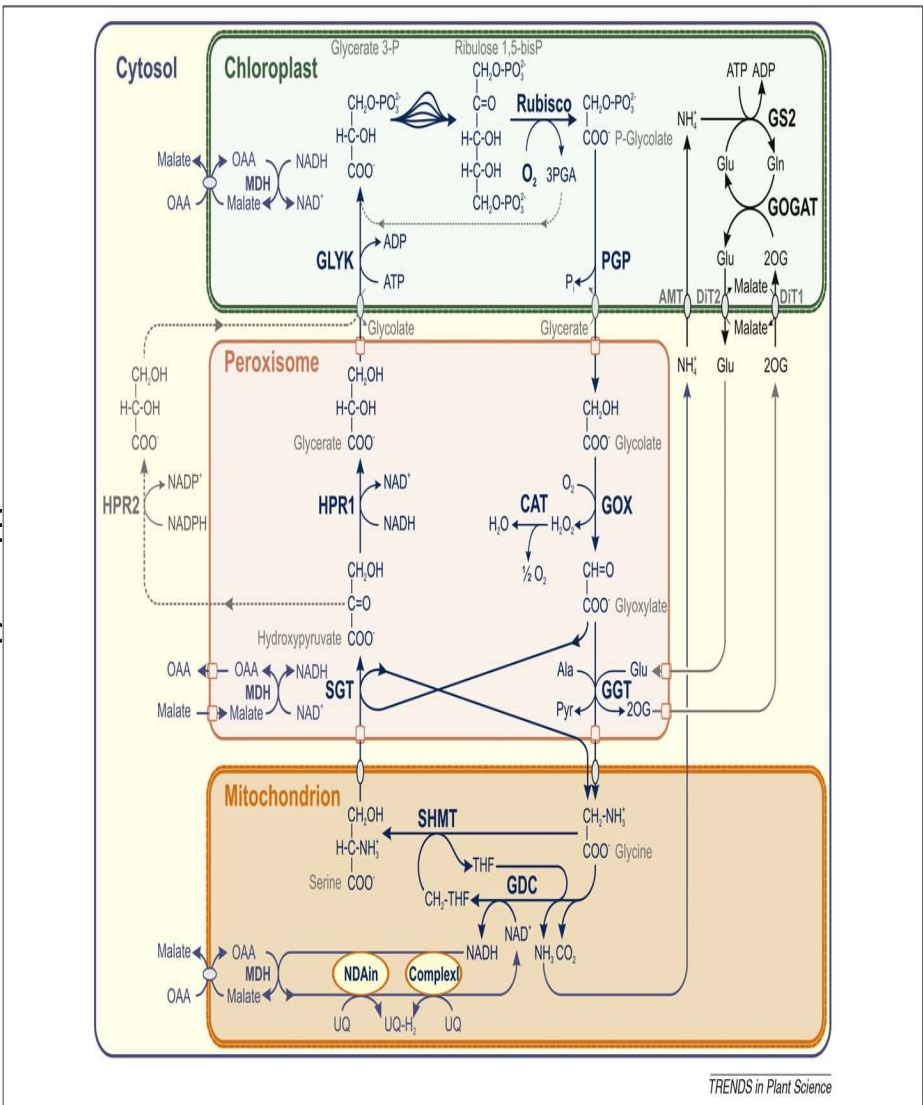


EIMo_3:
 1/1 "GLYCOLLATE" + 1/1 "L-ALPHA-ALANINE" + 1/2 "OXYGEN-MOLECULE" -> 1/1
 "PYRUVATE" + 1/1 "GLY"

per_RXN969:
 1/1 per_GLYCOLLATE + 1/1 "per_OXYGEN-MOLECULE" -> 1/1 "per_HYDROGEN-PEROXIDE"
 1/1 per_GLYOX

per_CATRNX: (Water ignored)
 2/1 "per_HYDROGEN-PEROXIDE" -> 1/1
 "per_OXYGEN-MOLECULE"

per_ALANINEGLYOXYLATEAMINOTRANSFERASE
 N:
 1/1 "per_L-ALPHA-ALANINE" + 1/1 per_GLYOX ->
 1/1 per_PYRUVATE + 1/1 per_GLY



Elementary modes in Peroxisome compartment

EIMo_0:

1/1 "MAL" + 1/1 "GLYCOLLATE" + 1/2 "OXYGEN-MOLECULE" + 1/1 "SER" -> 1/1
"GLYCERATE" + 1/1 "GLY" + 1/1 "OXALACETIC_ACID"

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EIMo_1:

1/1 "GLYCOLLATE" + 1/1 "GLT" + 1/2 "OXYGEN-MOLECULE" -> 1/1 "2-KETOGLUTARATE"
+ 1/1 "GLY"

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EIMo_2:

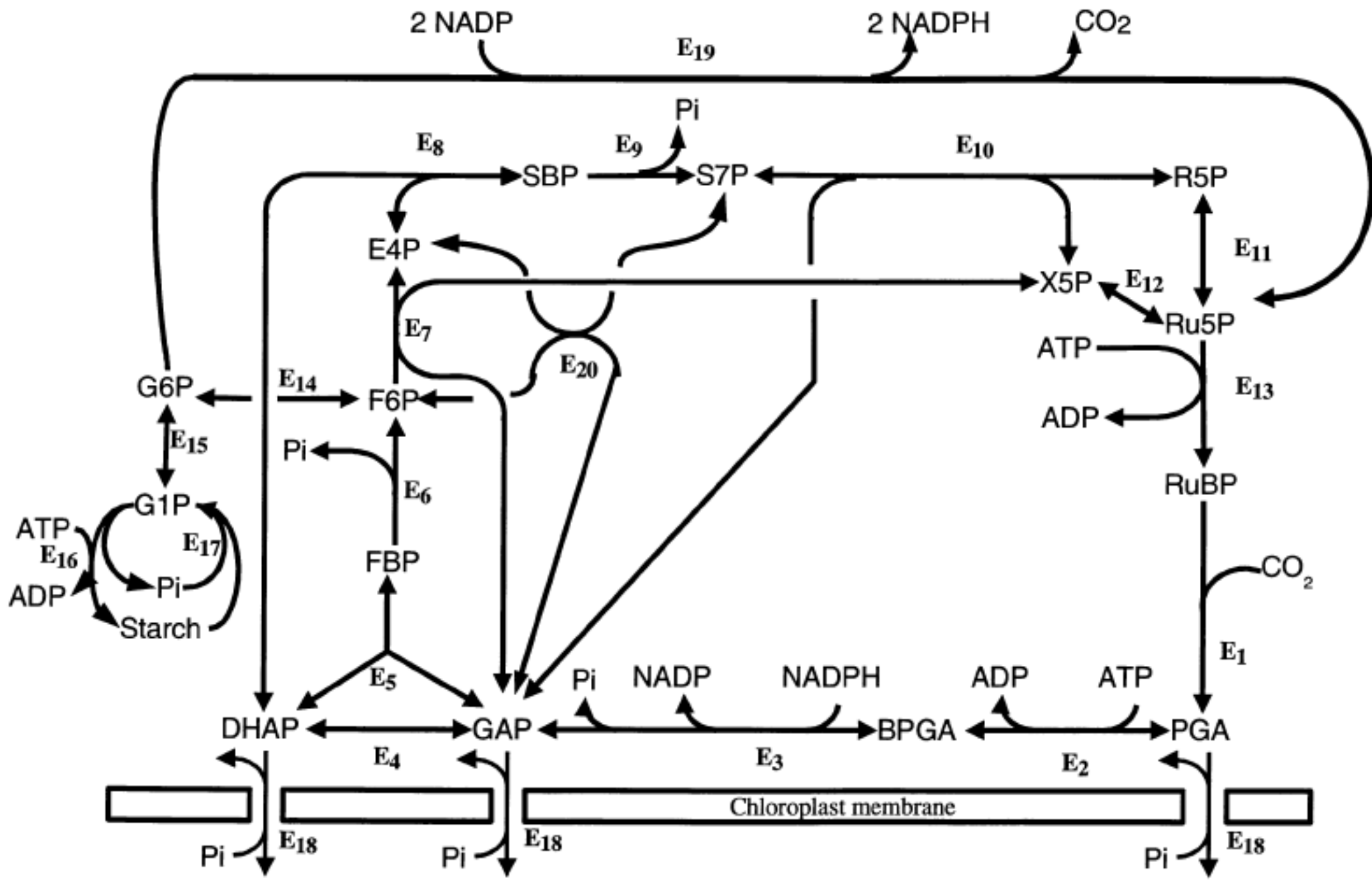
1/1 "SER" + 1/1 "GLYCOLLATE" + 1/2 "OXYGEN-MOLECULE" -> 1/1 "GLY" + 1/1 "OH-PYR"

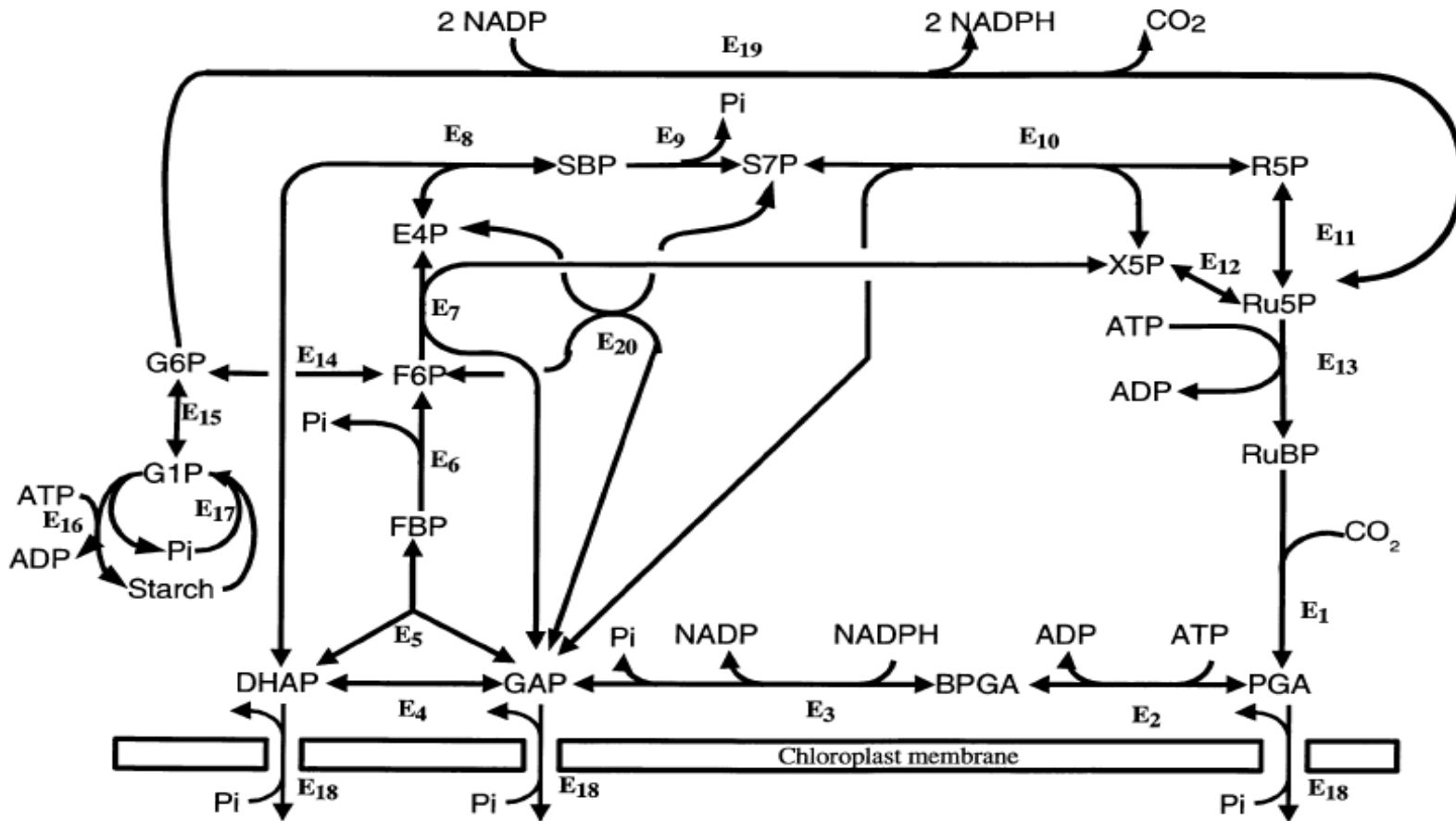
~

EIMo_3:

1/1 "GLYCOLLATE" + 1/1 "L-ALPHA-ALANINE" + 1/2 "OXYGEN-MOLECULE" -> 1/1
"PYRUVATE" + 1/1 "GLY"

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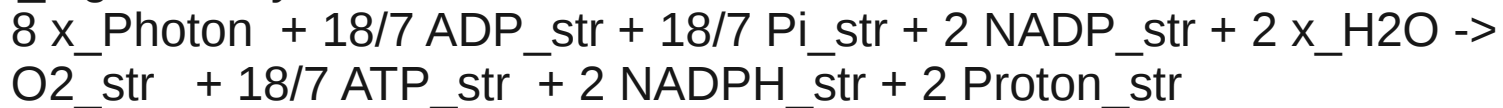


chl_LightCyc:



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chl_LightNonCyc:



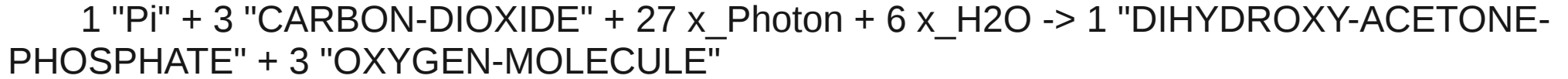
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EIMo_0:



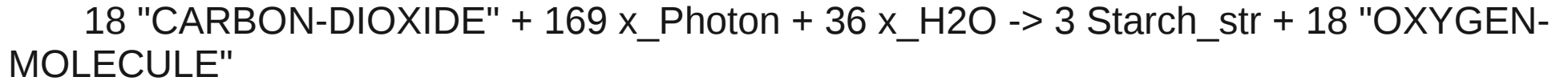
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EIMo_1:



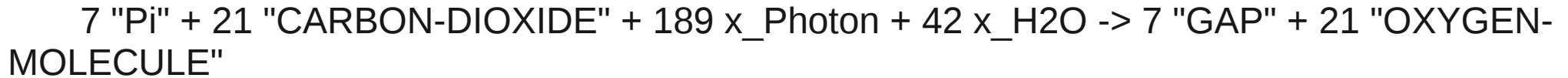
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EIMo_2:



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EIMo_3:



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Product	Photon needed (1 unit C-fixation)	Photon needed (1 unit product)		
PGA	7.89	23.66		
GAP	9.0	27.0		
DHAP	9.0	27.0		
Starch	9.38	56.3		

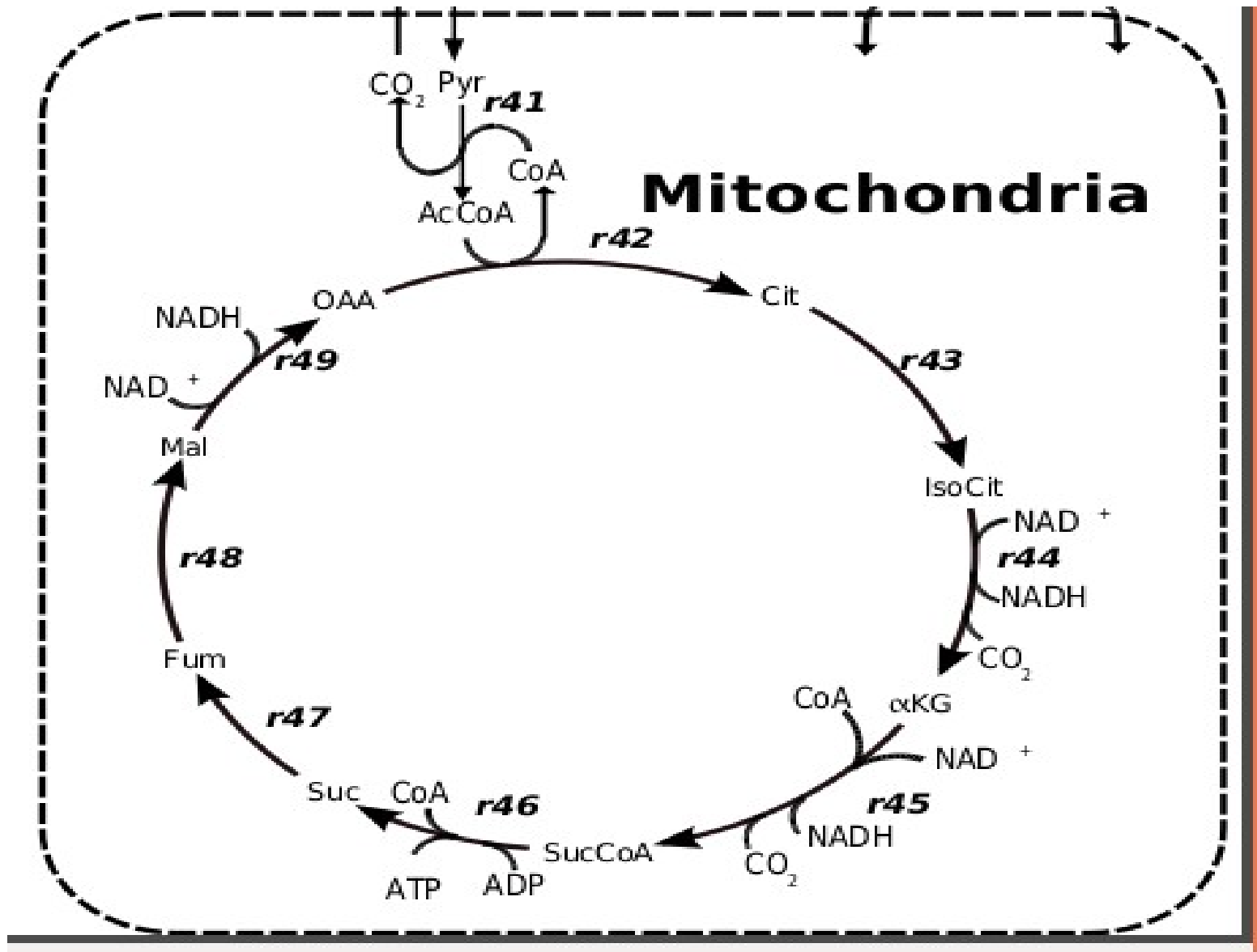
PR:
2 "GLYCOLLATE" <> 1 "GLYCERATE" + "CARBON-DIOXIDE" + x_PR

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156 x_Photon + 30 x_H2O -> 6 x_PR + 3 "OXYGEN-MOLECULE"

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{'chl_Ald1': 42, 'chl_Ald2': 42, 'chl_X5Piso': 84,
'chl_RuBPOxid': 84, 'chl_TKL1': 42, 'chl_TKL2': 42,
'chl_Ru5Pk': 126, 'PR': 42, 'chl_TPI': 84, 'chl_FBPase': 42,
'chl_SBPase': 42, 'chl_R5Piso': 42, 'chl_LightNonCyc': 105,
'chl_glycollate_tx': 84, 'chl_GLY3KIN': 42, 'chl_GPH': 84,
'chl_CO2_tx': 42, 'chl_PGK': 210, 'chl_glycerate_tx': 42,
'chl_Rubisco': 42, 'chl_LightCyc': 18, 'chl_G3Pdh': 210,
'chl_O2_tx': -21}



EM for Mitochondria

TCA cycle + mitochondrial reactions involved with photorespiration (described in 1st slide) + ETC

Making CO₂ unidirectional (it can go out only from mit)

Total EM=197

Metabolites/Transporter	Consumed	Produced
2-Ketoglutarate	26	91
SUC	87	31
CIT	42	38
FUM	27	49
MAL	30	46
OXALACETIC_ACID	85	25
Pyruvate	117	0
CARBON-DIOXIDE	0	119
OXYGEN-MOLECULE	183	
ATP	8 (all involved SUC as substrate)	117
ADP	117	8
SER	0	24

Different energy producing EM with same composition

- a. 1 WATER + 2 GLY + 1 OXALACETIC_ACID + 1 PROTON -> 1 SER + 1 MAL + 1 CARBON-DIOXIDE + 1 AMMONIA
- b. 2 GLY + 1 OXALACETIC_ACID + 1 PROTON -> 1 FUM + 1 AMMONIA + 1 CARBON-DIOXIDE + 1 SER
- c. 4 GLY + 1 OXYGEN-MOLECULE + 2 Pi + 2 ADP -> 2 SER + 2 CARBON-DIOXIDE + 2 ATP + 2 AMMONIA
- d. 4 GLY + 1 OXYGEN-MOLECULE + 5 Pi + 5 ADP -> 2 SER + 2 CARBON-DIOXIDE + 5 ATP + 2 AMMONIA

c. {'mit_amonia_tx': 2, 'mit_AOX': 1, '**mit_Complex_V**': 2, 'mit_GCVMULTI': 2, 'mit_SER_GLY_tx': 2, 'mit_GLYOHMETRANS': 2, 'mit_ATP_tx': 2, 'mit_CO2_tx': 2, '**mit_Complex_I**': 2, 'mit_O2_tx': 1}

d. {'mit_amonia_tx': 2, 'mit_CO2_tx': 2, '**mit_Complex_III**': 2, '**mit_Complex_V**': 5, 'mit_GCVMULTI': 2, 'mit_SER_GLY_tx': 2, 'mit_GLYOHMETRANS': 2, 'mit_ATP_tx': 5, '**mit_Complex_I**': 2, 'mit_O2_tx': 1, '**mit_Complex_IV**': 1}

3 PYRUVATE + 3 OXYGEN-MOLECULE + 6 Pi + 3 OXALACETIC_ACID + 6 ADP -> 3 WATER + 6 PROTON + 6 CARBON-DIOXIDE + 3 2-KETOGLUTARATE + 6 ATP

3 PYRUVATE + 3 OXYGEN-MOLECULE + 15 Pi + 3 OXALACETIC_ACID + 15 ADP -> 3 WATER + 6 PROTON + 6 CARBON-DIOXIDE + 3 2-KETOGLUTARATE + 15 ATP

1st Case: {'mit_CO2_tx': 6, 'mit_AconDHatase': 3, 'mit_Pyr_tx': 3, '**mit_Complex_V': 6**, 'mit_IsoCitDH': 3, 'mit_CitSynth': 3, '**mit_OAA_tx': 3**, 'mit_AOX': 3, 'mit_AKG_tx': -3, 'mit_ATP_tx': 6, 'mit_AconHydr': 3, '**mit_Complex_I': 6**, 'mit_PyrDH': 3, 'mit_O2_tx': 3}

2nd Case: {'mit_CO2_tx': 6, 'mit_AconDHatase': 3, '**mit_Complex_III': 6**, 'mit_Pyr_tx': 3, '**mit_Complex_V': 15**, 'mit_IsoCitDH': 3, 'mit_CitSynth': 3, 'mit_OAA_tx': 3, 'mit_AKG_tx': -3, 'mit_ATP_tx': 15, 'mit_AconHydr': 3, '**mit_Complex_I': 6**, 'mit_PyrDH': 3, 'mit_O2_tx': 3, '**mit_Complex_IV': 3**}

chl_LightCyc:

14 x_Photon + 6 ADP_str + 6 Pi_str -> 6 ATP_str

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chl_LightNonCyc:

8 x_Photon + 18/7 ADP_str + 18/7 Pi_str + 2 NADP_str + 2 x_H2O ->

O2_str + 18/7 ATP_str + 2 NADPH_str + 2 Proton_str

~

```
print el.ReacsOf("ElMo_0")
```

```
{'chl_Rubisco': 126, 'chl_PGA_tx': 42, 'chl_Ald1': 42, 'chl_Ald2': 42, 'chl_LightCyc': 11, 'chl_TPI': 84, 'chl_LightNonCyc': 105, 'chl_X5Piso': 84, 'chl_CO2_tx': 126, 'chl_FBPase': 42, 'chl_SBPase': 42, 'chl_PGK': 210, 'chl_R5Piso': 42, 'chl_O2_tx': -105, 'chl_TKL1': 42, 'chl_TKL2': 42, 'chl_Ru5Pk': 126, 'chl_G3Pdh': 210}
```

```
>>> print el.ReacsOf("ElMo_1")
```

```
{'chl_Rubisco': 42, 'chl_Ald1': 14, 'chl_Ald2': 14, 'chl_LightCyc': 3, 'chl_TPI': 42, 'chl_LightNonCyc': 42, 'chl_X5Piso': 28, 'chl_CO2_tx': 42, 'chl_FBPase': 14, 'chl_SBPase': 14, 'chl_PGK': 84, 'chl_R5Piso': 14, 'chl_DHAP_tx': 14, 'chl_O2_tx': -42, 'chl_TKL1': 14, 'chl_TKL2': 14, 'chl_Ru5Pk': 42, 'chl_G3Pdh': 84}
```

```
>>> print el.ReacsOf("ElMo_4")
```

```
{'chl_Ald1': 42, 'chl_Ald2': 42, 'chl_X5Piso': 84, 'chl_RuBPOxid': 84, 'chl_TKL1': 42, 'chl_TKL2': 42, 'chl_Ru5Pk': 126, 'PR': 42, 'chl_TPI': 84, 'chl_FBPase': 42, 'chl_SBPase': 42, 'chl_R5Piso': 42, 'chl_LightNonCyc': 105, 'chl_glycollate_tx': 84, 'chl_GLY3KIN': 42, 'chl_GPH': 84, 'chl_CO2_tx': 42, 'chl_PGK': 210, 'chl_glycerate_tx': 42, 'chl_Rubisco': 42, 'chl_LightCyc': 18, 'chl_G3Pdh': 210, 'chl_O2_tx': -21}
```