Supplementary Materials: Evaluation of Phenolic Compounds and Carotenoids Content and Mycotoxins Occurrence in Grains of Seventeen Barley and Eight Oat Cultivars Grown under Organic Management

Renata Kazimierczak, Dominika Średnicka-Tober, Danuta Leszczyńska, Anna Nowacka, Ewelina Hallmann, Marcin Barański, Klaudia Kopczyńska and Bogusław Gnusowski

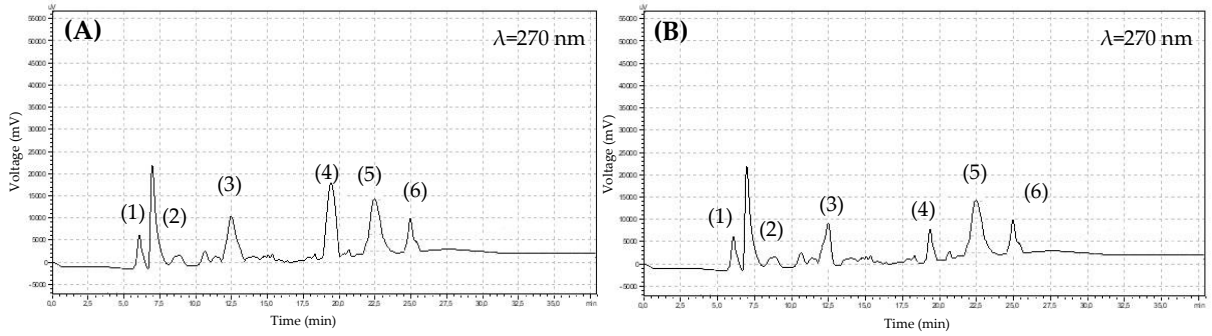

Figure S1. Chromatograms showing retention time for phenolic acids identified in organic oat grains (**A**): (1) gallic acid (0.40 μg mL^{-1}), (2) *t*-cinnamic acid (0.40 μg mL^{-1}), (3) caffeic acid (0.30 μg mL^{-1}), (4) ferulic acid (9.59 μg mL^{-1}), (5) sinapic acid (0.28 μg mL^{-1}), (6) *p*-coumaric acid (0.82 μg mL^{-1}); and in organic barley grains (**B**): (1) gallic acid (0.30 μg mL^{-1}), (2) *t*-cinnamic acid (0.10 μg mL^{-1}), (3) caffeic acid (0.08 μg mL^{-1}), (4) ferulic acid (4.07 μg mL^{-1}), (5) sinapic acid (0.27 μg mL^{-1}), (6) *p*-coumaric acid (0.79 μg mL^{-1}).

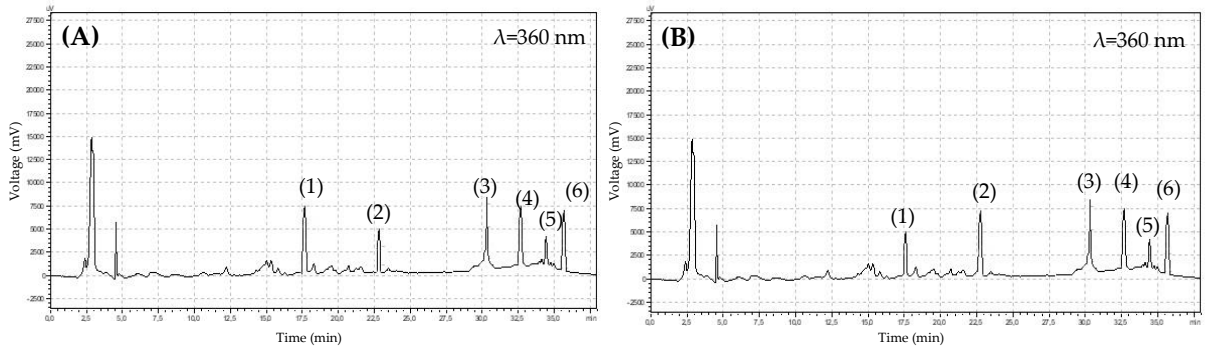

Figure S2. Chromatograms showing retention time for flavonoids identified in organic oat grains (**A**): (1) quercetin-3-*O*-rutinoside (1.29 μg mL^{-1}), (2) kaempferol-3-*O*-glucoside (0.78 μg mL^{-1}), (3) luteolin (0.42 μg mL^{-1}), (4) quercetin (0.46 μg mL^{-1}), (5) apigenin (1.16 μg mL^{-1}), (6) kaempferol (1.18 μg mL^{-1}); and in organic barley grains (**B**): (1) quercetin-3-*O*-rutinoside (0.62 μg mL^{-1}), (2) kaempferol-3-*O*-glucoside (0.65 μg mL^{-1}), (3) luteolin (0.50 μg mL^{-1}), (4) quercetin (0.65 μg mL^{-1}), (5) apigenin (1.91 μg mL^{-1}), (6) kaempferol (2.04 μg mL^{-1}).

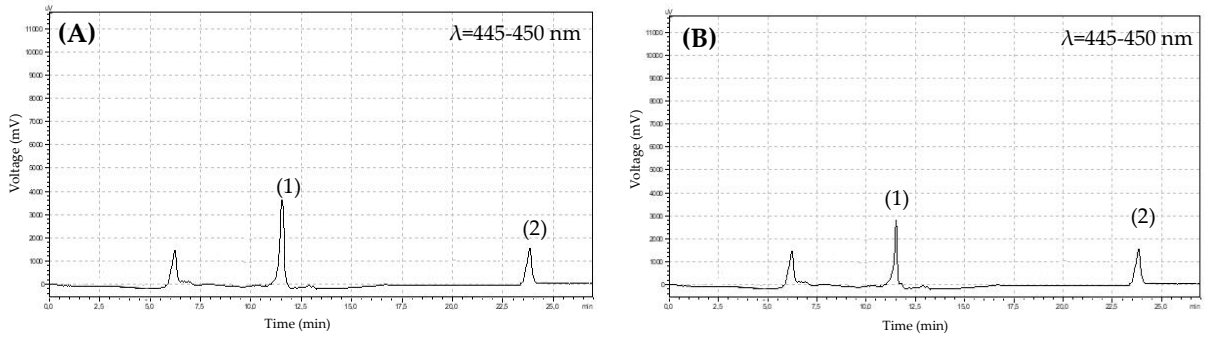

Figure S3. Chromatograms showing retention time for carotenoids in organic oat grains (**A**): (1) lutein (1.73 μg mL^{-1}), (2) β-carotene (0.03 μg mL^{-1}); and in organic barley grains (**B**): (1) lutein (1.33 μg mL^{-1}), (2) β-carotene (0.03 μg mL^{-1}).

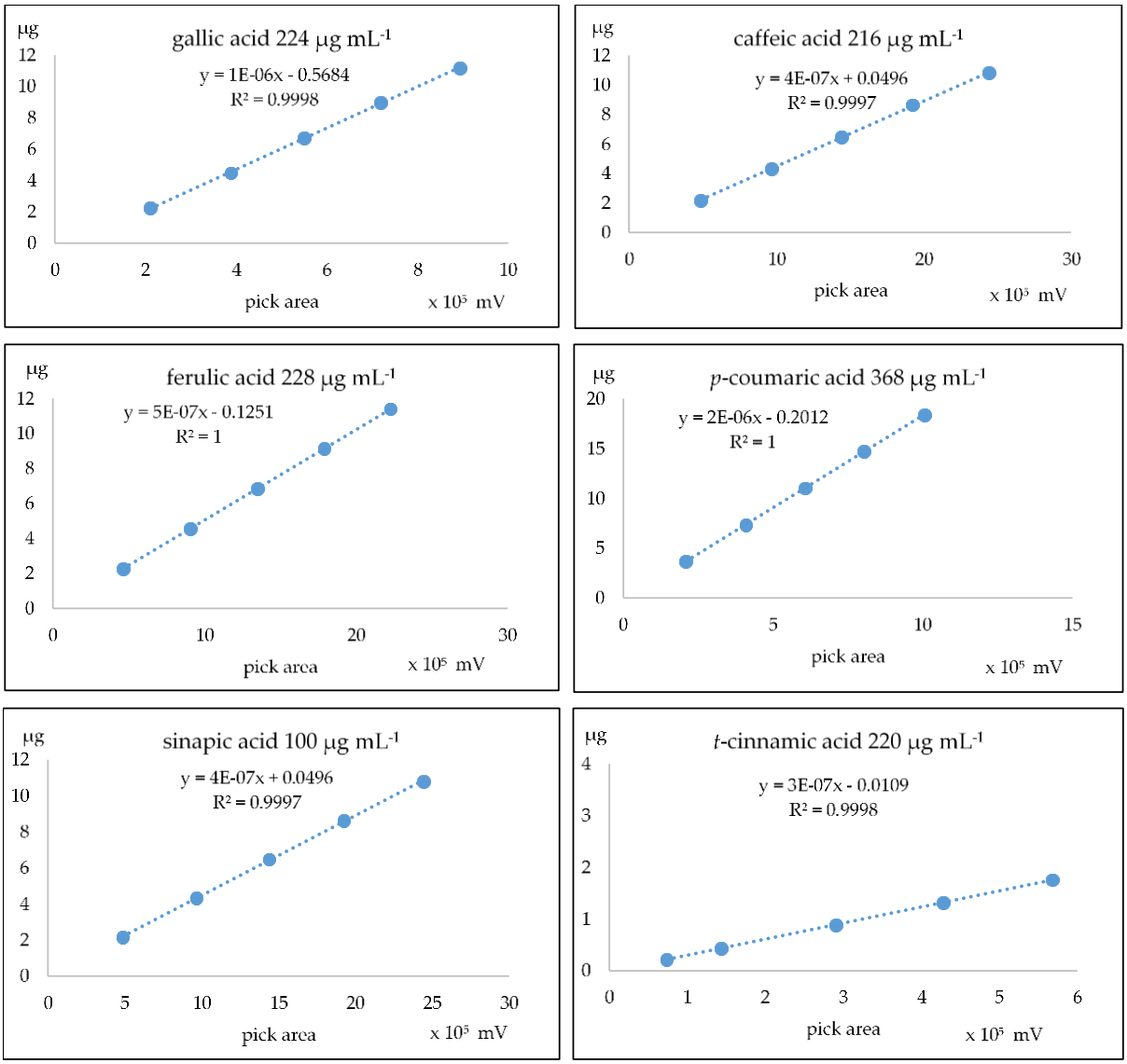

Figure S4. Standard curves with R^2 for all identified phenolic acids in cereal grains.

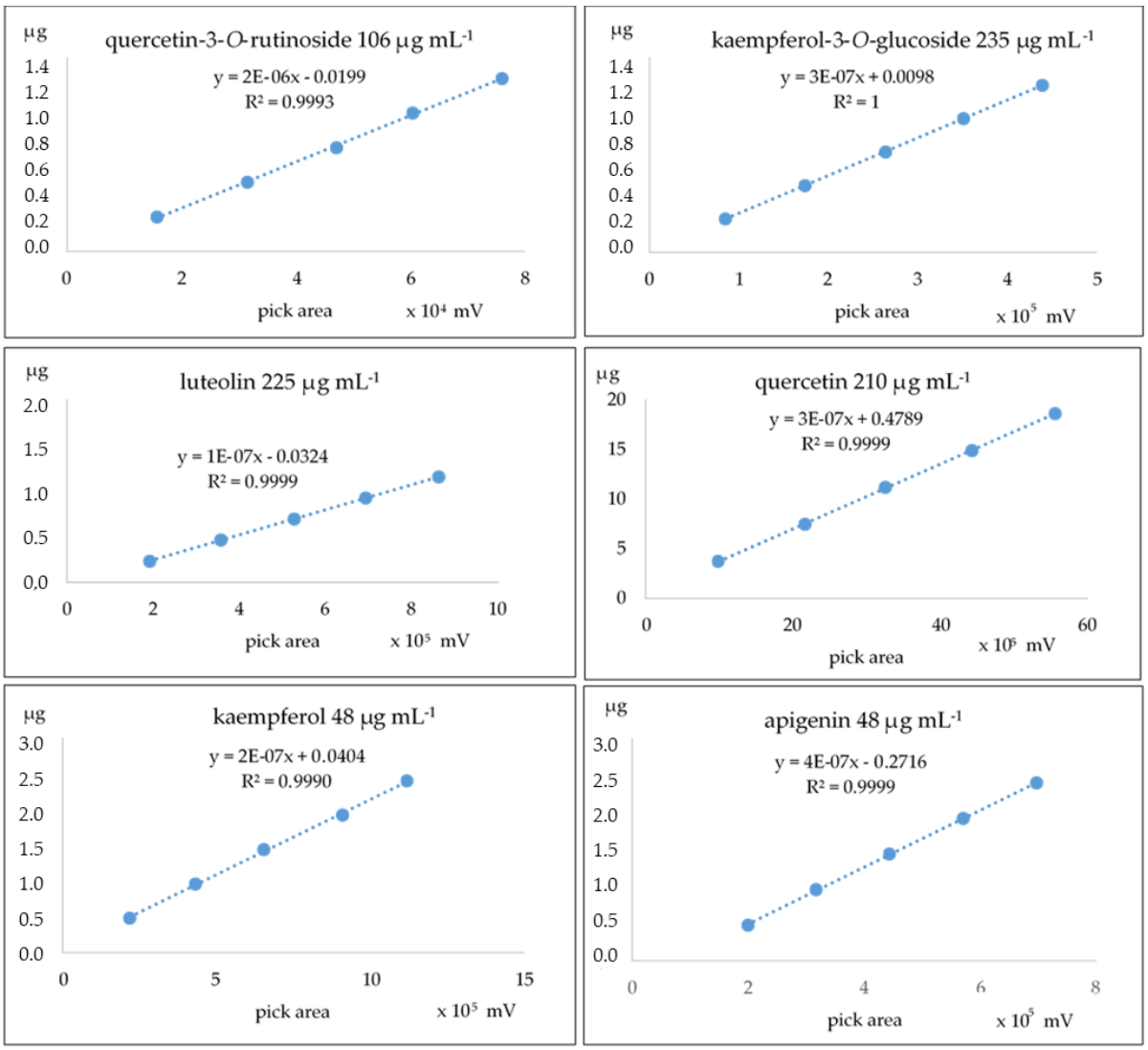

Figure S5. Standard curves with R^2 for all identified flavonoids in cereal grains.

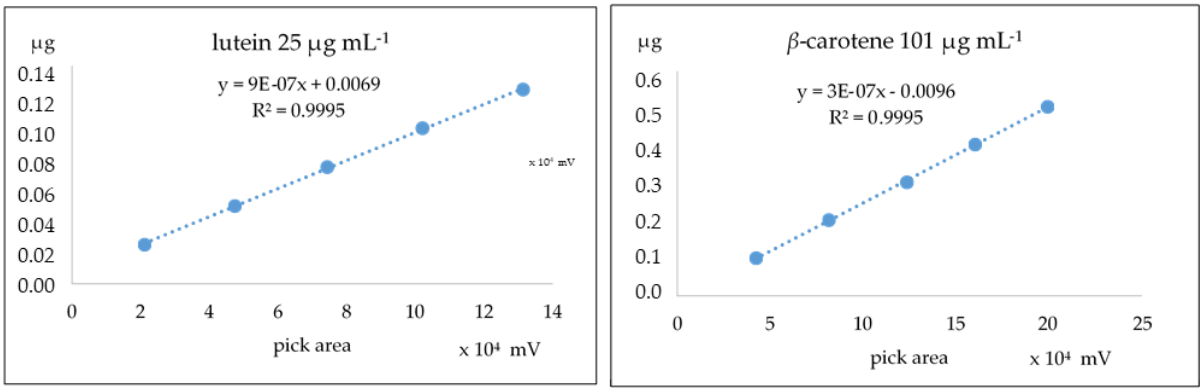

Figure S6. Standard curves with R^2 for the identified carotenoids in cereal grains.

Table S1. Multiple reaction monitoring (MRM) transitions with retention times, ion ratio, declustering potential, collision energy and cell exit potential used to detect target mycotoxins using a single method with negative and positive polarity.

Mycotoxin	MRM (qualifier)	MRM (qualifier)	Ratio	DP1 [1] (V)	CE2 [2] (V)	CXP3 [3] (V)	RT4 [4] (min)	Polarity
Aflatoxin B1 (AFLB1)	313/285	313/241	0.81	135/135	31/49	16/12	6.51	ESI+
Aflatoxin B2 (AFLB2)	315/287	315/259	0.74	141/141	35/39	14/14	6.31	ESI+
Aflatoxin G1 (AFLG1)	329/243	329/200	0.62	140/140	37/54	14/12	6.12	ESI+
Aflatoxin G2 (AFLG2)	331/313	331/189	0.43	150/150	33/54	16/10	5.89	ESI+
Aflatoxin B1–13C17 (AFLB1–13C17)	330/301			141	33	16	6.50	ESI+
Deoxynivalenol (DON)	341/265	341/295	0.94	-40/-40	-14/-14	-15/-17	3.18	ESI-
3-acetyldeoxynivalenol (3-AcDON)	383/337	383/307	0.80	-45/-45	-12/-12	-19/-19	5.29	ESI-
15-acetyldeoxynivalenol (15-AcDON)	339/231	339/137	0.65	96/96	10/10	15/15	5.27	ESI+
Fumonisin B1 (FB1)	722/334	722/704	0.60	126/126	39/53	32/18	7.48	ESI+
Fumonisin B2 (FB2)	706/336	706/688	0.49	126/126	49/37	18/32	8.25	ESI+
HT-2 toxin	447/345	447/285	0.79	136/136	25/27	18/16	7.18	ESI+
T-2 toxin	489/245	489/387	0.63	231/231	35/29	12/20	7.65	ESI+
Ochratoxin (OTA)	404/239	404/221	0.31	81/81	31/47	12/12	7.99	ESI+
Nivalenol (NIV)	357/281	357/311	1.20	-5/-5	-10/-20	-14/-11	1.84	ESI-
Zearalenone (ZEA)	317/175	317/273	0.70	-135/-135	-32/-26	-11/-17	7.98	ESI-

[1] Declustering potential (DP); [2] Collision energy (CE); [3] Cell exit potential (CXP); [4] Retention time (RT)

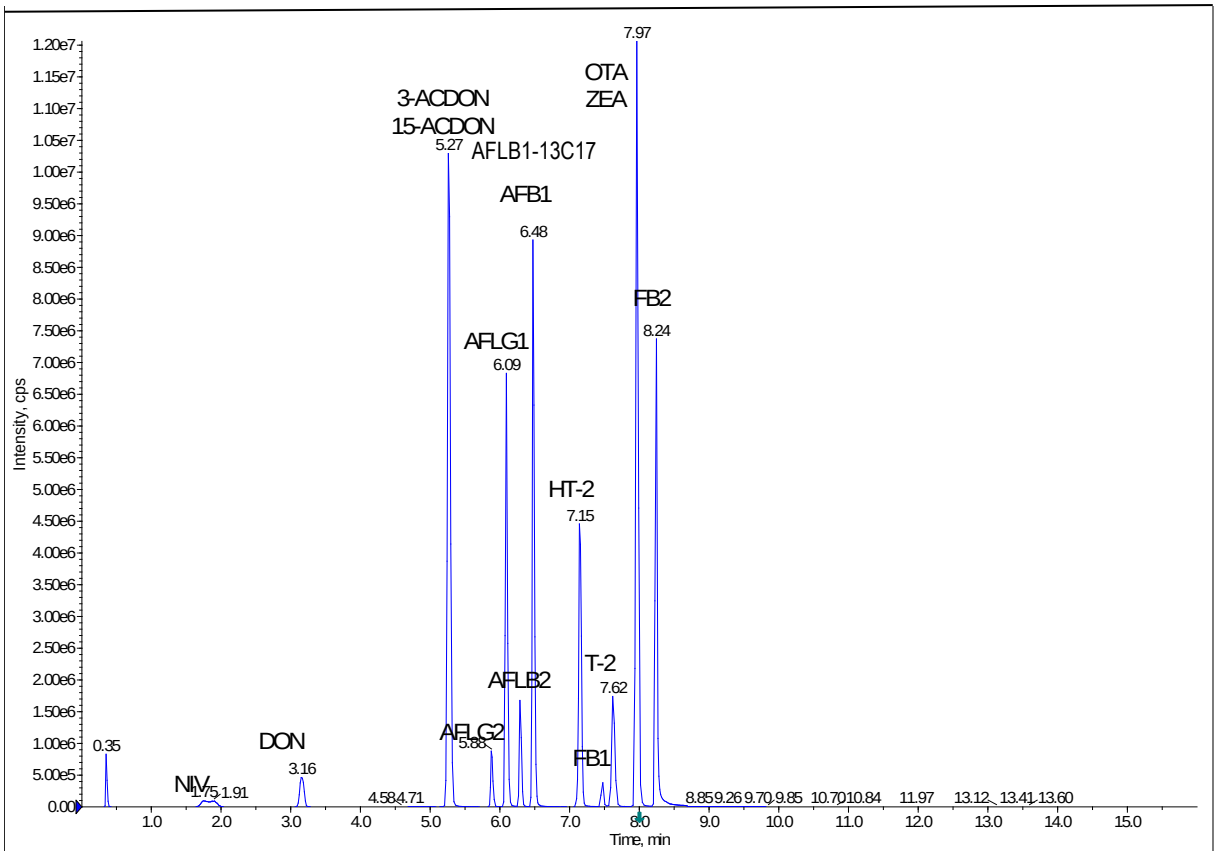

Figure S7. Total ion chromatogram of mycotoxins.

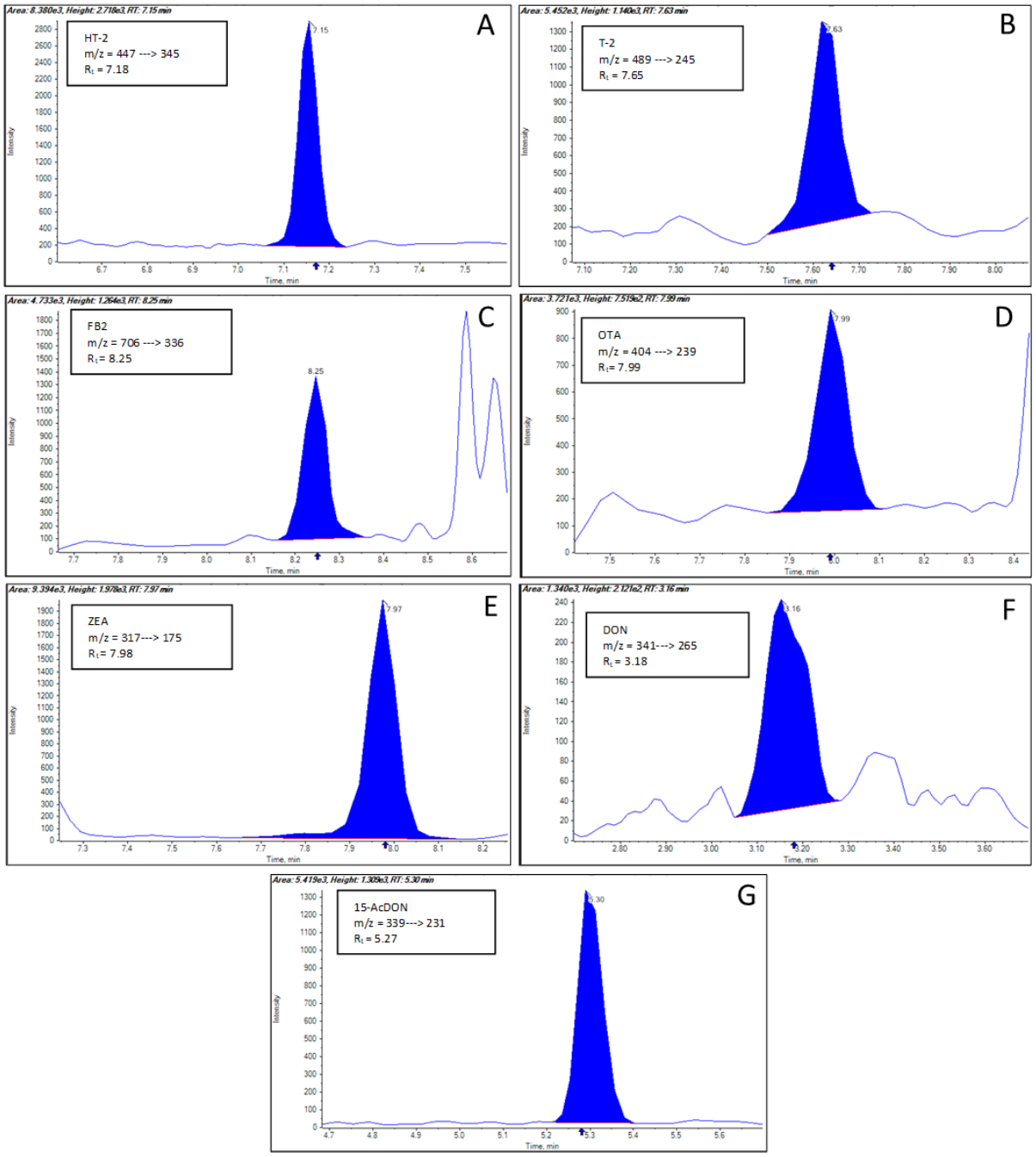

Figure S8. LC-MS/MS chromatograms of mycotoxins in representative grain samples: A - HT-2 toxin (HT-2) (3.42 μg kg^{-1}); B - T-2 toxin (T-2) (3.55 μg kg^{-1}); C - fumonisin B2 (FB2) (33.74 μg kg^{-1}); D - ochratoxin A (OTA) (1.53 μg kg^{-1}); E - zearalenone (ZEA) (8.00 μg kg^{-1}); F - deoxynivalenol (DON) (58.71 μg kg^{-1}) (barley, Soldo); G - 15-acetyldeoxynivalenol (15-AcDON) (2.28 μg kg^{-1}) (oat, Arden).