

Investigation of multimycotoxins by LC-MS/MS in maize semolina chips

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Electronic supplementary material

Supplementary Tables S1–S3

Table S1. Tandem mass spectrometry (MS-MS) ion transitions

Mycotoxin	Precursor ion <i>m/z</i>	Product ion <i>m/z</i>	Ret. time (min)	Delta ret. time (min)	Fragmentor (V)	Collision energy (V)	Cell accelerator voltage (V)	Polarity
AFB ₁	313.2	269.9	4.80	1.08	130	28	7	positive
AFB ₁	313.2	257.0	4.80	1.08	130	24	7	positive
AFB ₁	313.2	285.2	4.80	1.08	130	12	7	positive
AFB ₂	315.1	287.0	4.64	1.18	130	24	7	positive
AFB ₂	315.1	259.0	4.64	1.18	130	32	7	positive
AFB ₂	315.1	243.0	4.64	1.18	130	44	7	positive
AFG ₁	329.1	311.0	4.43	1.06	100	20	7	positive
AFG ₁	329.1	282.9	4.43	1.06	100	24	7	positive
AFG ₁	329.1	243.1	4.43	1.06	100	28	7	positive
AFG ₂	331.0	313.0	4.25	0.73	90	24	7	positive
AFG ₂	331.0	245.0	4.25	0.73	90	32	7	positive
AFG ₂	331.0	216.9	4.25	0.73	90	40	7	positive
CIT	251.1	233.0	5.39	1.13	88	12	7	positive
CIT	251.1	205.0	5.39	1.13	88	28	7	positive
CIT	251.1	91.0	5.39	1.13	88	50	7	positive
DON	297.1	249.1	2.39	2.82	90	8	7	positive
DON	297.1	231.0	2.39	2.82	90	8	7	positive
DON	297.1	202.9	2.39	2.82	90	12	7	positive
FB ₁	722.4	704.3	5.11	0.99	116	32	7	positive
FB ₁	722.4	352.2	5.11	0.99	116	40	7	positive
FB ₁	722.4	334.2	5.11	0.99	116	44	7	positive
FB ₂	706.4	337.1	5.66	0.60	90	32	7	positive
FB ₂	706.4	319.0	5.66	0.60	90	36	7	positive
HT-2 toxin	442.2	263.2	5.30	0.96	80	8	7	positive
HT-2 toxin	442.2	197.2	5.30	0.96	80	12	7	positive
OTA	404.1	358.0	5.98	1.01	102	12	7	positive
OTA	404.1	238.9	5.98	1.01	102	24	7	positive
OTA	404.1	220.9	5.98	1.01	102	40	7	positive
T-2 toxin	484.2	305.0	5.63	1.06	88	8	7	positive
T-2 toxin	484.2	215.0	5.63	1.06	88	16	7	positive
T-2 toxin	484.2	185.0	5.63	1.06	88	20	7	positive
ZEN	317.2	273.1	6.07	1.05	130	12	7	negative
ZEN	317.2	175.1	6.07	1.05	130	20	7	negative

AFB₁ – aflatoxin B₁; AFB₂ – aflatoxin B₂; AFG₁ – aflatoxin G₁; AFG₂ – aflatoxin G₂; CIT – citrinin; DON – deoxynivalenol; FB₁ – fumonisin B₁; FB₂ – fumonisin B₂; FB₁ – fumonisin B₁; FB₂ – fumonisin B₂; OTA – ochratoxin A; ZEN – zearalenone; ret. – retention

Table S2. Recovery results in multitoxin analysis

Mycotoxin	LOD ($\mu\text{g}\cdot\text{kg}^{-1}$)	LOQ ($\mu\text{g}\cdot\text{kg}^{-1}$)	Recovery rate (%)	Standard uncertainty (%)
DON	29.50	95.00	91.6	13.5
AFG ₂	0.24	0.78	96.8	15.6
AFG ₁	0.22	0.74	92.9	29.1
AFB ₂	0.26	0.82	94.7	17.5
AFB ₁	0.24	0.78	95.2	16.9
FB ₁	31.10	103.00	97.7	12.2
HT-2 toxin	3.32	11.10	103.5	18.5
CIT	30.40	101.00	99.7	14.3
T-2 toxin	3.16	10.60	102.6	16.9
FB ₂	17.10	57.00	90.5	17.5
OTA	0.26	0.85	94.2	12.5
ZEN	2.94	9.80	94.0	13.9

AFB₁ – aflatoxin B₁; AFB₂ – aflatoxin B₂; AFG₁ – aflatoxin G₁; AFG₂ – aflatoxin G₂; CIT – citrinin; DON – deoxynivalenol; FB₁ – fumonisin B₁; FB₂ – fumonisin B₂; FB₁ – fumonisin B₁; FB₂ – fumonisin B₂; OTA – ochratoxin A; ZEN – zearalenone; LOD – limit of detection; LOQ – limit of quantification

Table S3. R^2 and regression equations

Mycotoxin	R^2	Regression equation
DON	0.9966	$y = 151.92x - 3\,103.2$
AFG ₂	0.9984	$y = 1\,297.9x - 245.7$
AFG ₁	0.9995	$y = 3\,158.9x - 544.43$
AFB ₂	0.9990	$y = 3\,586x - 28$
AFB ₁	0.9987	$y = 1\,445.7x - 198.24$
FB ₁	0.9900	$y = 2\,504.2x - 44\,501$
HT-2 toxin	0.9952	$y = 129.57x + 23.176$
CIT	0.9945	$y = 97\,629x - 195\,108$
T-2 toxin	0.9975	$y = 2\,770.5x - 72\,452$
FB ₂	0.9915	$y = 823.2x - 16\,704$
OTA	0.9930	$y = 278\,759x - 77\,871$
ZEN	0.9926	$y = 268.51x - 320.81$

AFB₁ – aflatoxin B₁; AFB₂ – aflatoxin B₂; AFG₁ – aflatoxin G₁; AFG₂ – aflatoxin G₂; CIT – citrinin; FB₁ – fumonisin B₁; FB₂ – fumonisin B₂; DON – deoxynivalenol; FB₁ – fumonisin B₁; FB₂ – fumonisin B₂; OTA – ochratoxin A; ZEN – zearalenone; R^2 – correlation coefficient