

Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Simultaneous determination of major type A and B trichothecenes, zearalenone and certain modified metabolites in Finnish cereal grains with a novel liquid chromatography-tandem mass spectrometric method

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Table S1 Method performance characteristics and validation parameters determined in barley

Analyte	SSE (%)	LOD (µg/kg)	LOQ (µg/kg)	R ²	Ion ratio (Quan/Qual)	Apparent recovery ± RSD _R (%) (n = 18)		
						Low	Medium	High
3Ac-DON	109	3.4	10.2	0.993	0.3	110 ± 19	97 ± 9	99 ± 6
DON	78	1.2	3.6	0.995	1.4	102 ± 15	99 ± 12	90 ± 7
DON3Glc	74	2.8	8.4	0.994	1.1	93 ± 18	103 ± 27	101 ± 3
HT2	116	3.1	9.3	0.999	1.1	98 ± 6	102 ± 5	102 ± 6
HT2-3-Glc	121	4.1	12.3	0.993	0.6	100 ± 22	94 ± 26	102 ± 9
NIV	81	3.1	9.3	0.995	1.3	95 ± 15	99 ± 10	100 ± 9
NIV3Glc	59	3.5	10.5	0.989	4.9	90 ± 35	92 ± 23	96 ± 29
T2	107	2.5	7.5	0.999	0.8	96 ± 6	103 ± 4	103 ± 4
ZEN	84	2.0	6.0	0.999	1.2	115 ± 15	115 ± 5	116 ± 4
ZEN14Glc	89	0.1	0.3	0.998	2.4	93 ± 9	98 ± 26	99 ± 4
ZEN14Sulf	100	0.1	0.3	0.999	7.6	98 ± 8	102 ± 4	102 ± 4
ZEN16Glc	88	1.0	3.0	0.992	2.8	96 ± 29	97 ± 16	98 ± 8
α-ZEL	73	0.1	0.3	0.998	1.1	98 ± 10	99 ± 5	102 ± 4
α-ZEL14Glc	86	0.8	2.4	0.996	2.3	103 ± 18	103 ± 11	103 ± 5
β-ZEL	73	0.2	0.6	0.998	1.2	106 ± 12	98 ± 7	100 ± 8
β-ZEL14Glc	93	0.2	0.6	0.999	8.7	102 ± 7	102 ± 6	103 ± 4

Notes: SSE, signal suppression/enhancement ratio; LOD, limit of detection; LOQ, limit of quantification; R², coefficient of determination; Quan, quantifier ion; Qual, qualifier ion; RSD_R, inter-day precision

Table S2 Method performance characteristics and validation parameters determined in oats

Analyte	SSE (%)	LOD (µg/kg)	LOQ (µg/kg)	R ²	Ion ratio (Quan/Qual)	Apparent recovery ± RSD _R (%) (n = 18)		
						Low	Medium	High
3Ac-DON	122	5.1	15.3	0.988	0.3	97 ± 29	92 ± 15	98 ± 7
DON	77	1.8	5.4	0.996	2.7	91 ± 11	98 ± 10	100 ± 11
DON3Glc	114	3.9	11.7	0.989	1.1	96 ± 13	99 ± 7	94 ± 13
HT2	75	2.9	8.7	0.997	1.0	96 ± 16	100 ± 20	101 ± 8
HT2-3-Glc	62	4.2	12.6	0.986	0.6	101 ± 29	84 ± 7	106 ± 17
NIV	85	3.4	10.2	0.982	1.4	106 ± 18	111 ± 15	100 ± 15
NIV3Glc	93	5.3	15.9	0.989	4.5	114 ± 28	93 ± 10	87 ± 20
T2	101	2.6	7.8	0.999	1.0	98 ± 11	100 ± 27	100 ± 7
ZEN	79	3.1	9.3	0.999	1.3	92 ± 13	92 ± 17	96 ± 10
ZEN14Glc	53	0.2	0.6	0.995	4.0	111 ± 16	104 ± 9	106 ± 12
ZEN14Sulf	116	0.1	0.3	0.998	6.9	103 ± 8	101 ± 12	101 ± 9
ZEN16Glc	75	0.3	0.9	0.989	4.4	108 ± 24	102 ± 12	106 ± 9
α-ZEL	69	0.3	0.9	0.997	1.1	92 ± 14	92 ± 18	97 ± 9
α-ZEL14Glc	110	2.5	7.5	0.990	2.5	115 ± 21	99 ± 13	101 ± 11
β-ZEL	92	0.4	1.2	0.997	1.2	100 ± 15	94 ± 22	97 ± 8
β-ZEL14Glc	105	5.1	15.3	0.995	9.1	97 ± 29	92 ± 15	98 ± 7

Notes: SSE, signal suppression/enhancement ratio; LOD, limit of detection; LOQ, limit of quantification; R², coefficient of determination; Quan, quantifier ion; Qual, qualifier ion; RSD_R, inter-day precision