Supporting Information

Release of resource constraints allows greater carbon allocation to secondary metabolites and storage in winter wheat

Authors: Jianbei Huang, Almuth Hammerbacher, Lenka Forkelová, Henrik Hartmann

Table S1 Carbon (C) and nitrogen (N) concentrations and C/N ratios in leaves, stems, and roots of winter wheat (*Triticum aestivum* cv. Genius) for the three [CO_2] treatments: 680 ppm [CO_2], 390 ppm [CO_2] and 170 ppm [CO_2]. Values represent the means (SD) of three individual chambers. Different letters indicate significant differences between [CO_2] treatments ($P<0.05$, Tukey's HSD).

		Leaf			Stem			Root		
Developmental periods	CO_2 (ppm)	C concentration (%)	N concentration (%)	C/N ratio	C concentration (%)	N concentration (%)	C/N ratio	C concentration (%)	N concentration (%)	C/N ratio
	680	39.9 (0.1) a	5.9 (0.1) a	6.8 (0.1) b	36.2 (0.3) a	4.8 (0.1) a	7.5 (0.1) a	29.0 (5.5) a	3.5 (0.6) a	8.4 (0.2) ab
3L	390	39.5 (0.4) ab	5.7 (0.1) a	6.9 (0.1) b	36.2 (0.7) a	4.7 (0.1) a	7.6 (0.1) a	31.4 (2.5) a	3.8 (0.3) a	8.2 (0.4) b
	170	39.1 (0.3) b	5.3 (0.2) b	7.4 (0.2) a	35.6 (0.4) a	4.7 (0.2) a	7.6 (0.3) a	30.3 (1.0) a	3.4 (0.1) a	8.9 (0.1) a
	680	40.7 (0.3) a	4.2 (0.2) b	9.8 (0.6) a	38.4 (0.3) a	3.5 (0.2) b	10.9 (0.8) a	37.1 (1.0) a	2.4 (0.2) b	15.7 (1.5) a
6L	390	39.2 (0.4) b	5.0 (0.0) a	7.8 (0.1) b	36.2 (0.4) b	4.7 (0.0) a	7.7 (0.1) b	31.3 (1.2) b	3.5 (0.2) a	9.1 (0.2) b
	170	37.2 (0.4) c	4.7 (0.2) a	8.0 (0.2) b	34.6 (0.2) c	4.7 (0.2) a	7.4 (0.4) b	25.1 (2.8) c	2.7 (0.4) b	9.4 (0.5) b
	680	39.8 (0.7) a	4.0 (0.4) a	10.0 (1.1) a	36.0 (0.7) a	3.4 (0.4) b	10.7 (1.3) a	35.2 (3.1) a	2.4 (0.4) a	15.2 (2.2) a
8L	390	40.0 (1.2) a	4.5 (0.3) a	8.9 (0.7) a	35.3 (0.5) a	3.8 (0.3) b	9.3 (0.8) ab	32.7 (5.3) a	2.9 (0.3) a	11.5 (1.5) ab
	170	36.5 (0.6) b	4.4 (0.2) a	8.3 (0.3) a	33.0 (0.1) b	4.5 (0.1) a	7.4 (0.2) b	24.2 (4.7) a	2.5 (0.5) a	9.9 (0.2) b

Table S2 Molecular formula, molecular weight, and C fraction of standards that are used for quantification of secondary metabolites in leaves, stems, and roots of winter wheat (*Triticum aestivum* cv. Genius).

Secondary metabolites	Standards for quantification	Molecular formula	Molecular weight (g mol^{-1})	The fraction of C
Ferulic acid-based	Feruoylputrescine	$C_{14}H_{20}N_2O_3$	264.32	0.636
Luteolin-based	Luteolin 6-C-glucoside	$C_{21}H_{20}O_{11}$	448.38	0.562
Apigenin-based	apigenin 6-C-glucoside	$C_{21}H_{20}O_{10}$	432.38	0.583
Chrysoeriol-based	Chrysoeriol	$C_{16}H_{12}O_6$	300.26	0.639
Tricin-based	Chrysoeriol	$C_{16}H_{12}O_6$	300.26	0.639
Putrescine-based	Feruoylputrescine	$C_{14}H_{20}N_2O_3$	264.32	0.636
DIMBOA-Glc-based	DIMBOA-Glc	$C_{15}H_{19}NO_{10}$	373	0.483
HDMBOA-Glc-based	HDMBOA-Glc	$C_{16}H_{21}NO_{10}$	387	0.496

Fig. S1 Concentrations of Ferulic acid-based (a), Luteolin-based (b), chrysoeriol-based (c) and tricin-based (d) and apigenin-based (e) secondary metabolites in leaves of winter wheat (*Triticum aestivum* cv. Genius) for the three [CO_2] treatments: 680 ppm [CO_2] (squares, blue line); 390 ppm [CO_2] (circles, black line); 170 ppm [CO_2] (triangles, red line). Values are the means (mg g^{-1}) of three individual chambers; error bars represent $\pm$ 1 SD. Significant differences between 680 ppm and 170 ppm [CO_2] treatments compared to ambient [CO_2] (390 ppm) are indicated by filled symbols (P<0.05, Tukey's HSD).

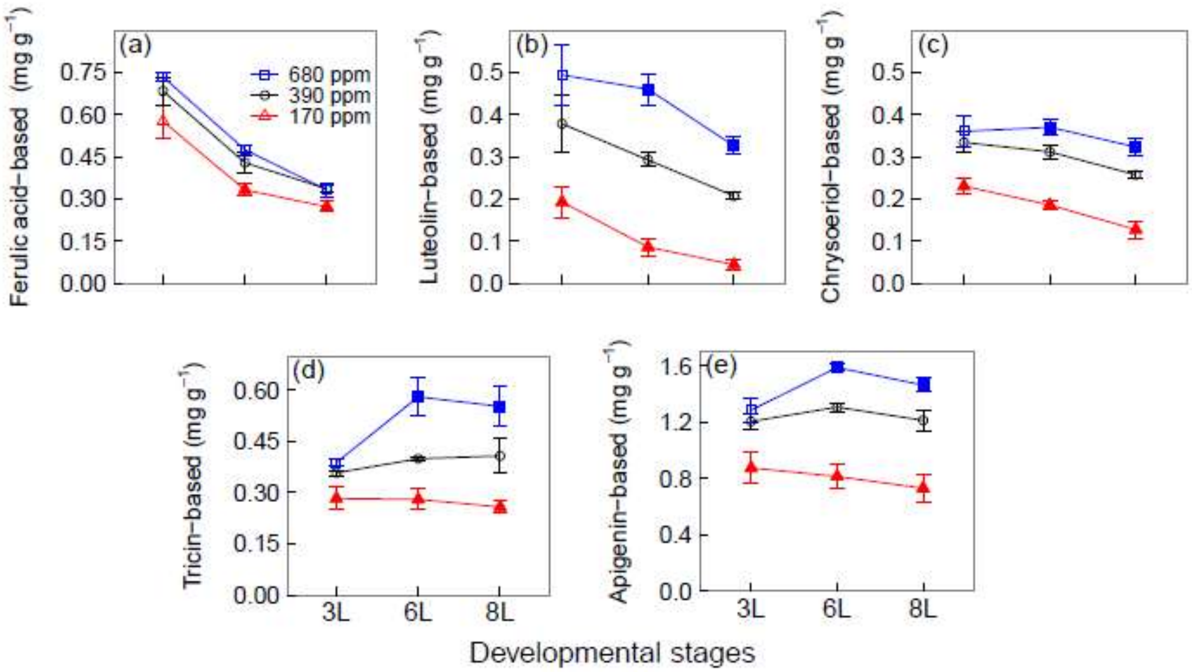

Fig. S2 Concentrations of Putrescine-based (a), DIMBOA-Glc-based (b),and HDMBOA-Glc-based (c) secondary metabolites in roots of winter wheat (*Triticum aestivum* cv. Genius) for the three [CO_2] treatments: 680 ppm [CO_2] (squares, blue line); 390 ppm [CO_2] (circles, black line); 170 ppm [CO_2] (triangles, red line). Values are the means (mg g^{-1}) of three individual chambers; error bars represent $\pm$ 1 SD. Significant differences between 680 ppm and 170 ppm [CO_2] treatments compared to ambient [CO_2] (390 ppm) are indicated by filled symbols ($P<0.05$, Tukey's HSD).

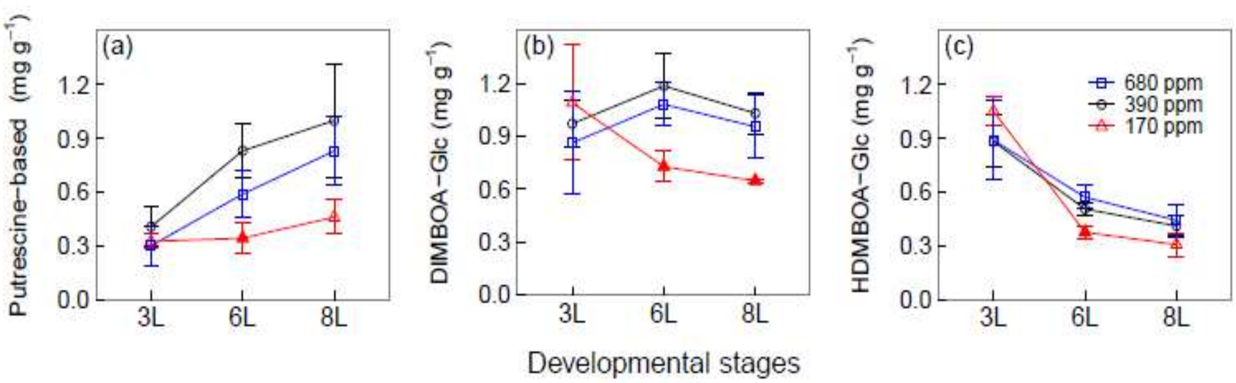

Fig. S3 Correlations between leaf nonstructural carbohydrate (NSC) concentrations (mg g^{-1}) and leaf assimilation rate (nmol CO_2 g^{-1} S^{-1}) (a), and correlations between whole-plant NSC concentrations (mg g^{-1}) and respiration rate (nmol CO_2 g^{-1} S^{-1}) (b) in winter wheat (*Triticum aestivum* cv. Genius) for the three [CO_2] treatments: 680 ppm [CO_2] (squares, blue line); 390 ppm [CO_2] (circles, black line); 170 ppm [CO_2] (triangles, red line). Values are the means of three individual chambers; error bars are ± 1 SD.

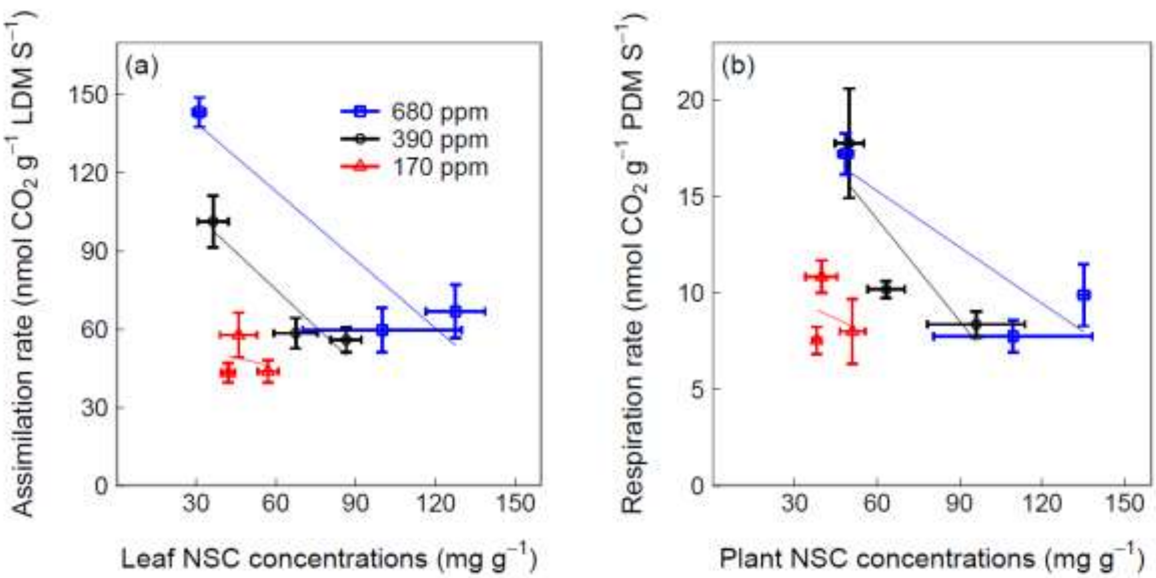

Fig. S4 Correlations between leaf nitrogen (N) concentrations (mg g^{-1}) and assimilation rate (nmol CO_2 g^{-1} S^{-1}) in winter wheat (*Triticum aestivum* cv. Genius) for the three [CO_2] treatments: 680 ppm [CO_2] (squares, blue line); 390 ppm [CO_2] (circles, black line); 170 ppm [CO_2] (triangles, red line). Values are the means of three individual chambers; error bars are ± 1 SD.