

Table S1. Shown are p-values of an ANOVA for genotype and daytime in plants grown at elevated CO₂ concentration (1000 ppm). Only p-values < 0.05 are given (n=5).

Metabolite	geno	daytime	geno x daytime
Starch		<0.0001	
Ala	<0.0001	<0.0001	
PyrF	0.0330	0.0007	
Asp	0.0008	0.0267	
Ser	<0.0001	0.0152	0.0040
Gly	0.0022	0.0001	0.0179
Arg		0.0152	
Glc		<0.0001	
Frc		<0.0001	
Suc	0.0021	<0.0001	
Mal		0.0002	
Fum	0.0004	0.0026	0.0143
MF	0.0035	0.0004	0.0248
Cit	0.0073	0.0081	
NH ₄	0.0004	0.0175	

Table S2. Shown are p-values of an ANOVA for genotype and daytime in plants shifted from elevated CO₂ concentration (1000 ppm) to ambient (ca. 450 ppm). Only p-values < 0.05 are given (n=5).

Metabolite	geno	daytime	geno x daytime
Starch	0.0476	<0.0001	
Ala	0.0086		
Val		0.0371	
Leu			0.0466
PyrF	0.0237		
Ile		0.0479	
Asp	<0.0001	0.0055	
Thr		0.0095	
Trp			0.0094
AroF			0.0091
Ser	<0.0001	0.0040	0.0062
Gly	<0.0001	<0.0001	<0.0001
Glu	0.0061	0.0002	0.0305
Pro	0.0021		
His		0.0165	
KgF	0.0189		
Glc	0.0001	<0.0001	0.0007
Frc	0.0012	<0.0001	0.0131
Suc	0.0000	<0.0001	0.0081
Mal	0.0007	<0.0001	
Fum	<0.0001	<0.0001	
MF	<0.0001	<0.0001	
Cit	0.0027	0.0012	
NH ₄	<0.0001	<0.0001	0.0007

Table S3. ODE system for modeling dynamics in primary metabolites. All terms extended by `_par` are model parameters to be identified. All terms extended by `_var` are model variables that were given for certain time points. Terms carrying no extension are constants calculated from C/N ratios in metabolite pools. Because pools vary in composition for the different genotype x CO₂ treatments, these constants are different for the different conditions.

```

d/dt HP      = NPS_var/6.0 + (1-alpha_par)*Gly_var*kgd_par - starchb_par*HP_var +
               starchd_par*Starch_var - ks_par*HP_var - kmf_par*HP_var - kaal_par*HP_var +
               Ser_var*hpr_par
d/dt Starch  = starchb_par*HP_var - starchd_par*Starch_var
d/dt Sugar   = (6/cSugar)*ks_par*HP_var - ex1_par*Sugar_var
d/dt MF      = (6/4)*kmf_par*HP_var - Resp_var/6.0 + alpha_par*Gly_var*kgd_par -
               kcit_var*MF_par
d/dt Cit     = (4/6)*kcit_var*MF_par - kakg_var*Cit_par + Glu_var*v0_par - Cit_var*kasf_par
d/dt AA1     = (6/cAA1)*HP_var*kaal_par - AA1_var*ex3_par
d/dt Ser     = (Gly_var/2.0)*kgd_par - Ser_var*hpr_par - Ser_var*ex4_par - Ser_var*kshmt_par
d/dt Gly     = v0_par*(NPS_var/2.0) - kgd_par*Gly_var + Ser_var*kshmt_par
d/dt AsF     = (6/cASF)*Cit_var*kasf_par - ex5_par*AsF_var
d/dt Glu     = kglu_par*aKG_var + Gln_var*kglu_par - Glu_var*kglu_par - Glu_var*kkgf_par -
               Glu_var*v0_par
d/dt Gln     = kglu_par*Glu_var - Gln_var*kglu_par
d/dt KgF     = (5/cKGF)*kkgf_par*Glu_var - KgF_var*ex2_par
d/dt aKG     = (6/5)*Cit_var*kakg_par - kglu_par*aKG_var
d/dt NH4     = knew_par - knh4*NH4_var+Gly_var*kgd_par

```

Constants for Col-0 at elevated CO₂

```

cSugar      = 8.9
cAA1        = 4.5
cAsF        = 4.2
cKgf        = 5.6
knkgf       = 0.461*kkgf_par
knasf       = (0.326*(4/4.2)*MF_var*kasf_par)/Glu_var
knaa1       = (0.247*(6/4.5)*HP_var+kaal_par)/Glu_var
knpr        = v0_par/Glu_var
knh4        = ((knkgf+knasf+knaa1+knpr)*Glu_var)/NH4_var

```

#Constants for hpr1-1 at elevated CO₂

```

cSugar      = 8.7
cAA1        = 4.6
cAsF        = 4.4
cKgf        = 5.7
knkgf       = 0.493*kkgf_par
knasf       = (0.321*(4/4.4)*MF_var*kasf_par)/Glu_var
knaa1       = (0.244*(6/4.6)*HP_var+kaal_par)/Glu_var
knpr        = v0_par/Glu_var
knh4        = ((knkgf+knasf+knaa1+knpr)*Glu_var)/NH4_var

```

#Constants for Col-0 at ambient CO₂

```

cSugar      = 9.2
cAA1        = 4.8
cAsF        = 4.2
cKgf        = 5.6
knkgf       = 0.451*kkgf_par
knasf       = (0.358*(4/4.2)*MF_var*kasf_par)/Glu_var
knaa1       = (0.244*(6/4.5)*HP_var+kaal_par)/Glu_var
knpr        = v0_par/Glu_var
knh4        = ((knkgf+knasf+knaa1+knpr)*Glu_var)/NH4_var

```

#Constants for hpr1-1 at ambient CO2

```
cSugar      = 8.0
cAA1        = 5.0
cAsF        = 4.3
cKgF        = 5.7
knkgf       = 0.507*kkgf_par
knasf       = (0.371*(4/4.3)*MF_var*kasf_par)/Glu_var
knaa1       = (0.242*(6/5)*HP_var+kaa1_par)/Glu_var
knpr        = v0_par/Glu_var
knh4        = ((knkgf+knasf+knaa1+knpr)*Glu_var)/NH4_var
```