Plant Physiology Maarleveld et al. 2014 - Supplemental Data S2

FAME batch commands to reproduce results

Using the special drop-down menu FAME displays when the *Synechocystis* model is loaded, the reader can apply appropriate settings to the model to reproduce the results shown in this manuscript. Alternatively, one can copy the commands shown in the remainder of this section into FAME's "Batch Commands" box. Note that the "Run" command must still explicitly be given after applying any of the settings, and that to prevent previous changes from affecting results, one should preferably apply these settings on freshly loaded models.

All figures: Color bar

To make sure the color bar is the same for all simulations, we use two dummy reactions and four dummy species to set fixed minimal and maximal predicted flux values. The following batch commands are used to do this; this applies to all figures in the manuscript. In the SETCONSTRAINTS commands, the first value corresponds to the lower bound, and the second value to the upper bound. n this case, for example, "SETCONSTRAINTS maxdraw 50.0 50.0" means that we fix the reaction with ID "maxdraw" to 50. Detailed information about FAME's batch commands may be found in the tool's manual, which can be accessed online at http://f-a-m-e.org/.

```
ADDSPECIES a c 1
ADDSPECIES b c 1
ADDREACTION maxdraw a <=> b
SETCONSTRAINTS maxdraw 50.0 50.0
ADDSPECIES test1 c 1
ADDSPECIES test2 c 1
ADDREACTION mindraw test1 <=> test2
SETCONSTRAINTS mindraw 0.000000001 0.000000001
```

To generate the expression color bar in Figure 4, we used the following "custom gene expression settings". Note that these are not batch commands, and that they already come pre-loaded with the *Synechocystis* model and map.

```
minValueForColorBar: -3.422331198
maxValueForColorBar: 6.499373721
```

Figure 2A

The following constraints and objectives are used to reproduce autotrophic growth.

```
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -50 0
SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -3.7 0
SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_Sink_glycogen 0 INF
SETCONSTRAINTS R_BiomassAuto 0 INF
ADDOBJECTIVE R_BiomassAuto maximize
DELOBJECTIVE R_BiomassHetero
```

Figure 2B

The following constraints and objectives are used to reproduce growth on glycogen. Here, we set R_PROAKGOX1r to zero to simulate the absence of the L-proline degradation pathway. Note that our solver predicted R_GND to be about 10^-13, which is essentially zero. To obtain better figures (i.e. a better color bar), we also set R_GND to zero.

```
SETCONSTRAINTS R_PROAKGOX1r 0 0
SETCONSTRAINTS R_GND 0 0
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -3.7 0
SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_Sink_glycogen -0.1 INF
SETCONSTRAINTS R_BiomassHetero 0 INF
DELOBJECTIVE R_BiomassAuto
ADDOBJECTIVE R_BiomassHetero maximize
```

Figure 2C

The following constraints and objectives are used to reproduce growth on glycogen. Here, we allow a flux through R_PROAKGOX1r to simulate the presence of a reaction that converts L-proline to hydroxyproline.

```
SETCONSTRAINTS R_PROAKGOX1r 0 INF
SETCONSTRAINTS R_GND 0 INF
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -3.7 0
SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_Sink_glycogen -0.1 INF
SETCONSTRAINTS R_BiomassHetero 0 INF
DELOBJECTIVE R_BiomassAuto
ADDOBJECTIVE R_BiomassHetero maximize
```

Figure 3B and S-2 A

The following constraints and objectives are used to reproduce the carbon and light limiting autotrophic growth state.

```
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -26.01 0

SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -1.9 0

SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0

SETCONSTRAINTS R_Sink_glycogen 0 INF

SETCONSTRAINTS R_BiomassAuto 0 INF

ADDOBJECTIVE R_BiomassAuto maximize

DELOBJECTIVE R_BiomassHetero
```

Figure 3C

The following constraints and objectives are used to reproduce the light limiting autotrophic growth state.

```
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -10 0

SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -3.7 -3.7

SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0

SETCONSTRAINTS R_Sink_glycogen 0 INF

SETCONSTRAINTS R_BiomassAuto 0 INF

ADDOBJECTIVE R_BiomassAuto maximize

DELOBJECTIVE R_BiomassHetero
```

Figure 3D

The following constraints and objectives are used to reproduce the carbon limiting autotrophic growth state.

```
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -50 -50

SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -0.5 0

SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0

SETCONSTRAINTS R_Sink_glycogen 0 INF

SETCONSTRAINTS R_BiomassAuto 0 INF

ADDOBJECTIVE R_BiomassAuto maximize

DELOBJECTIVE R_BiomassHetero
```

Figure 5B and S-2 B

The following constraints and objectives are used to reproduce the carbon and light limiting state in which 23BD is produced. Note that we first fix the specific growth rate at 10% of its maximum for these conditions (Figure 3B).

```
SETCONSTRAINTS R_BiomassAuto 0.00453707332157 0.00453707332157
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -26.01 0
SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -1.9 0
SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_Sink_glycogen 0 INF
ADDOBJECTIVE R_23BDD maximize
DELOBJECTIVE R_BiomassAuto
DELOBJECTIVE R_BiomassHetero
```

Figure 5C

The following constraints and objectives are used to reproduce the light limiting 23BD production state. Note that we first fix the specific growth rate at 10% of its maximum for these conditions (Figure 3C).

```
SETCONSTRAINTS R_BiomassAuto 0.00174435708172 0.00174435708172
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -10 0
SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -3.7 -3.7
SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_Sink_glycogen 0 INF
ADDOBJECTIVE R_23BDD maximize
DELOBJECTIVE R_BiomassAuto
DELOBJECTIVE R_BiomassHetero
```

Figure 5D

The following constraints and objectives are used to reproduce the carbon limiting 23BD production state. Note that we first fix the specific growth rate at 10% of its maximum for these conditions (Figure 3D).

```
SETCONSTRAINTS R_BiomassAuto 0.00119396666357 0.00119396666357
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -50 -50
SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -0.5 0
SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_Sink_glycogen 0 INF
ADDOBJECTIVE R_23BDD maximize
```

```
DELOBJECTIVE R_BiomassAuto
DELOBJECTIVE R_BiomassHetero
```

Figure S-1 A

The following constraints and objectives are used to reproduce the carbon limiting autotrophic growth state with a quinol oxidase knock-out.

```
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -50 -50
SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -0.5 0
SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_Sink_glycogen 0 INF
SETCONSTRAINTS R_CYTBDu 0 0
SETCONSTRAINTS R_CYTBDpp 0 0
ADDOBJECTIVE R_BiomassAuto maximize
DELOBJECTIVE R_23BDD maximize
DELOBJECTIVE R_BiomassHetero
```

Figure S-1 B

The following constraints and objectives are used to reproduce the carbon and light limiting autotrophic growth state where the alternative electron pathways cannot carry any flux.

```
SETCONSTRAINTS R_EX_photon_LPAREN_e_RPAREN_ -26.01 0
SETCONSTRAINTS R_EX_hco3_LPAREN_e_RPAREN_ -1.9 0
SETCONSTRAINTS R_EX_glc_LPAREN_e_RPAREN_ 0 0
SETCONSTRAINTS R_Sink_glycogen 0 999999
SETCONSTRAINTS R_BiomassAuto 0 999999
ADDOBJECTIVE R_BiomassAuto maximize
DELOBJECTIVE R_BiomassHetero
SETCONSTRAINTS R_CYTBDu 0 0
SETCONSTRAINTS R_CYTBDpp 0 0
SETCONSTRAINTS R_NDH1_1u 0 0
SETCONSTRAINTS R_NDH1_1p 0 0
SETCONSTRAINTS R_NDH1_2u 0 0
SETCONSTRAINTS R_NDH1_2p 0 0
SETCONSTRAINTS R_NDH1_3u 0 0
SETCONSTRAINTS R_NDH2_syn 0 0
SETCONSTRAINTS R_NDH2_pp 0 0
```

```
SETCONSTRAINTS R_NDH1_4pp 0 0

SETCONSTRAINTS R_NADH5 0 0

SETCONSTRAINTS R_CYO1b_syn 0 0

SETCONSTRAINTS R_CYO1b2_syn 0 0

SETCONSTRAINTS R_CYO1bpp_syn 0 0

SETCONSTRAINTS R_CYO1b2pp_syn 0 0

SETCONSTRAINTS R_MEHLER 0 0

SETCONSTRAINTS R_H2ASE_syn 0 0

SETCONSTRAINTS R_FQR 0 0

SETCONSTRAINTS R_SUCD2u 0 0

SETCONSTRAINTS R_SUCD4 0 0
```