

Table S1. Statistical analysis of the time variation of leaf photosynthesis (An) and leaf water soluble carbohydrates (WSCs) during the grain filling period, and WSCs (g 100 g DW⁻¹) in flag leaves of the four cereal species shown in Figure 1 and 2, respectively.

Leaf photosynthesis (An) and leaf water soluble carbohydrates (WSCs) during the grain filling period					
Trait	water regime	Triticale	Bread wheat	Durum wheat	Barley
An ($\mu\text{mol m}^{-2} \text{s}^{-1}$)	WW	$y = -0.0015x^2 - 0.3084x + 25.959$	$y = -0.0196x^2 + 0.6333x + 14.306$	$y = -0.0364x^2 + 0.9699x + 14.515$	$y = -0.035x^2 + 0.8631x + 7.8679$
	WL	$y = 0.001x^2 - 0.3891x + 24.054$	$y = -0.0044x^2 - 0.0852x + 16.736$	$y = -0.0322x^2 + 0.6752x + 14.208$	$y = -0.0475x^2 + 1.132x + 3.3052$
Leaf WSC (g 100gDW ⁻¹)	WW	$y = -0.02x^2 + 1.3485x - 13.955$	$y = -0.0173x^2 + 1.1678x - 12.195$	$y = -0.0278x^2 + 1.2674x - 7.8762$	$y = -0.0012x^2 + 0.2897x + 1.3235$
	WL	$y = -0.0358x^2 + 2.0371x - 20.246$	$y = -0.0367x^2 + 2.0815x - 21.591$	$y = -0.0321x^2 + 1.3912x - 8.4343$	$y = -0.0048x^2 + 0.3044x + 3.0261$
WSCs (g 100 g DW ⁻¹) in flag leaves of the four cereal species					
WSC		Triticale	Bread wheat	Durum wheat	Barley
Glucose		$y = -0.0032x^2 + 0.1576x - 0.7892$	$y = -0.003x^2 + 0.1619x - 1.1684$	$y = -0.0002x^2 + 0.021x + 0.1113$	$y = 0.0044x^2 - 0.1049x + 1.9803$
Fructose		$y = -0.0035x^2 + 0.1918x - 1.5259$	$y = -0.0071x^2 + 0.3954x - 4.0319$	$y = 0.0003x^2 + 0.0065x + 0.0829$	$y = 0.0042x^2 - 0.0939x + 1.5208$
Sucrose		$y = -0.0176x^2 + 1.0739x - 11.533$	$y = -0.0164x^2 + 0.9827x - 10.56$	$y = -0.0214x^2 + 0.9035x - 5.6063$	$y = -0.0119x^2 + 0.472x - 1.2847$
Maltose		$y = -0.0044x^2 + 0.3188x - 3.9596$	$y = 0.0033x^2 - 0.1373x + 2.0515$	$y = -0.0173x^2 + 0.7891x - 6.9203$	$y = 0.0064x^2 - 0.2036x + 1.9038$

Table S2. Effect of water deficit on the water-soluble carbohydrate content (g 100 g DW⁻¹) in leaves and grain, from the grain filling stage to maturity (in days after anthesis; DAA). Values are differences between the water-limited (WL) and the well-watered (WW) regime. Values corresponds to the WL regime.

WL	no effect		WW							
Leaves					Grain development					
Triticale (DAA)	15	22	29	36	15	22	29	36	43	64
Gluc	0.42***	0.32	0.43	-0.64	0.14	-0.68***	-0.34	0.26	-0.34	0.16
Fruc	0.30*	0.39	0.48*	-0.52	0.02	-0.66***	-0.25	-0.09	-0.41	1.09
Suc	0.35	0	-0.1	-0.11	-0.04	-0.21	-0.1	-0.18	-0.01	0
Malt		0.33	0.24	-0.11	-0.26	-0.53**	1.09*	-0.08	0.1	-0.01
Bread wheat (DAA)	15	22	29	36	15	22	29	26	43	64
Gluc	0.41	0.26	1.11*	-0.47	-0.11	-0.17	-0.22	0.05	-0.12	-0.24*
Fruc	0.71***	0.81	2.27**	-0.36	-0.1	-0.16	-0.14	0.02	-0.03	-0.25*
Suc	-0.29	-0.11	-0.17	-0.24*	-0.08	-0.03	-0.14	-0.03	0.01	-0.2
Malt		0.06	-0.15	-0.07	-0.3	-0.05	0.03	-0.17	-0.06	-0.12**
Durum wheat (DAA)	8	15	22	29	8	15	22	29	36	57
Gluc	0.37	-0.09	-0.05	1.95	-0.13	-0.15	-0.34	-0.15	-0.01	-0.18*
Fruc	0.21	0.02	2.06	0.47	-0.47	-0.15	-0.16	-0.41*	-0.13	-0.11**
Suc	-0.2	0.04	-0.1	-0.21	-0.34	0.02	0.08	0.02	-0.21	0.11
Malt		0.35	0.02	-0.36	0.37	-0.07	-0.16	-0.36	-0.21	-0.02
Barley (DAA)	4	11	18	25	4	11	18	25	32	53
Gluc	0.67	0.91*	0.3	-0.23		-0.50*	0.07	0.51	-0.22	-0.34*
Fruc	0.41	1.19**	0.32	-0.12		-0.40**	0.39	-0.78	0.39	-0.41
Suc	2.47**	0.04	0.01	0.02		-0.16	0.17	0.1	0.17	-0.05
Malt		-0.45	0.72*	0.67		-0.06	0.32	-0.11	-0.46	0.03

Statistical differences ($p < 0.05$ *; $p < 0.01$ **; $p < 0.001$ ***)

Table S3. Statistical analysis of the time variation of different water-soluble carbohydrates (WSCs) (g 100 g DW⁻¹) in grain for the four cereal species shown in Figure 3.

WSC	Triticale	Bread wheat	Durum wheat	Barley
Glucose	$y = 0.0004x^2 - 0.0556x + 1.8417$	$y = 2E-05x^2 - 0.0125x + 0.7056$	$y = -0.0003x^2 - 0.0031x + 0.9282$	$y = 0.0005x^2 - 0.0563x + 1.6519$
Fructose	$y = 0.0016x^2 - 0.1679x + 4.3619$	$y = 0.0004x^2 - 0.0534x + 1.7715$	$y = 0.0005x^2 - 0.0679x + 2.1308$	$y = 0.0016x^2 - 0.1482x + 3.385$
Sucrose	$y = 0.0013x^2 - 0.1633x + 6.1733$	$y = 0.0013x^2 - 0.1534x + 5.4881$	$y = 0.0006x^2 - 0.1275x + 5.7514$	$y = -7E-05x^2 - 0.0734x + 4.8525$
Maltose	$y = -0.0004x^2 + 0.031x - 0.1454$	$y = -0.0007x^2 + 0.0562x - 0.4585$	$y = -0.0009x^2 + 0.059x - 0.2231$	$y = -0.0002x^2 + 0.0073x + 0.4861$

Table S4. Statistical analysis of the relationships between starch in grain, and water-soluble carbohydrates (WSCs) in grain (A, B) and mean grain weight (C, D) for the four cereal species under the well-watered (WW) and water-limited (WL) regimes shown in Figure 4.

	WW	WL
WSC		
Triticale	$y = 6E-07x^2 - 0.0043x + 10.02$	$y = 4E-07x^2 - 0.0037x + 9.89$
Bread wheat	$y = 3E-07x^2 - 0.0032x + 9.12$	$y = 5E-07x^2 - 0.0034x + 8.38$
Durum wheat	$y = -1E-06x^2 + 0.0021x + 7.17$	$y = -2E-06x^2 + 0.0043x + 4.51$
Barley	$y = 2E-08x^2 - 0.0017x + 8.51$	$y = -7E-07x^2 + 0.0016x + 5.83$
Grain weight		
Triticale	$y = 2.1045x^2 + 5.2178x + 2.2501$	$y = 5.0352x^2 - 3.1975x + 5.8235$
Bread wheat	$y = 1.0299x^2 + 13.707x - 9.1689$	$y = -5.6353x^2 + 40.67x - 30.724$
Durum wheats	$y = 6.3273x^2 - 8.5674x + 5.7824$	$y = 4.2552x^2 - 2.5776x + 5.9184$
Barley	$y = 3.1155x^2 - 4.83x + 7.4019$	$y = 2.3194x^2 - 0.296x + 6.8797$

Table S5. Effect of water deficit on amino acid concentration ($\mu\text{mol g DW}^{-1}$) in leaves and grain, from the grain filling stage to harvest (in days after anthesis; DAA). Values are differences between the water-limited (WL) and well-watered (WW) regime. Value corresponds to the WL regime.

	Leaves				Grain development					
	15	22	29	36	15	22	29	36	43	64
Triticale (DAA)										
Arg	0.18	0.25	0.09*	0.08	0.2	-0.95*	-0.13	0.14	-0.37	0.06
Asn		-0.01	0.01	0.07	-0.64	-0.75	0.05	0.71	0.98	0.62
Asp	-0.29	-0.06	0.03	0.01	0.2	-0.25	-0.16	0.02	-0.06	0.16
GABA	-0.06	0	-0.01	-0.01	0.06	-0.48	-0.04	0.02	-0.05	0.01
Gln	-0.1	0.01	0.03**	0.08	-0.16	0.5	0.2	-0.04	-0.25	0.02
Glu	-0.44	-0.03	0.01	-0.02	0.42	2.13	-1.15	0.83	-0.25	0.09
Gly	-0.39	0.01	0.01	0.03	0.51	2.75*	-0.52	-0.01	-0.74	0.01
His	-0.06	-0.01	-0.02		0.04	-0.11*	-0.02	0.01	0.24	0.02
Ile	-0.13	0.05	0.06	0.09	0.47	-0.26	-0.63	-0.31	-0.46	0.01
Leu	-0.11	0.06	0.05	0.07	-1.68	-0.47	-0.51	0.17	-0.27	0.02
Lys	-0.02	0	0.01	0	0.08	0.02	-0.13	0.04	-0.18	0.04
Met	-0.06	-0.01	0	0	0.05	-0.07	-0.02	0.02	-0.06	-0.01
Phe	-0.15	0.05	0.07	0.07	0.11	-0.05	-0.24	0.06	-0.08	0.01
Pro	-0.39	-0.02	0.05	0.03	1.48	-4.36*	-0.48	0.25	-0.16	0.2
Ser	0.1	-0.06	0.04	0.05	0.3	-0.14	-0.38	0.09	-0.52	0.01
Thr	-0.07	-0.02	0	0.03	-0.07	0.07	-0.17	0.12	-0.24	-0.03
Tyr	-0.12	0.01	0.02	0.05	-0.03	-0.22	-0.14	-0.01	-0.04	0.02
Val	-0.15	0.07	0.06	0.21	0.39	0.26	-0.57	0.18	-0.45	0.04
Bread wheat (DAA)										
Arg	-0.27	-0.17	0	0.02	1.08	-0.02	-0.39	0.03	0.12	0.02
Asn	0.20*	0.25	-0.01	0.37	3.08	-0.42	-0.48	3.21*	-0.97	-0.6
Asp	-0.24	-0.04	0.01	-0.01	1.08*	-0.09	-0.44*	0	-0.19	-0.09
GABA	-0.09	0.01	-0.01	-0.05	1.37	-0.13	-2.2	-0.04	0	0.02
Gln	-0.04	0.13	0.03	0.08	3.86	-0.4	0.07	0.1	0.42	-0.12
Glu	-0.12	-0.01	0.01	-0.04	2.60*	0.2	-1.27	-0.13	0.64	-0.31
Gly	0.03*	0.01	0	0	1.56	0.33	-1.33*	-0.13	0.48	-0.04
His	0.04				0.04	-0.03	-0.06	0.01	-0.03	-0.05
Ile	0.07	0.11	0.11	0.03	0.85**	0.11	-0.78	-0.45	0.03	0.01
Leu	0.09	0.09*	0.19	0.04	0.65**	-0.04	-0.80*	-0.21	0.05	0
Lys	0.12	0.02	0.03*	-0.03	0.53**	-0.01	-0.28	-0.03	0.05	-0.03
Met	0.03	0.01	0.02	-0.04	0.26*	-0.05*	-0.06	0	0.01	-0.01
Phe	0.12*	0.10*	0.12	0.07	0.55*	-0.06	-0.34*	-0.02	0.04	-0.01
Pro	-0.07	-0.02	0.14	0	2.71*	-0.73	0.01	-0.05	0.09	-0.01
Ser	-0.07	-0.05	-0.02	0.06	0.52**	-0.03	-0.64*	-0.07	0.14	-0.02
Thr	-0.05	0.03	-0.22	0.01	0.96**	0	-0.34	-0.01	0.06	-0.09
Tyr	0.04	0.07	0.07	0	1.09	-0.02	-0.31*	-0.06	-0.06	0
Val	0.13*	0.14	0.09	0.06	2.06**	0	-1.00*	-0.24	0.14	-0.01
Durum wheat (DAA)										
Arg	-0.1	-0.02	0	0.06	-0.07	-0.25	-0.74	-0.58	-1.29	0.03*
Asn		0.26	-0.01	0.14	7.46	-1.74	-2.26	2.70*	0.25	0.88**

Asp	0.42	0	0.01	0.02	-0.5	-0.52*	-0.12	0.90**	-0.76	0.09
GABA	0.18	-0.15	-0.01	0	-0.45	-0.13	-0.29	-0.06	-0.21	0.03
Gln	0.2	0.02	0.03	0.05	5.07	0.19	-1.39	-0.13	-0.35	
Glu	0.27	-0.02	0.01	0.01	-0.08	-0.81		1.85	-0.13	0.12
Gly	0.34	-0.03	0	0.05	0.32	-0.34	-0.93	-1.48	-0.58	0.15
His	0.01					-0.09**	-0.07	-0.03	-0.1	
Ile	0.01	-0.03	0.11	0.07	0.54	-0.19	0.14	-1.58*	-0.32	0.01
Leu	0.02	-0.02	0.19	0.11	0.51	-0.88*	-0.71	-0.93	-0.18	0.01
Lys	0.01	-0.02	0.03*	0.01	0.12	-0.21	-0.26	-0.3	-0.07	
Met	-0.01	-0.01	0.02	0	-0.02	0.02	-0.02	-0.07	-0.01	0
Phe	0.07	-0.01	0.12	0.07	-0.21	-0.41	-0.38	-0.22	-0.03	0
Pro	0.02	-0.07	0.14	0.1	-0.15	-1.24	-2.34	-0.04	-0.48	0.03
Ser	0.78	0.01	-0.02	0.19	0.06	-0.49	-0.24	-0.37	-0.07	0.02
Thr	0.08	-0.01	-0.22	0.03	-0.01	-0.4	-0.48	-0.04	-0.1	
Tyr	0.05	-0.02	0.07	0.03	1.24	-0.24	-0.59	-0.36	0.22	-0.03
Val	0.08	-0.01	0.09	0.1	-0.02	-0.61	-0.7	-1.24	-0.74	0.02
Barley (DAA)	4	11	18	25	4	11	18	25	32	53
Arg	0.16	0.23	0.26*	-0.01		0.17	0.65	-0.95	-0.15	-0.43
Asn		0.01	0.01*	0.01		9.81	4.74	-2.03	3.61	-0.46
Asp	0.07	0.04	0.02	-0.05		0.48	-0.15	-0.32*	0.1	-0.42
GABA	0.01			0.01		0.08	-0.15	-0.12	-0.09	-0.1
Gln	-0.08	0.02	0.03*	0		2.43	-0.38	-1.37	-0.39	-0.17
Glu	-0.02	-0.04	0.06	-0.05		0.61	-1.03	-1.59	0.23	0
Gly	-0.28	-0.01	0.03	0		1.69	-1.7	-1.81	-1.64	-0.01
His	0.03	0	0.01			0	-0.01	-0.04	-0.03	0.05***
Ile	-0.11	0.04	0.02	0		-0.18	-1.29	-1.32	0.01	-0.34
Leu	-0.13	0.04	0.01	0		0.93	-1.37	-0.42	-0.38	0
Lys	-0.08	0	0	-0.01		0.27	-0.6	-0.14	-0.16	0
Met	0.02	0	0	-0.01		0.2	-0.1	-0.11	-0.04	-0.03
Phe	0	0	0.05	-0.02		0.1	-0.84	-0.55	-0.18	0.01
Pro	-0.11	-0.05	0.19*	0.1		5.18*	0.79	-1.01	-0.03	0.02
Ser	-0.02	0.09	0.07*	0		1.43	0.06	-0.01	-1.98*	-0.02
Thr	0.09	0	0.04	-0.02		1.16	-2.22	-1.21*	-1.07	0.02
Tyr	0.02	0	0.02	-0.01		0.05	-0.72	-0.56	-0.12	-0.1
Val	-0.08	0.02	0.07	-0.02		1.53	-1.01	-1.63	-0.96	0.01

Statistical differences ($p<0.05$ *; $p<0.01$ **, $p<0.001$ ***)

Table S6. Statistical analysis of time variation (expressed as days after anthesis, DAA) of the total amino acid (AA) concentration in leaves and grain, and grain weight. Fig. 7 A, B, C and D.

Trait	Env	Triticale	R2	Bread wheat	R2	Durum wheat	R2	Barley	R2
Grain	WW	$y = 33.824\ln(x) - 91.272$	0.95	$y = 39.706\ln(x) - 113.22$	0.95	$y = 21.828\ln(x) - 50.038$	0.82	$y = 15.959\ln(x) - 28.08$	0.68
weight	WL	$y = 31.734\ln(x) - 80.884$	0.96	$y = 40.078\ln(x) - 112.36$	0.93	$y = 20.777\ln(x) - 45.75$	0.85	$y = 15.621\ln(x) - 25.541$	0.81
AA	WW	$y = -0.5826x + 50.957$	0.82	$y = -0.4243x + 39.981$	0.9	$y = -1.1652x + 71.942$	0.96	$y = -1.5659x + 87.413$	0.83
grain	WL	$y = -0.5552x + 49.151$	0.84	$y = -0.7166x + 54.03$	0.66	$y = -1.1967x + 70.137$	0.78	$y = -1.9554x + 98.278$	0.73
AA	WW	$y = -0.2269x + 14.411$	0.84	$y = -0.1326x + 12.118$	0.99	$y = -0.2456x + 13.298$	0.9	$y = -0.3233x + 14.597$	0.88
leaves	WL	$y = -0.0896x + 10.762$	0.84	$y = -0.1011x + 11.672$	0.85	$y = -0.2907x + 15.191$	0.71	$y = -0.2252x + 13.034$	0.96

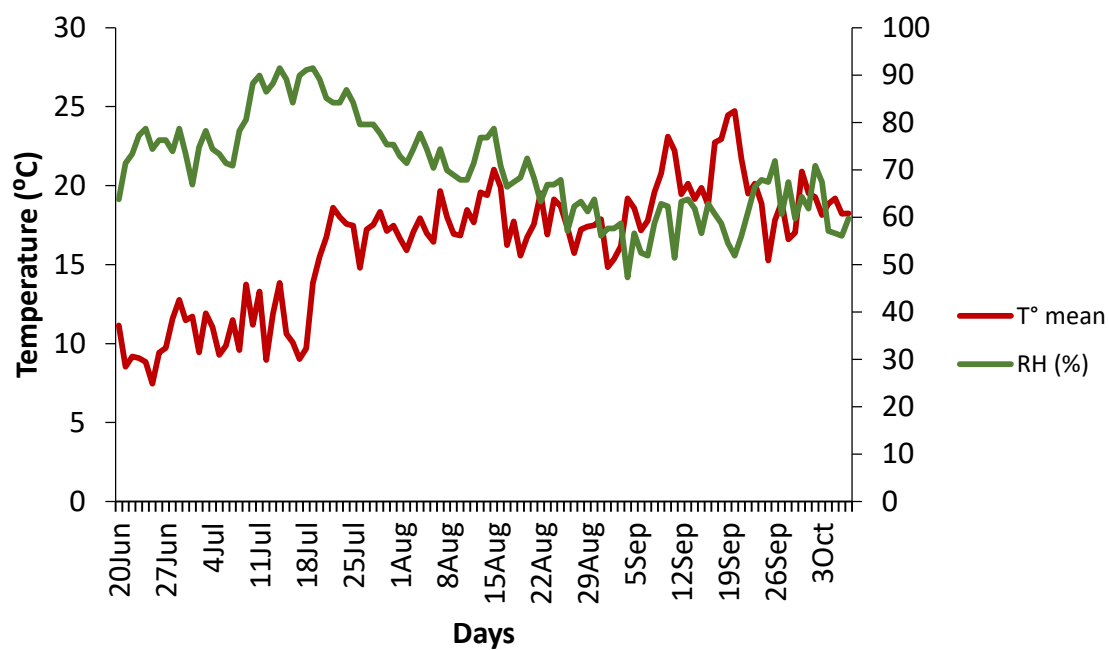


Figure S1. Temperature mean (T° mean) and relative humidity in the glasshouse in 2016. Data correspond to one week before the start of measurement.

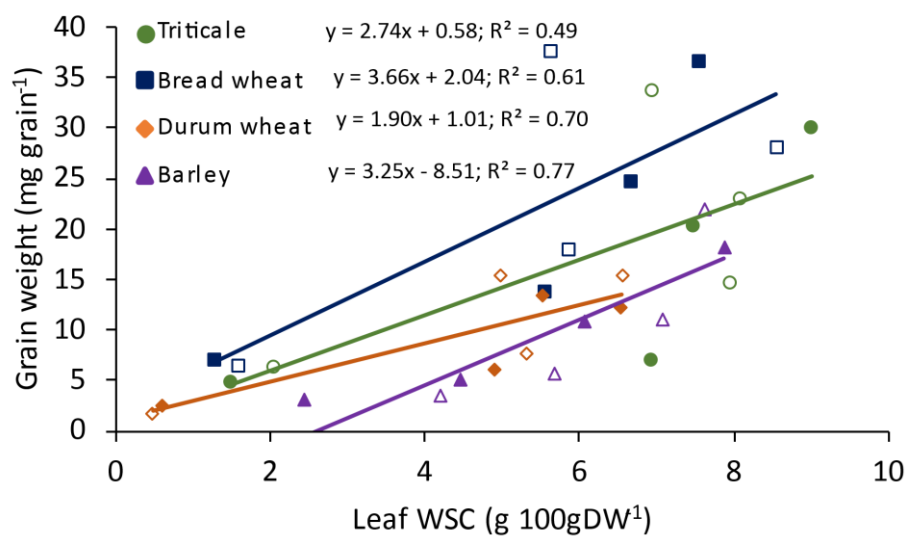


Figure S2. Relationship between water-soluble carbohydrate (WSC) content in leaves and the mean weight of the grain during the grain filling stage in triticale, bread wheat, durum wheat and barley, grown under water-limited (open symbols) and well-watered regimes (closed symbols). Values are means of three replicates. There were no statistically significant differences among the slopes.

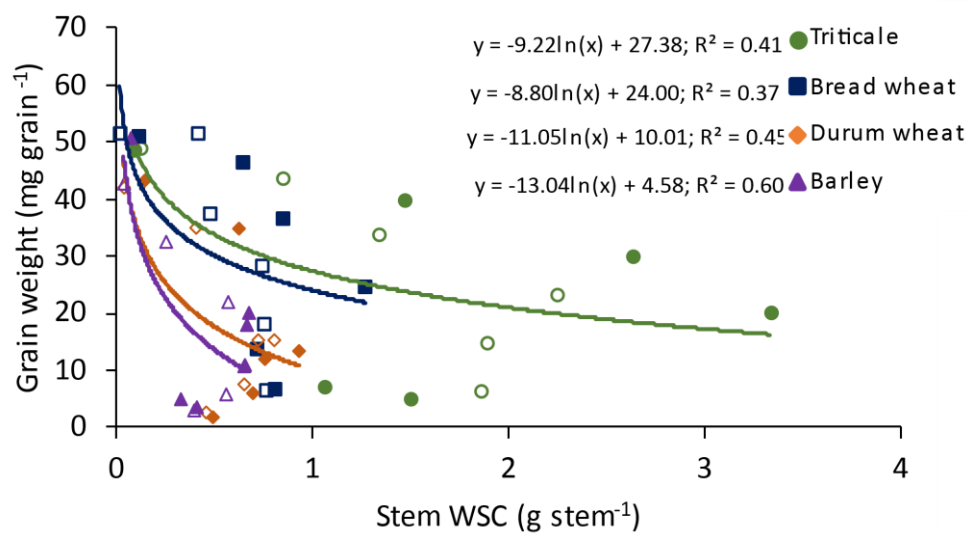
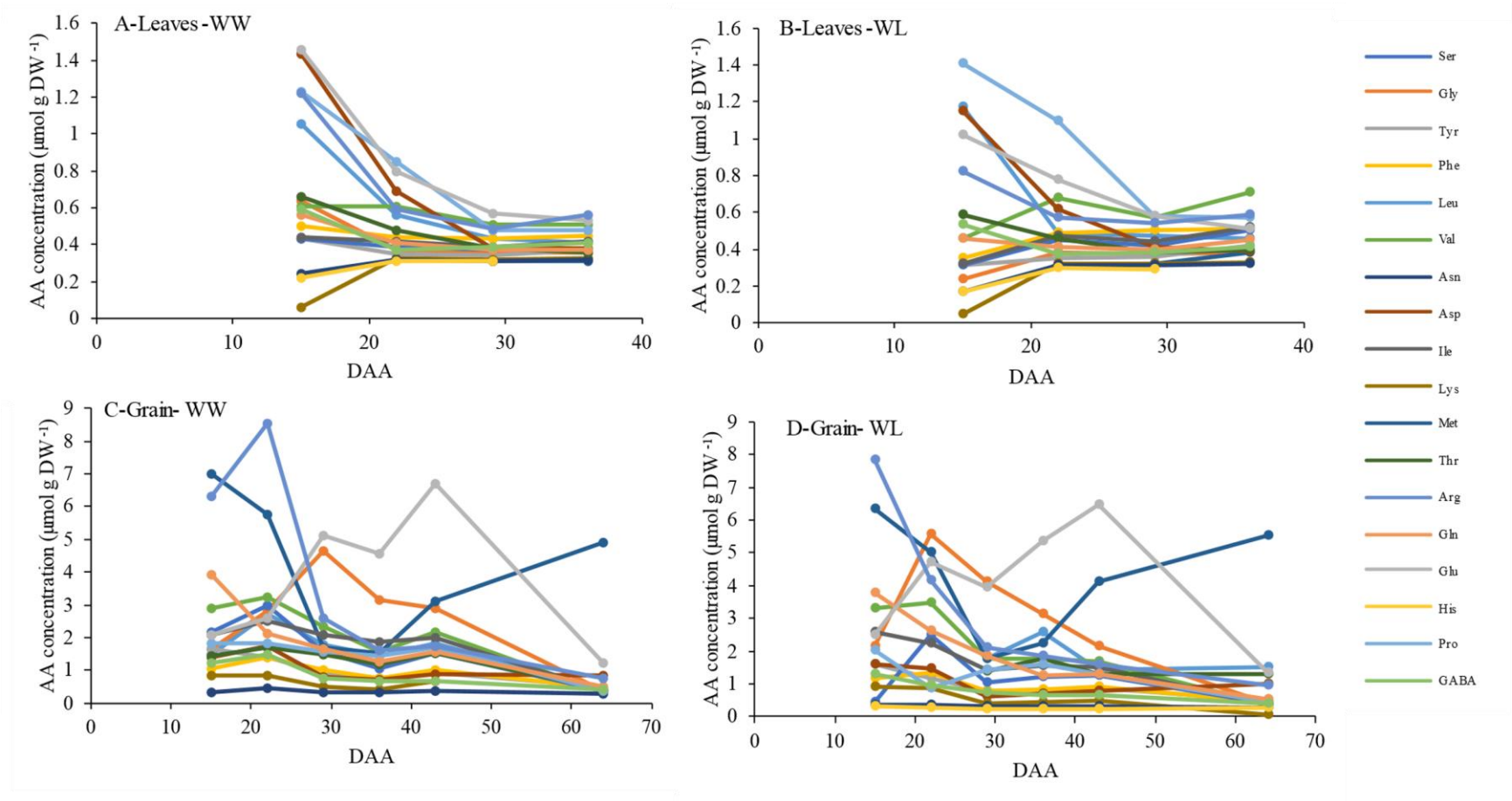
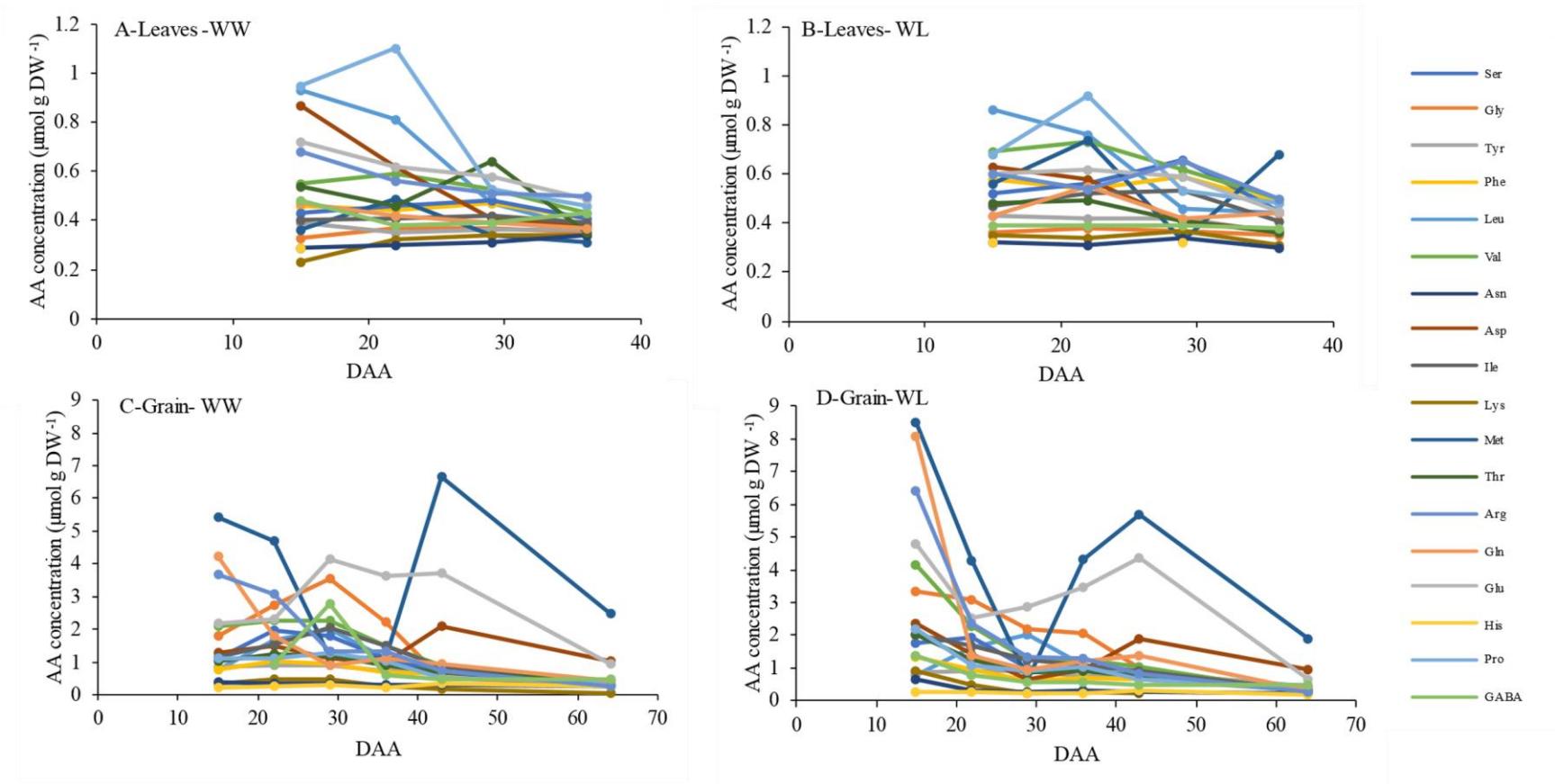


Figure S3. Relationship between water-soluble carbohydrate (WSC) content in stems and the weight of a single grain during the grain filling period, of the four cereals triticale, bread wheat, durum wheat and barley, grown under water-limited (open symbols) and well-watered (closed symbols) regimes. Values are means of three replicates.

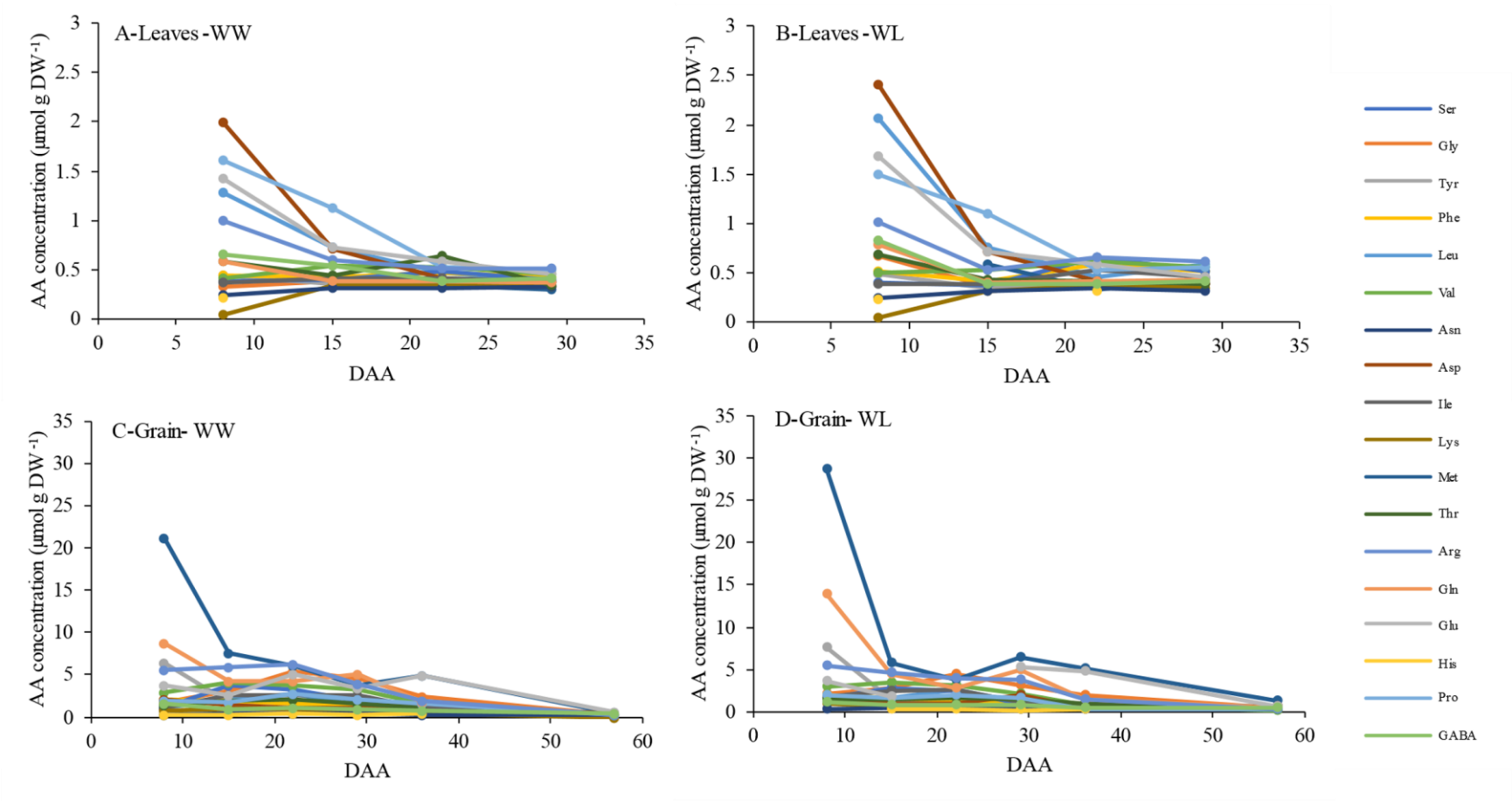
A) Triticale



B) Bread wheat



C) Durum wheat



D) Barley

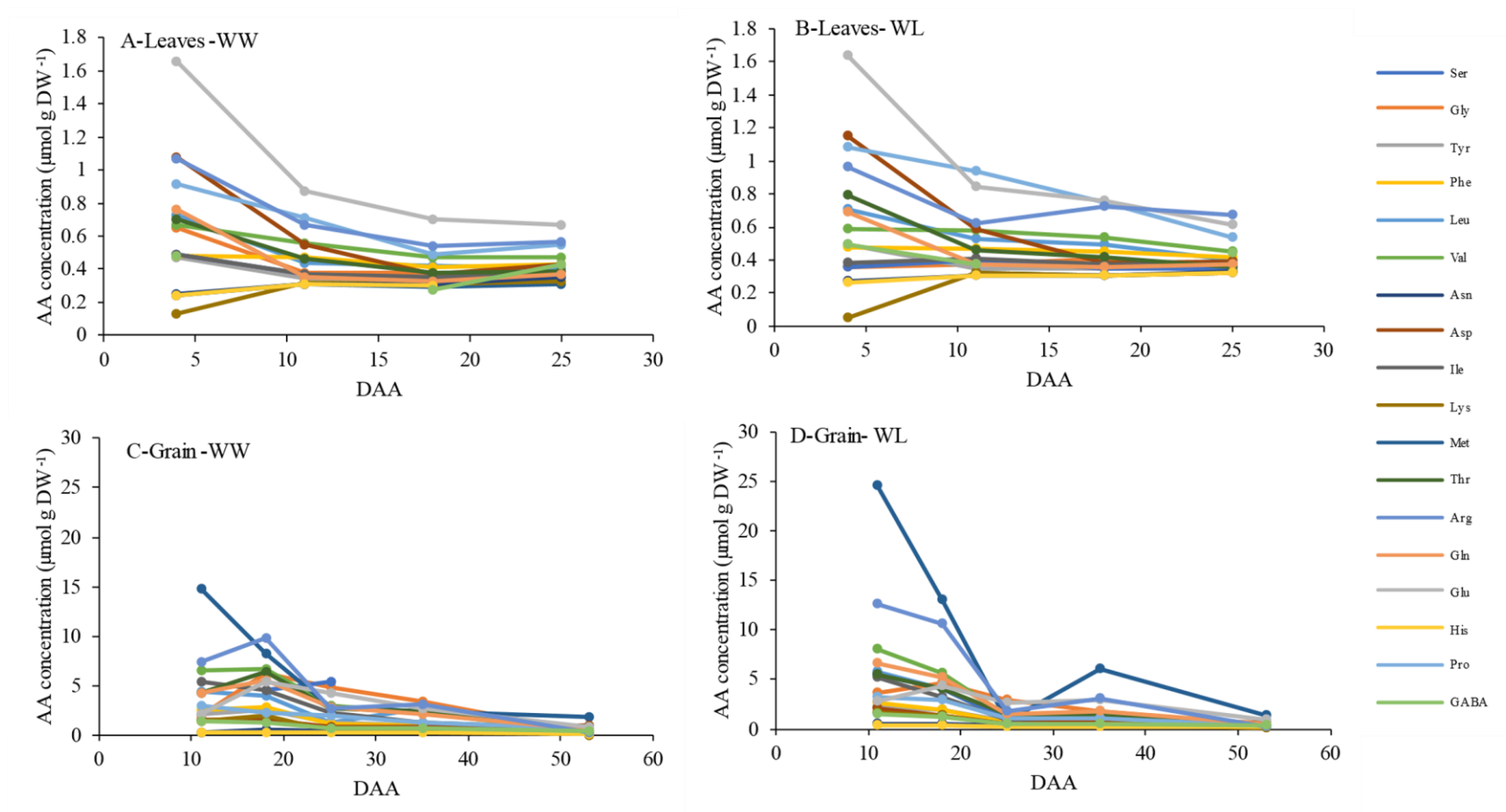


Figure S4. Concentration ($\mu\text{mol g DW}^{-1}$) of different amino acids in leaves and grain during the grain filling stage (in days after anthesis DAA) in triticale (A), bread wheat (B), durum wheat (C) and barley (D), grown under well-watered (WW) and water-limited (WL) regimes. Representation of the data sets has been separated according to species and plant part (leaves or grain) for better visualisation of the data.