The calculation method of the Gibbs free energy per carbon fixation

The Gibbs free energy profiles were based on calculations and estimates made using eQuilibrator software[8] (http://equilibrator.weizmann.ac.il/). Specially paramaters were listed in following parts.

(1) physiological conditions: at pH 7.0, with ionic strength I = 0.1 M, and the concentrations of all substrates, set to 1 mM.

(2) without ATP conditions: at pH 7.0, with ionic strength I = 0.1 M, and the concentrations of all substrates except ATP, set to 1 mM, the concentration of ATP, set 0.

(3) 0.1mM ATP conditions: pH 7.0, ionic strength I = 0.1 M, and the concentrations of all substrates except ATP, set to 1 mM, the concentration of ATP, set 0.1mM.

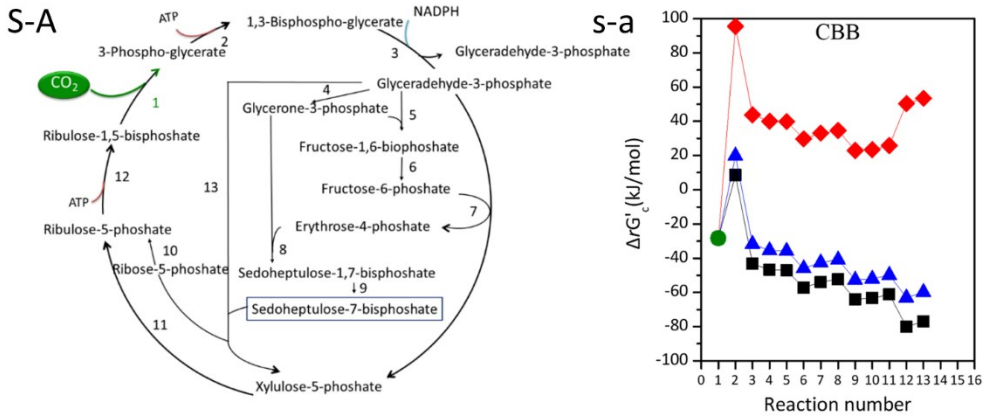
(4) Different ionic strength conditions: at pH 7.0, with ionic strength I = 0.05 M/0.2M, and the concentrations of all substrates, set to 1 mM.

To compare these different pathways with products containing different numbers of carbon atoms, we calculated the Gibbs free energy of reaction per mol of fixed carbon ($\Delta_r G'^{m}$). The calculation method is as follows.

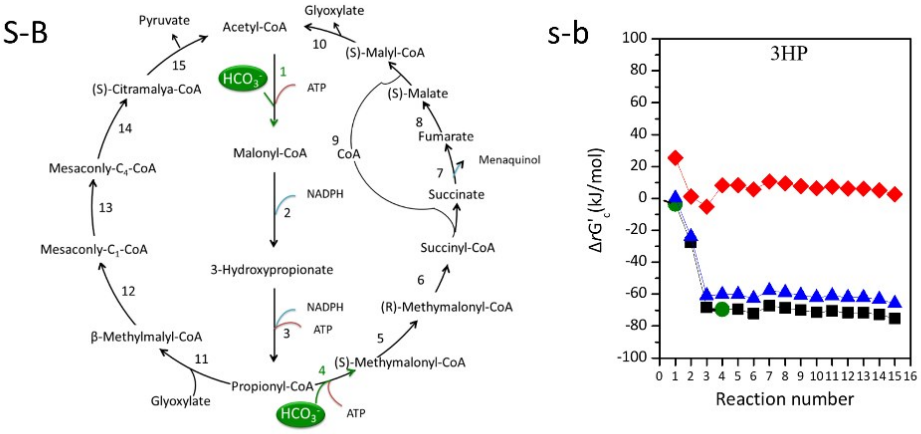
For example, in the CBB pathway, three mol of CO_2 are used to produce one mol of G3P, and we calculated the Gibbs free energy ($\Delta_r G'^{m}$) per reaction on online, and that value of $\Delta_r G'^{m}$ per reaction was then divided by three to obtain the Gibbs free energy of reaction per mol of fixed carbon ($\Delta_r G'^{m}/3$)

Figure S Profiles of ten CFPs and summary of metabolic characteristics.

(S-A, s-a) the CBB cycle; (S-B, s-b) the 3HP cycle; (S-C, s-c) the 3HP/4HB cycle; (S-D, s-d) the 4HB cycle; (S-E, s-e) the WL pathway; (S-F, s-f) the rTCA cycle; (S-G, s-g) the WL-rGly pathway; (S-H, s-h) the modified serine cycle; (S-I, s-i) the CETCH cycle; (S-J, s-j) the SACA pathway.

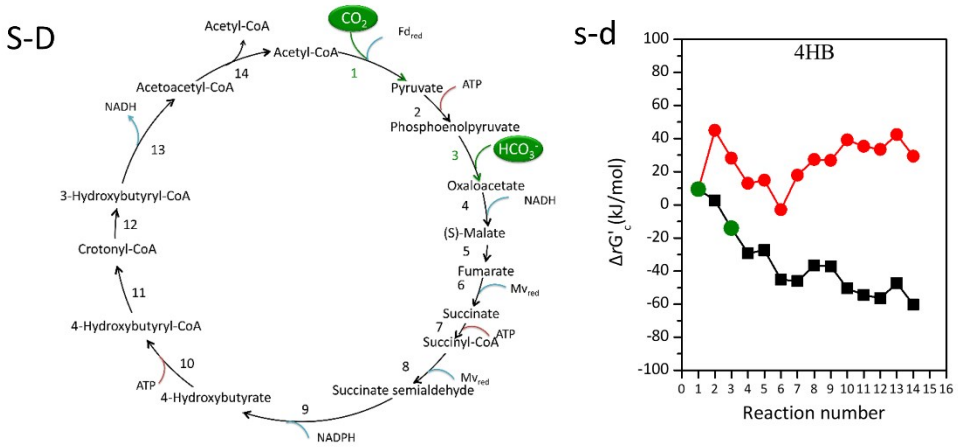


Reaction: $3CO_2 + 9ATP + 6NADPH \rightarrow$ Glyeradehyde-3-phosphate + 9ADP + 9Pi + $6NADP^+$
Representative strains: Plant, Algae, Cyanobacteria
The oxygen requirement of the strain: Aerobic
Energy source: Light
ATP requirement of per mol carbon: 3
Reducing equivalent requirement of per mol carbon: 3
Carbon fixation enzymes: Rubisco (EC: 2.1.1.127)

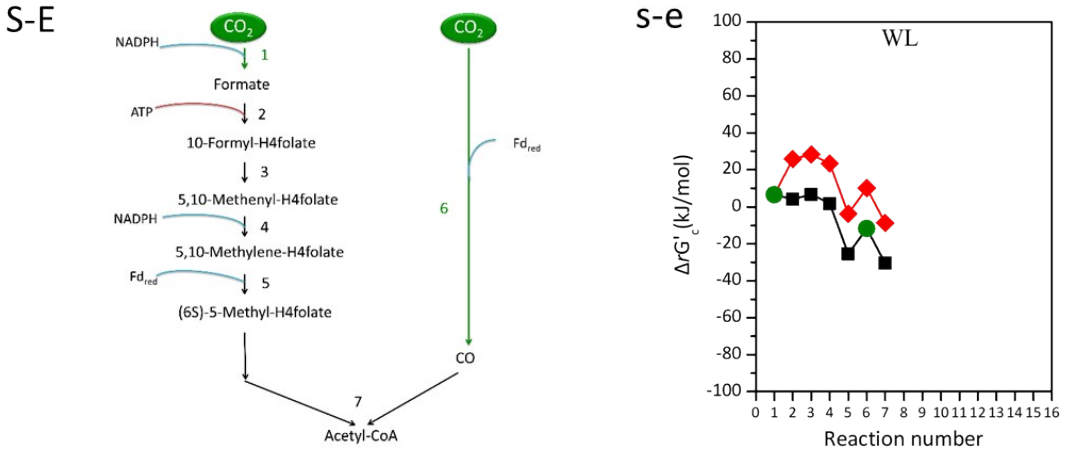


Reaction: $3HCO_3^-$+ 5 ATP+ 5NAD(P)H→Pyruvate + 3ADP + 2AMP + 3Pi + 2PPi + 5$NAD(P)^+$
Representative strains: *Chloroflexus aurantiacus*
The oxygen requirement of the strain: Aerobic
Energy source: Light
ATP requirement of per mol carbon: 1.67
Reducing equivalent requirement of per mol carbon: 1.67
Carbon fixation enzymes: Acetyl-CoA carboxylase (EC: 6.4.1.2) Propionyl-CoA carboxylase (EC: 6.4.1.3)

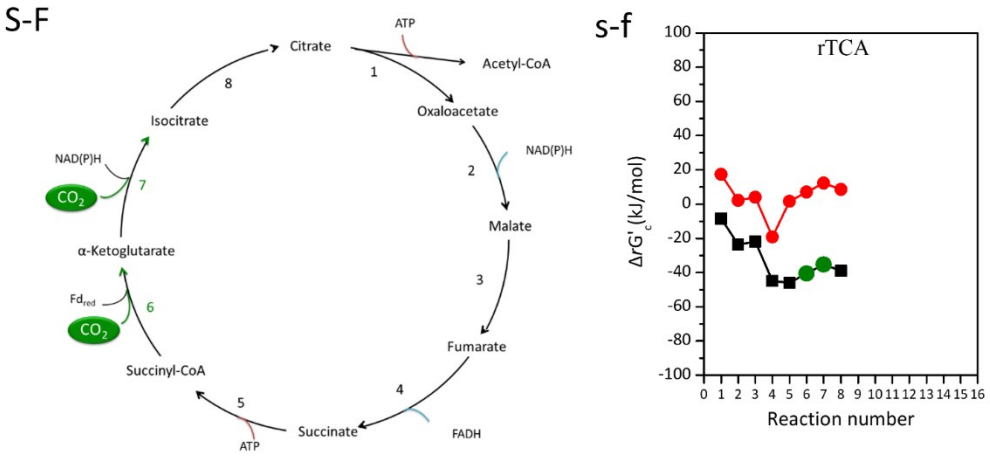
Reaction: $2HCO_3^- + 4ATP + 4NAD(P)H + CoASH \rightarrow AcCoA + 3ADP + 3Pi + AMP + PPi + 4NAD(P)^+$
Representative strain: *Metallosphaera sedula*
The oxygen requirement of the strain: Aerobic
Energy source: Hydrogen, Sulfur
ATP requirement of per mol carbon: 2
Reducing equivalent requirement of per mol carbon: 2
Carbon fixation enzymes: Acetyl-CoA carboxylase (EC: 6.4.1.2) Propionyl-CoA carboxylase (EC: 6.4.1.3)



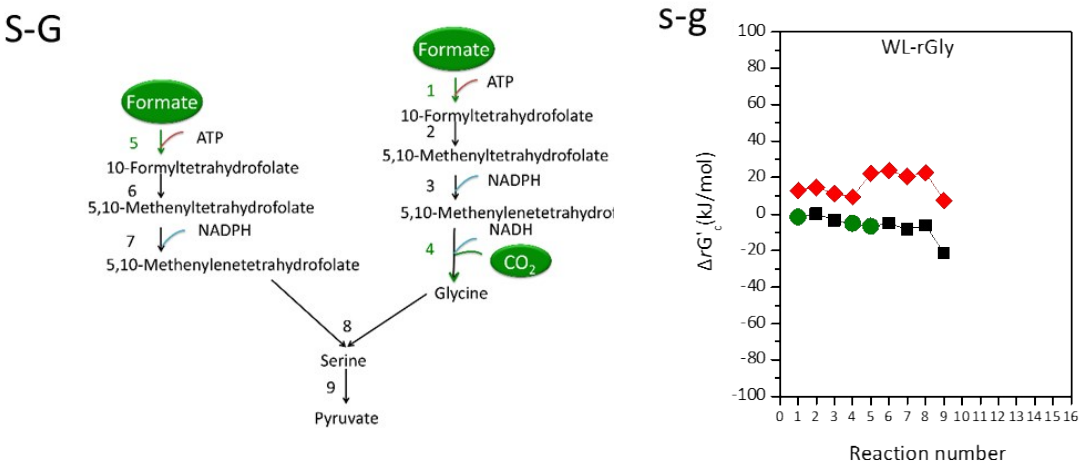
Reaction: CO_2 + HCO_3^- + NAD(P)H + 2Fd(red) + 3ATP + 4MVred + CoASH→AcCoA + 2ADP + AMP + 2Pi + 2PPi + $NAD(P)^+$ + 2Fdox + 4MVox
Representative strain: *Ignicoccus hospitalis*
The oxygen requirement of the strain: Anaerobic
Energy source: Hydrogen, sulfur
ATP requirement of per mol carbon: 1.5
Reducing equivalent requirement of per mol carbon: 2
Carbon fixation enzymes: Pyruvate synthase (EC: 1.2.7.1) Phosphoenolpyruvate carboxylase (EC: 4.1.1.31)



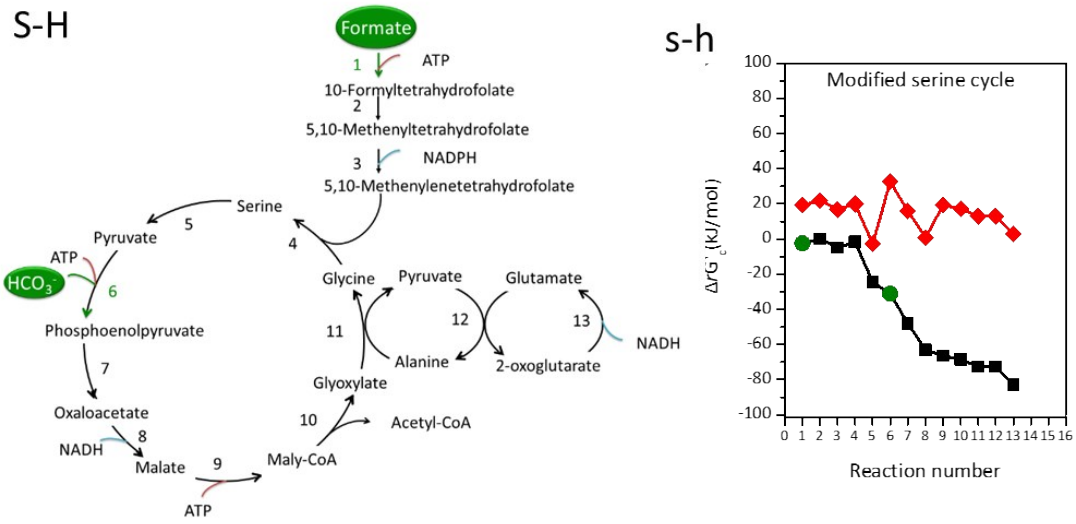
Reaction: $2CO_2$ + ATP + 2NAD(P)H + 2Fdred + CoASH→AcCoA + ADP + Pi + $2NADP^+$ + 2Fdox
Representative strain: *Clostridium ljungdahlii*
The oxygen requirement of the strain: Anaerobic
Energy source: Hydrogen
ATP requirement of per mol carbon: 0.5
Reducing equivalent requirement of per mol carbon: 1.5
Carbon fixation enzymes: Formate dehydrogenase (EC: 1.2.1.2) CO dehydrogenate/Acetyl-CoA synthase (EC: 2.3.1.169)



Reaction: $2CO_2 + 2ATP + 2NAD(P)H + FADH_2 + 2Fdred + CoASH \rightarrow AcCoA + 2ADP + 2Pi + 2NAD(P)^+ + FAD^+ + 2Fdox$
Representative strain: *Chlorobiumthiosulfatophilum*
The oxygen requirement of the strain: Anaerobic
Energy source: Light, Sulfur
ATP requirement of per mol carbon: 1
Reducing equivalent requirement of per mol carbon: 2
Carbon fixation enzymes: 2-Oxoglutarate synthase (EC: 1.2.7.3) Isocitrate dehydrogenase (EC: 1.1.1.87)

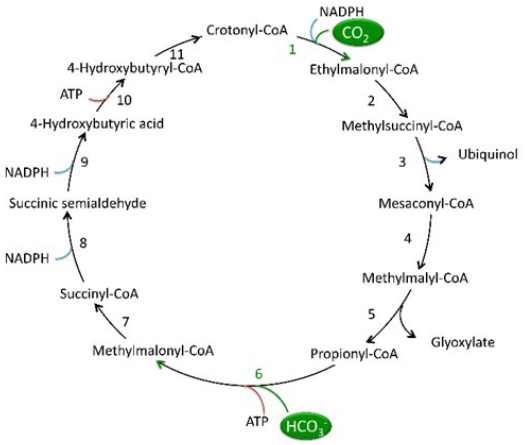


Reaction: CO_2 + 2Formate + 2ATP + 3NAD(P)H→Pyruvate + 2ADP + 2Pi + 3NAD(P)$^+$
Representative strain: *E. coli*, Yeast
The oxygen requirement of the strain: Aerobic
Energy source: Formate, glucose, pyruvate
ATP requirement of per mol carbon: 0.67
Reducing equivalent requirement of per mol carbon: 1
Carbon fixation enzymes: Formate-tetrahydrofolate ligase (EC 6.3.4.3) Glycine decarboxylase (EC 1.4.4.2)

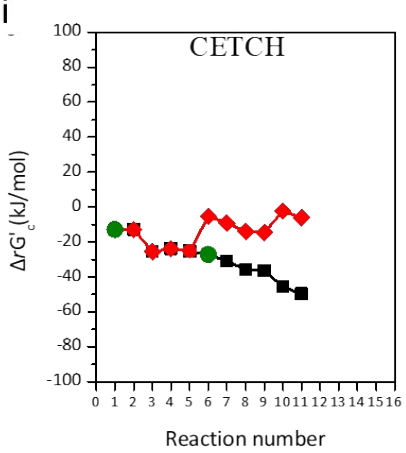


Reaction: HCO_3^- + Formate + 3ATP + 3NAD(P)H→Acetyl-CoA + 3ADP + 3Pi + 3NAD(P)$^+$
Representative strain: *E. coli*
The oxygen requirement of the strain: Aerobic
Energy source: Formate, glucose, pyruvate
ATP requirement of per mol carbon: 1.5
Reducing equivalent requirement of per mol carbon: 1.5
Carbon fixation enzymes: Formate-tetrahydrofolate ligase (EC 6.3.4.3) Phosphoenolpyruvate carboxylase (EC: 4.1.1.31)

S-I

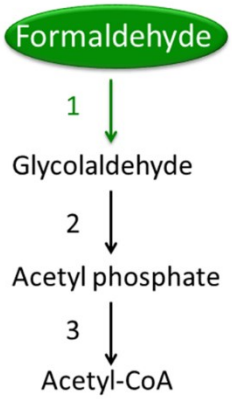


s-i

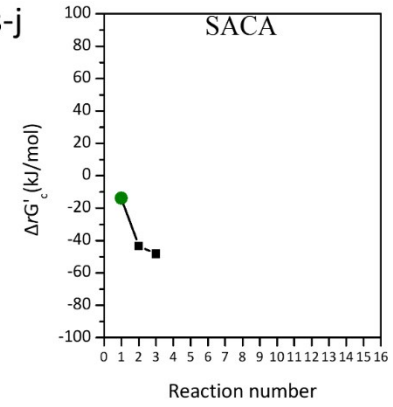


Reaction: HCO_3^- + CO_2 + 2ATP + 3NAD(P)H + Ubiquinone→Glyoxylate + 3ADP + 3Pi + 3$NAD(P)^+$ + Ubiquinol
Metabolic behavior (classical strain): Aerobic (*in vitro*)
Representative strain: --
The oxygen requirement of the strain: --
Energy source: ATP, NAD(P)H
ATP requirement of per mol carbon: 1
Reducing equivalent requirement of per mol carbon: 1
Carbon fixation enzymes: Enoyl-CoA carboxylases/reductases(--)

S-J



s-j



Reaction: 2 formaldehyde→Acetyl-CoA
Representative strain: *E. coli*
The oxygen requirement of the strain: Aerobic
Energy source: no
ATP requirement of per mol carbon: 0
Reducing equivalent requirement of per mol carbon: 0
Carbon fixation enzymes: Glycolaldehyde synthase(--)