Supporting Tables

Supporting Table S1. Mycotoxin Information (Name, CAS Registry Number, Molecular Structure, Formula, and Weight), Precursor Ion and Weight, and Retention Times used in the UHPLC-High Resolution Mass Spectrometry Analysis of Finished Grain and Nut Products

Supporting Table S2. Resolution studies for mycotoxins in acetonitrile/water. Mass accuracies (ppm) of molecular ions of each mycotoxin evaluated in the study based on mycotoxin type, resolution (17,500, 35,000, 70,000 and 140,000) and concentration (1, 10 and 100 ng/mL). Each mass accuracy result is an average ± standard deviation from triplicate experiments.

Supporting Table S3. Resolution studies for mycotoxins in peanut matrix extracted with acetonitrile/water. Mass accuracies (ppm) of molecular ions of each mycotoxin evaluated in the study based on mycotoxin type, resolution (17,500, 35,000, 70,000 and 140,000) and concentration (1, 10 and 100 ng/mL). Each mass accuracy result is an average ± standard deviation from triplicate experiments.

Supporting Table S4. Resolution studies for mycotoxins in wheat matrix extracted with acetonitrile/water. Mass accuracies (ppm) of molecular ions of each mycotoxin evaluated in the study based on mycotoxin type, resolution (17,500, 35,000, 70,000 and 140,000) and concentration (1, 10 and 100 ng/mL). Each mass accuracy result is an average ± standard deviation from triplicate experiments.

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Supporting Table S5. % Average Abundances, % RSDs and % Differences of M+1 and M+2 isotopes (and M+3 isotope for ochratoxin A) relative to the M isotopes for mycotoxin analysis in this study obtained from mycotoxins fortified at 1, 10 and 100 ng/mL in acetonitrile/water and acetonitrile/water extracts obtained from peanut and wheat matrices (n = 9 each at each level and different matrices). % Difference is defined by 100 x [Average Abundance – Theoretical Abundance]/Theoretical Abundance.

Supporting Table S6. Mycotoxin concentrations (average ± standard deviation, n = 3) found in finished cereal and nut products. (-) indicates none of the mycotoxins were detected with the Q-Orbitrap method. Numerical values labeled in red (avg ± SD) are LC-MS/MS results obtained from *J. Agric. Food Chem.* **2013**, *61*, 4771-4782.

Supporting Table S7. Experimental Masses and Mass Accuracies of Ions used in the Identification of Mycotoxins in Solvent (50:50 Acetonitrile:Water Mixture).

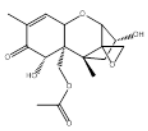
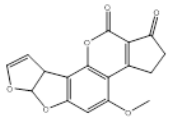
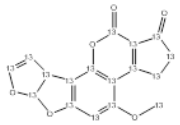
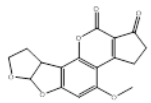
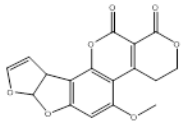
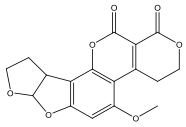
Supporting Table S8. Experimental Masses and Mass Accuracies of Ions used in the Identification of Mycotoxins in Peanut Matrix extracted with 50:50 Acetonitrile:Water Mixture.

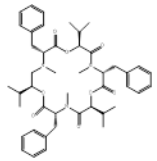
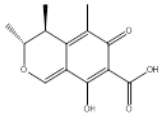
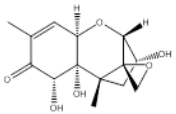
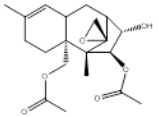
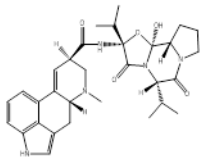
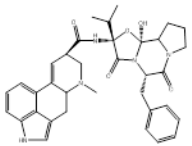
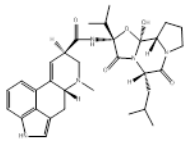
Supporting Table S9. Experimental Masses and Mass Accuracies of Ions used in the Identification of Mycotoxins in Wheat Matrix extracted with 50:50 Acetonitrile:Water Mixture.

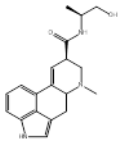
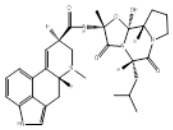
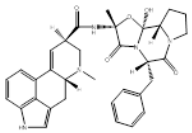
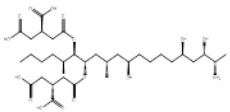
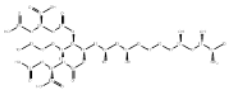
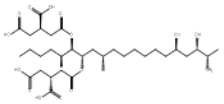
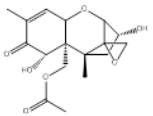
Supporting Table S10. Experimental Masses and Mass Accuracies of Ions used in the Identification of Isotope-labeled Mycotoxins in Solvent (50:50 Acetonitrile:Water) and Peanut and Wheat Matrices extracted with 50:50 Acetonitrile:Water Mixture.

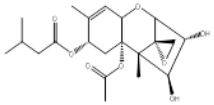
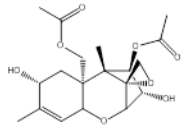
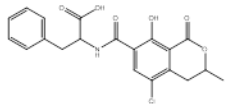
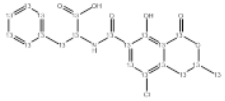
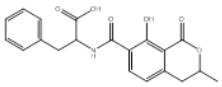
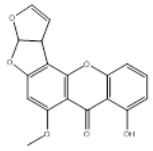
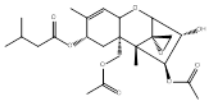
Supporting Table S11. Molecular ions and % ion ratios used to identify mycotoxins, including proposed molecular formulae and theoretical masses. Average ion ratios (% Avg) and relative standard deviations (RSD) based on triplicate results each of the mycotoxins fortified in solvent (acetonitrile:water) and acetonitrile:water extracts from peanut and wheat matrices at 1, 10 and 100 ng/mL. The % ion ratio was determined by the ratio of the ion signal responses extracted of the ion to the response with the signal of the molecular or fragment ion (indicated in bold) of the highest signal intensity.

Supporting Table 1. Mycotoxin Information (Name, CAS Registry Number, Molecular Structure, Formula, and Weight), precursor Ion and Weight, and Retention Times used in the UHPLC-High Resolution Mass Spectrometry Analysis of Finished Grain and Nut Products

Compound	CAS Number	Molecular Structure	Molecular Formula	Molecular Weight	Precursor Ion	Precursor Ion Weight	Retention Time (min)
5-Acetyl Deoxynivalenol	88337-96-6		$C_{17}H_{22}O_7$	338.13655	$[M+NH_4]^+$	356.17038	6.37
Aflatoxin B_1	1162-65-8		$C_{17}H_{12}O_6$	312.06339	$[M+H]^+$	313.07066	7.49
($^{13}C_{17}$)-Aflatoxin B_1	1217449-45-0		$^{13}C_{17}H_{12}O_6$	329.12042	$[M+H]^+$	330.12770	7.50
Aflatoxin B_2	7220-81-7		$C_{17}H_{14}O_6$	314.07904	$[M+H]^+$	315.08631	7.35
Aflatoxin G_1	1165-39-5		$C_{17}H_{12}O_7$	328.05830	$[M+H]^+$	329.06558	7.11
Aflatoxin G_2	7241-98-7		$C_{17}H_{14}O_7$	330.07395	$[M+H]^+$	331.08123	6.94

Compound	CAS Number	Molecular Structure	Molecular Formula	Molecular Weight	Precursor Ion	Precursor Ion Weight	Retention Time (min)
Beauvreicin	26048-05-5		$C_{45}H_{57}N_3O_9$	783.40948	$[M+NH_4]^+$	801.44331	9.69
Citrinin	518-75-2		$C_{13}H_{14}O_5$	250.08412	$[M+H]^+$	251.09140	7.47
Deoxynivalenol	51481-10-8		$C_{15}H_{20}O_6$	296.12599	$[M+H]^+$	297.13326	5.07, 5.20
Diacetoxyscirpenol	2270-40-8		$C_{19}H_{26}O_7$	366.16785	$[M+NH_4]^+$	384.20168	7.28
Ergocornine	564-36-3		$C_{31}H_{39}N_5O_5$	561.29512	$[M+H]^+$	562.30240	7.52, 7.84
Ergocristine	511-08-0		$C_{35}H_{39}N_5O_5$	609.29512	$[M+H]^+$	610.30240	7.89, 8.13
Ergocryptine	511-09-1		$C_{32}H_{41}N_5O_5$	575.31077	$[M+H]^+$	576.31805	7.80, 8.04

Compound	CAS Number	Molecular Structure	Molecular Formula	Molecular Weight	Precursor Ion	Precursor Ion Weight	Retention Time (min)
Ergometrine	60-79-7		$C_{19}H_{23}N_3O_2$	325.17903	$[M+H]^+$	326.18630	5.48, 5.53
Ergosine	561-94-4		$C_{30}H_{37}N_5O_5$	547.27947	$[M+H]^+$	548.28675	7.34, 7.41
Ergotamine	113-15-5		$C_{33}H_{35}N_5O_5$	581.26382	$[M+H]^+$	582.27110	7.47, 7.56
Fumonisin B_1	116355-83-0		$C_{34}H_{59}NO_{15}$	721.38847	$[M+H]^+$	722.39575	8.06
($^{13}C_{34}$)-Fumonisin B_1			$^{13}C_{34}H_{59}NO_{15}$	755.50253	$[M+H]^+$	756.50981	8.07
Fumonisin B_2	116355-84-1		$C_{34}H_{59}NO_{14}$	705.39356	$[M+H]^+$	706.40083	8.67
Fusarenon-X	88337-96-6		$C_{17}H_{22}O_8$	354.13147	$[M+H]^+$	355.13874	5.63, 5.72

Compound	CAS Number	Molecular Structure	Molecular Formula	Molecular Weight	Precursor Ion	Precursor Ion Weight	Retention Time (min)
HT-2	26934-87-2		$C_{22}H_{32}O_8$	424.20972	$[M+NH_4]^+$	442.24354	7.83
Neosolaniol	36519-25-2		$C_{19}H_{26}O_8$	382.16332	$[M+NH_4]^+$	400.19659	5.82, 5.89
Ochratoxin A	303-47-9		$C_{20}H_{18}ClNO_6$	403.08226	$[M+H]^+$	404.08954	8.54
($^{13}C_{20}$)-Ochratoxin A			$^{13}C_{20}H_{18}ClNO_6$	423.14936	$[M+H]^+$	424.15664	8.54
Ochratoxin B	4825-86-9		$C_{20}H_{19}NO_6$	369.12124	$[M+H]^+$	370.12851	8.10
Sterigmatocystin	10048-13-2		$C_{18}H_{12}O_6$	324.06339	$[M+H]^+$	325.07066	9.13
T-2	21259-20-1		$C_{24}H_{34}O_9$	466.22028	$[M+NH_4]^+$	484.25411	8.19

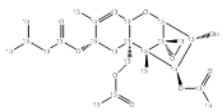
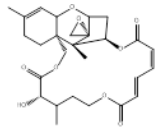
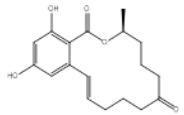
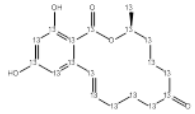
Compound	CAS Number	Molecular Structure	Molecular Formula	Molecular Weight	Precursor Ion	Precursor Ion Weight	Retention Time (min)
($^{13}C_{24}$)-T-2			$^{13}C_{24}H_{34}O_9$	490.30080	$[M+NH_4]^+$	508.33462	8.19
Verrucarin A	3148-09-2		$C_{27}H_{34}O_9$	502.22028	$[M+NH_4]^+$	520.25411	8.24
Zearalenone	17924-92-4		$C_{18}H_{22}O_5$	318.14672	$[M+H]^+$	319.15400	8.74
($^{13}C_{18}$)-Zearalenone			$^{13}C_{18}H_{22}O_5$	336.20711	$[M+H]^+$	337.21439	8.73

Table S2. Resolution studies for mycotoxins in acetonitrile/water. Mass accuracies (ppm) of molecular ions of each mycotoxin evaluated in the study based on mycotoxin type, resolution (17,500, 35,000, 70,000 and 140,000) and concentration (1, 10 and 100 ng/mL (ppb)). Each mass accuracy result is an average ± standard deviation from triplicate experiments.

Compound	Molecular ion	Theoretical mass	17,500			35,000			70,000			140,000		
			1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb
15-Acetyl Deoxynivalenol	$[M+H]^+$	339.14383	-1.9±1.6	-1.5±0.4	-2.0±0.2	-3.2±1.2	-2.5±0.4	-2.5±0.3	-0.4±0.9	0.5±0.4	-0.2±0.2	0.8±0.5	0.0±0.2	-0.6±0.2
Aflatoxin B_1	$[M+H]^+$	313.07066	-1.8±0.2	-2.3±0.5	-2.9±0.4	-2.5±0.2	-2.8±0.3	-2.9±0.1	0.0±0.2	0.2±0.3	-0.8±0.3	-0.1±0.3	-0.5±0.3	-1.4±0.1
Aflatoxin B_2	$[M+H]^+$	315.08631	-1.6±0.2	-2.0±0.2	-2.9±0.2	-2.3±0.2	-2.7±0.5	-2.9±0.3	0.3±0.1	0.0±0.3	-0.8±0.2	0.2±0.4	-0.6±0.2	-1.4±0.2
Aflatoxin G_1	$[M+H]^+$	329.06558	-1.4±0.3	-2.2±0.3	-2.8±0.3	-2.2±0.3	-2.4±0.1	-2.8±0.1	0.2±0.1	0.2±0.4	-0.7±0.3	0.2±0.5	-0.3±0.1	-1.2±0.3
Aflatoxin G_2	$[M+H]^+$	331.08123	-1.4±0.4	-2.0±0.3	-2.5±0.2	-2.3±0.3	-2.3±0.1	-2.7±0.2	0.2±0.4	0.1±0.1	-0.6±0.3	0.0±0.4	-0.3±0.2	-1.2±0.5
Beauvreicin	$[M+NH_4]^+$	801.44331	-2.3±1.5	-1.9±0.3	-2.5±0.4	-2.7±0.9	-2.3±0.3	-2.4±0.3	0.4±0.1	-0.2±0.0	-0.4±0.3	0.0±0.4	-0.6±0.1	-1.0±0.1
Citrinin	$[M+H]^+$	251.09140	-1.4±0.1	-2.2±0.6	-2.5±0.1	-2.3±0.2	-2.5±0.2	-2.5±0.4	0.5±0.0	0.4±0.2	-0.7±0.4	0.2±0.5	-0.5±0.2	-1.0±0.1
Deoxynivalenol	$[M+H]^+$	297.13326	-2.1±0.4	-2.5±0.3	-2.5±0.2	-2.9±0.4	-2.4±0.4	-2.4±0.5	0.1±0.3	0.4±0.3	-0.1±0.1	0.6±0.2	-0.3±0.3	-0.8±0.1
Diacetoxyscirpenol	$[M+NH_4]^+$	384.20168	-1.3±0.2	-1.6±0.2	-2.5±0.2	-2.0±0.1	-2.2±0.3	-2.5±0.2	0.4±0.2	0.5±0.1	-0.3±0.1	0.3±0.2	-0.1±0.3	-0.9±0.2
Ergocornine	$[M+H]^+$	562.30240	-1.9±0.6	-1.5±0.2	-2.1±0.3	-1.7±0.4	-2.4±0.3	-2.5±0.2	0.7±0.2	0.6±0.2	-0.2±0.3	0.3±0.4	-0.2±0.1	-0.7±0.2
Ergocristine	$[M+H]^+$	610.30239	-2.4±0.6	-3.1±0.1	-2.4±0.2	-2.6±0.2	-2.0±0.2	-2.5±0.5	0.7±0.4	0.6±0.4	-0.5±0.3	0.6±0.4	0.2±0.2	-0.7±0.3
Ergocryptine	$[M+H]^+$	576.31805	-1.0±0.7	-1.1±0.4	-2.3±0.3	-2.1±0.2	-1.9±0.3	-2.2±0.3	1.0±0.3	0.8±0.5	-0.3±0.3	0.7±0.3	0.3±0.2	-1.0±0.3
Ergometrine	$[M+H]^+$	326.18630	-0.7±0.4	-1.6±0.3	-2.3±0.1	-2.5±0.1	-2.6±0.5	-2.4±0.2	0.5±0.5	0.3±0.4	-0.3±0.2	0.1±0.4	-0.2±0.3	-0.9±0.4
Ergosine	$[M+H]^+$	548.28675	-1.4±0.5	-1.6±0.4	-2.1±0.3	-1.5±0.3	-1.9±0.2	-2.3±0.4	0.6±0.2	0.6±0.3	-0.3±0.3	0.8±0.3	0.0±0.4	-0.7±0.2
Ergotamine	$[M+H]^+$	582.27110	-1.7±1.6	-1.3±0.3	-2.0±0.4	-1.9±0.4	-2.3±0.4	-2.3±0.2	0.9±0.6	0.8±0.4	-0.2±0.2	0.5±0.4	-0.2±0.1	-0.9±0.1
Fumonisin B_1	$[M+H]^+$	722.39575	-1.8±0.4	-1.4±0.5	-2.2±0.1	-1.7±0.8	-1.9±0.1	-2.2±0.3	0.5±0.4	0.5±0.3	0.0±0.3	0.3±0.3	0.0±0.1	-0.8±0.2
Fumonisin B_2	$[M+H]^+$	706.40083	-1.2±0.9	-1.4±0.7	-2.2±0.1	-2.1±0.4	-2.0±0.0	-2.1±0.2	0.4±0.2	0.2±0.1	-0.2±0.4	0.2±0.3	-0.1±0.1	-0.8±0.3
Fusarenon-X	$[M+H]^+$	355.13874	-3.6±1.5	-2.7±0.6	-2.1±0.1	-3.8±0.6	-2.6±0.4	-2.4±0.1	-0.3±0.5	0.5±0.5	-0.2±0.3	0.6±0.6	-0.2±0.4	-0.5±0.3
HT-2	$[M+NH_4]^+$	442.24354	-1.3±0.5	-1.5±0.7	-2.0±0.3	-1.7±0.3	-1.8±0.3	-2.3±0.4	0.6±0.5	0.7±0.5	-0.1±0.2	0.5±0.4	0.2±0.1	-0.6±0.2
Neosolaniol	$[M+NH_4]^+$	400.19659	N.D.	-2.2±0.4	-2.3±0.1	-2.2±0.8	-1.8±0.3	-1.9±0.2	2.4±1.2	1.1±0.4	0.1±0.2	0.6±0.5	0.0±0.1	-0.5±0.3
Ochratoxin A	$[M+H]^+$	404.08954	-1.8±1.6	-1.4±0.3	-2.0±0.1	-1.8±1.0	-2.3±0.4	-1.9±0.3	0.5±0.4	0.3±0.4	0.1±0.5	0.3±0.3	0.1±0.1	-0.4±0.3
Ochratoxin B	$[M+H]^+$	370.12851	-0.9±0.4	-1.5±0.3	-2.5±0.4	-1.9±0.3	-2.1±0.2	-2.0±0.5	0.7±0.2	0.3±0.4	-0.1±0.3	0.4±0.3	-0.2±0.2	-0.7±0.1
Sterigmatocystin	$[M+H]^+$	325.07066	-1.1±0.3	-1.9±0.2	-2.7±0.1	-2.3±0.3	-2.5±0.2	-2.4±0.2	0.3±0.3	-0.2±0.3	-0.1±0.5	0.0±0.3	-0.7±0.3	-1.1±0.2
T-2	$[M+H]^+$	484.25411	-0.4±0.8	-1.3±0.4	-2.0±0.1	-1.8±0.6	-1.9±0.3	-1.9±0.4	0.9±0.5	0.6±0.3	0.1±0.3	0.5±0.3	0.3±0.2	-0.3±0.1
Verrucarin A	$[M+H]^+$	520.25411	-1.1±0.3	-1.5±0.4	-2.2±0.4	-1.8±0.2	-2.1±0.4	-1.9±0.5	0.9±0.2	0.5±0.2	0.1±0.3	0.7±0.3	0.1±0.2	-0.6±0.2
Zearalenone	$[M+H]^+$	319.15400	2.7±0.3	-2.5±0.6	-2.4±0.4	-1.3±0.4	-2.0±0.1	-2.1±0.3	0.6±0.2	0.1±0.2	-0.4±0.2	0.3±0.4	-0.2±0.2	-1.0±0.1

Table S3. Resolution studies for mycotoxins in peanut matrix extracted with acetonitrile/water. Mass accuracies (ppm) of molecular ions of each mycotoxin evaluated in the study based on mycotoxin type, resolution (17,500, 35,000, 70,000 and 140,000) and concentration (1, 10 and 100 ng/mL (ppb)). Each mass accuracy result is an average ± standard deviation from triplicate experiments.

Compound	Molecular ion	Theoretical mass	17,500			35,000			70,000			140,000		
			1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb
15-Acetyl Deoxynivalenol	$[M+H]^+$	339.14383	3.0±2.0	-2.1±2.0	-1.0±0.3	0.9±0.5	-0.6±0.5	-0.4±0.2	-0.4±0.9	-0.2±0.4	-0.2±0.2	-1.4±0.4	0.2±0.5	0.5±0.1
Aflatoxin B_1	$[M+H]^+$	313.07066	-0.7±0.4	-1.0±0.3	-1.5±0.2	-0.7±0.4	-1.0±0.3	-0.8±0.1	-0.1±0.2	-0.7±0.3	-0.9±0.1	0.2±0.1	-0.1±0.3	0.0±0.4
Aflatoxin B_2	$[M+H]^+$	315.08631	0.7±0.4	-0.4±0.3	-1.2±0.1	-0.2±0.4	-0.2±0.2	-0.8±0.3	-0.1±0.3	-0.4±0.4	-0.7±0.1	0.6±0.2	0.3±0.2	0.2±0.5
Aflatoxin G_1	$[M+H]^+$	329.06558	-0.3±0.3	-0.5±0.1	-1.2±0.3	-0.1±0.1	-0.2±0.3	-0.6±0.5	-0.4±0.5	-0.1±0.6	-0.4±0.3	0.8±0.2	0.5±0.2	0.1±0.4
Aflatoxin G_2	$[M+H]^+$	331.08123	-0.4±0.2	-0.5±0.3	-0.8±0.1	-0.4±0.1	-0.3±0.5	-0.5±0.3	-0.3±0.5	-0.3±0.4	-0.4±0.2	0.4±0.1	0.3±0.2	0.1±0.4
Beauvreicin	$[M+NH_4]^+$	801.44331	-1.6±1.4	-0.3±0.4	-1.0±0.1	-1.4±2.0	-0.2±0.3	-0.8±0.5	-0.4±0.6	-0.6±0.4	-0.7±0.1	0.5±0.6	0.0±0.2	0.3±0.4
Citrinin	$[M+H]^+$	251.09140	-0.4±0.3	-0.7±0.3	-1.1±0.2	-0.2±0.4	-0.2±0.2	-0.5±0.2	-0.1±0.4	-0.3±0.5	-0.8±0.2	0.7±0.1	0.2±0.2	0.2±0.5
Deoxynivalenol	$[M+H]^+$	297.13326	2.1±0.4	2.5±0.6	-0.9±0.6	2.1±0.7	1.9±0.5	-0.2±0.2	2.8±0.7	2.6±1.0	-0.3±0.3	-0.9±0.7	-1.5±0.6	0.6±0.1
Diacetoxyscirpenol	$[M+NH_4]^+$	384.20168	-0.9±2.5	-0.3±0.2	-0.7±0.2	-0.7±0.5	-0.2±0.5	-0.3±0.1	0.0±0.5	-0.3±0.5	-0.2±0.1	0.7±0.4	0.6±0.3	0.6±0.3
Ergocornine	$[M+H]^+$	562.30240	0.4±1.3	-0.3±0.5	-0.9±0.2	-0.1±0.6	-0.1±0.3	-0.5±0.2	0.2±0.6	-0.1±0.6	-0.4±0.1	1.0±0.2	0.5±0.2	0.5±0.4
Ergocristine	$[M+H]^+$	610.30239	-4.1±0.5	-1.5±0.5	-0.7±0.4	-0.9±1.2	0.0±0.4	-0.1±0.3	0.2±0.6	0.1±0.5	-0.4±0.2	1.1±0.3	0.7±0.4	0.6±0.5
Ergocryptine	$[M+H]^+$	576.31805	1.2±0.7	0.4±0.5	-0.7±0.3	-0.5±0.3	0.1±0.5	-0.2±0.3	0.7±0.4	0.3±0.6	-0.1±0.1	1.5±0.4	1.0±0.2	0.5±0.5
Ergometrine	$[M+H]^+$	326.18630	-2.2±1.6	-1.0±0.1	-1.2±0.2	-0.9±1.1	-0.7±0.2	-0.6±0.3	-0.1±0.3	-0.8±0.2	-0.7±0.1	0.0±0.4	0.0±0.5	0.0±0.2
Ergosine	$[M+H]^+$	548.28675	-0.1±1.2	0.0±0.1	-0.7±0.4	-0.1±0.8	0.4±0.3	0.0±0.2	0.2±0.4	0.1±0.6	-0.2±0.2	1.2±0.1	0.9±0.1	0.8±0.5
Ergotamine	$[M+H]^+$	582.27110	0.4±1.8	-0.1±0.4	-0.5±0.1	-1.0±0.8	0.2±0.2	-0.3±0.3	0.6±0.7	-0.2±0.4	-0.5±0.2	1.1±0.4	0.8±0.3	0.6±0.4
Fumonisin B_1	$[M+H]^+$	722.39575	0.7±2.5	-0.1±0.6	-0.6±0.1	0.2±0.8	0.0±0.3	-0.4±0.4	0.3±0.1	0.2±0.4	-0.2±0.1	1.1±0.3	0.8±0.2	0.5±0.5
Fumonisin B_2	$[M+H]^+$	706.40083	-1.0±1.5	-0.1±0.7	-0.9±0.1	-0.5±1.0	-0.2±0.2	-0.5±0.1	-0.2±0.3	0.0±0.3	-0.6±0.2	0.8±0.4	0.4±0.2	0.5±0.2
Fusarenon-X	$[M+H]^+$	355.13874	-2.2±1.2	-2.2±1.5	-0.4±0.2	-0.7±2.2	-0.5±0.6	-0.1±0.3	0.2±1.4	-0.2±0.3	-0.1±0.3	0.5±0.9	0.6±0.3	0.4±0.2
HT-2	$[M+NH_4]^+$	442.24354	-1.8±0.8	-1.0±1.0	-0.4±0.4	0.0±0.2	0.0±0.5	-0.2±0.3	0.0±0.3	0.3±0.3	0.2±0.1	0.8±0.3	0.6±0.3	0.7±0.5
Neosolaniol	$[M+NH_4]^+$	400.19659	N.D.	-0.9±0.4	-0.9±0.3	-0.7±0.9	-0.5±0.2	-0.2±0.2	0.8±0.2	-0.4±0.4	0.0±0.1	0.9±0.3	0.6±0.2	0.6±0.2
Ochratoxin A	$[M+H]^+$	404.08954	-3.8±1.1	-0.2±0.4	-0.7±0.1	-4.6±0.4	-0.6±0.5	-0.3±0.4	-0.7±1.1	0.0±0.2	-0.1±0.2	-1.3±0.4	0.5±0.1	0.8±0.3
Ochratoxin B	$[M+H]^+$	370.12851	-1.5±4.4	-0.4±0.6	-0.9±0.3	0.1±0.8	0.0±0.4	-0.2±0.5	0.0±0.4	0.0±0.6	-0.2±0.3	0.5±0.3	0.7±0.4	0.5±0.5
Sterigmatocystin	$[M+H]^+$	325.07066	-1.4±1.5	-0.5±0.7	-1.1±0.2	-0.8±0.3	-0.4±0.4	-0.4±0.3	-0.4±0.3	-0.6±0.3	-0.6±0.1	0.3±0.4	0.1±0.1	0.4±0.5
T-2	$[M+H]^+$	484.25411	-1.9±2.0	0.3±0.5	-0.7±0.4	0.4±0.7	0.0±0.2	0.0±0.2	0.2±0.4	0.4±0.5	0.2±0.2	1.4±0.3	0.9±0.3	1.1±0.3
Verrucarin A	$[M+H]^+$	520.25411	0.1±1.2	0.0±0.5	-0.9±0.5	0.4±0.5	0.2±0.3	0.1±0.4	0.4±0.4	0.3±0.4	0.0±0.2	1.2±0.3	1.1±0.2	1.0±0.2
Zearalenone	$[M+H]^+$	319.15400	2.2±0.5	0.0± 0.5	-0.8±0.2	0.0±0.5	-0.4±0.3	-0.3±0.2	-0.2±0.4	0.0±0.6	-0.3±0.1	0.4±0.2	0.4±0.2	0.5±0.2

Table S4. Resolution studies for mycotoxins in wheat matrix extracted with acetonitrile/water. Mass accuracies (ppm) of molecular ions of each mycotoxin evaluated in the study based on mycotoxin type, resolution (17,500, 35,000, 70,000 and 140,000) and concentration (1, 10 and 100 ng/mL (ppb)). Each mass accuracy result is an average ± standard deviation from triplicate experiments.

Compound	Molecular ion	Theoretical mass	17,500			35,000			70,000			140,000		
			1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb	1 ppb	10 ppb	100 ppb
15-Acetyl Deoxynivalenol	$[M+H]^+$	339.14383	-2.3±2.1	-2.4±0.4	-1.8±0.2	-2.0±1.4	-1.4±1.6	-0.1±0.1	0.0±0.5	0.2±0.2	0.6±0.2	0.2±0.8	-1.3±0.4	-0.9±0.1
Aflatoxin B_1	$[M+H]^+$	313.07066	-2.5±0.5	-2.3±0.5	-2.7±0.3	-1.5±0.4	-0.9±0.3	-1.1±0.1	-0.4±0.2	-0.2±0.3	-0.1±0.4	-0.7±0.2	-0.9±0.5	-1.6±0.2
Aflatoxin B_2	$[M+H]^+$	315.08631	-1.8±0.5	-2.0±0.4	-2.6±0.5	-1.3±0.2	-0.9±0.3	-1.2±0.2	-0.2±0.2	-0.1±0.1	0.3±0.3	-0.9±0.4	-0.9±0.4	-1.3±0.3
Aflatoxin G_1	$[M+H]^+$	329.06558	-1.7±0.3	-2.1±0.2	-2.6±0.2	-1.1±0.3	-1.1±0.3	-0.9±0.3	-0.1±0.1	0.1±0.4	0.5±0.4	-0.7±0.2	-0.9±0.2	-1.4±0.2
Aflatoxin G_2	$[M+H]^+$	331.08123	-2.7±0.4	-1.8±0.3	-2.2±0.4	-1.0±0.4	-0.9±0.7	-0.9±0.3	-0.1±0.2	0.1±0.3	0.6±0.3	-0.5±0.2	-0.7±0.2	-1.2±0.1
Beauvreicin	$[M+NH_4]^+$	801.44331	-2.0±3.6	-1.9±1.6	-2.4±0.2	-2.1±1.7	-0.5±0.6	-0.7±0.2	-0.1±0.4	0.0±0.1	0.6±0.1	-0.6±0.4	-1.3±0.4	-1.4±0.5
Citrinin	$[M+H]^+$	251.09140	-1.8±0.4	-1.8±0.3	-2.4±0.2	-1.0±0.2	-0.6±0.3	-0.8±0.1	0.0±0.3	-0.3±0.4	0.5±0.4	-0.4±0.3	-0.6±0.5	-1.2±0.1
Deoxynivalenol	$[M+H]^+$	297.13326	-3.4±0.8	-3.1±1.3	-2.3±0.8	-2.5±1.1	-1.3±1.4	-0.6±0.3	0.0±0.4	-0.1±0.2	0.6±0.4	-0.4±0.6	-0.7±0.5	-1.3±0.3
Diacetoxyscirpenol	$[M+NH_4]^+$	384.20168	-4.2±0.7	-1.4±0.7	-2.3±0.3	-1.0±0.4	-0.7±0.5	-0.7±0.2	0.1±0.3	0.2±0.4	0.6±0.2	-0.4±0.3	-0.7±0.3	-1.0±0.2
Ergocornine	$[M+H]^+$	562.30240	-2.3±1.1	-1.6±0.3	-2.1±0.4	-1.3±0.2	-0.9±0.7	-0.3±0.1	0.3±0.4	0.6±0.3	1.0±0.3	-0.1±0.2	-0.4±0.5	-1.0±0.2
Ergocristine	$[M+H]^+$	610.30239	-3.7±0.5	-2.8±0.8	-2.4±0.7	-2.1±1.2	-1.5±2.0	-0.6±0.1	0.3±0.1	0.3±0.3	0.7±0.4	-0.3±0.3	-0.4±0.3	-0.7±0.3
Ergocryptine	$[M+H]^+$	576.31805	-0.9±0.9	-0.9±0.3	-1.8±0.5	-0.5±1.2	-0.2±0.3	-0.4±0.1	0.4±0.3	0.6±0.4	1.1±0.3	-0.1±0.3	-0.3±0.3	-0.8±0.2
Ergometrine	$[M+H]^+$	326.18630	-1.2±0.4	-2.1±0.3	-2.0±0.5	-1.6±0.4	-1.1±1.0	-0.6±0.2	0.1±0.2	-0.1±0.4	0.7±0.4	-0.7±0.3	-1.2±0.1	-1.0±0.4
Ergosine	$[M+H]^+$	548.28675	-1.5±2.2	-1.5±0.4	-2.4±0.2	-0.7±0.3	-0.1±0.1	-0.6±0.3	0.5±0.3	0.2±0.4	0.9±0.6	-0.2±0.2	-0.4±0.5	-0.8±0.2
Ergotamine	$[M+H]^+$	582.27110	1.2±1.6	-1.4±0.5	-2.0±0.1	-1.7±0.6	0.1±0.5	-0.5±0.2	0.4±0.3	0.3±0.2	0.8±0.2	-0.2±0.4	-0.5±0.3	-0.9±0.1
Fumonisin B_1	$[M+H]^+$	722.39575	0.4±3.4	-1.5±1.2	-2.0±0.3	-1.4±0.3	-1.3±1.9	-0.6±0.0	0.3±0.4	0.4±0.3	0.8±0.4	-0.3±0.2	-0.8±0.2	-1.1±0.2
Fumonisin B_2	$[M+H]^+$	706.40083	-2.6±0.7	-1.9±0.3	-1.9±0.2	-0.8±0.4	-0.1±0.2	-0.9±0.1	0.2±0.2	0.3±0.7	1.0±0.1	-0.6±0.5	-1.0±0.4	-1.1±0.2
Fusarenon-X	$[M+H]^+$	355.13874	2.1±1.7	-2.5±1.0	-2.2±0.9	-3.6±0.7	-1.1±1.4	-0.3±0.2	-0.1±0.5	0.3±0.2	0.9±0.2	-0.5±0.4	-0.7±1.0	-1.1±0.4
HT-2	$[M+NH_4]^+$	442.24354	-2.4±1.0	-2.7±0.9	-1.6±0.3	-0.7±0.4	-0.4±0.3	-0.4±0.3	0.2±0.3	0.5±0.3	1.2±0.2	-0.7±0.3	-0.6±0.4	-0.8±0.2
Neosolaniol	$[M+NH_4]^+$	400.19659	N.D.	-3.1±1.3	-2.8±0.7	-2.8±0.8	-0.7±0.3	-0.4±0.4	1.6±0.5	0.0±0.3	2.0±0.5	-0.8±0.3	-1.4±0.2	-0.6±0.3
Ochratoxin A	$[M+H]^+$	404.08954	-1.3±2.4	-1.4±0.6	-1.9±0.2	-2.0±0.9	-0.5±0.3	-0.3±0.2	0.1±0.3	0.3±0.3	1.1±0.0	-0.7±0.1	-1.0±0.2	-1.1±0.2
Ochratoxin B	$[M+H]^+$	370.12851	-1.6±1.1	-1.7±0.2	-2.1±0.4	-1.2±0.4	-0.3±0.3	-0.5±0.2	0.2±0.1	0.2±0.3	0.7±0.4	-0.6±0.5	-1.2±0.7	-1.0±0.2
Sterigmatocystin	$[M+H]^+$	325.07066	-1.8±0.4	-2.2±0.2	-2.2±0.4	-1.5±0.5	-0.7±0.2	-0.7±0.1	0.1±0.2	-0.1±0.4	0.7±0.2	-1.0±0.1	-1.2±0.2	-1.2±0.5
T-2	$[M+H]^+$	484.25411	-0.8±2.8	-2.0±0.7	-1.8±0.2	-1.3±1.9	-0.2±0.3	-0.2±0.2	0.3±0.4	0.8±0.3	1.0±0.4	0.1±0.3	-0.4±0.4	-0.7±0.1
Verrucarin A	$[M+H]^+$	520.25411	-0.4±0.6	-0.9±0.2	-2.0±0.6	-0.4±0.1	0.1±0.3	-0.4±0.2	0.6±0.4	0.9±0.2	1.2±0.2	0.1±0.3	-0.3±0.2	-0.7±0.3
Zearalenone	$[M+H]^+$	319.15400	2.2±0.6	-3.4±0.4	-2.3±0.3	-1.0±0.4	-0.7±0.1	-0.9±0.1	0.2±0.2	0.3±0.5	0.7±0.1	-0.8±0.1	-0.8±0.2	-1.1±0.1

Table S5. % Average Abundances, % RSDs and % Differences of M+1 and M+2 isotopes (and M+3 isotope for ochratoxin A) relative to the M isotopes for mycotoxin analysis in this study obtained from mycotoxins fortified at 1, 10 and 100 ng/mL in acetonitrile/water and acetonitrile/water extracts obtained from peanut and wheat matrices (n = 9 each at each level and different matrices). % Difference is defined by 100 x [Average Abundance – Theoretical Abundance]/Theoretical Abundance.

Compound	Adduct	Theoretical Mass	Theoretical Abundance	1 ng/mL			10 ng/mL			100 ng/mL		
				Average Abundance	% RSD	% Difference	Average Abundance	% RSD	% Difference	Average Abundance	% RSD	% Difference
15-Acetyl Deoxynivalenol	$[M + H]^+$	339.14383	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	340.14718	18.4	ND	-	-	18.1	0.6	-1.6	19.0	1.3	3.7
	$[M + 2 + H]^+$	341.15054	1.6	ND	-	-	4.7	16.1	192.7	2.8	2.9	69.2
Aflatoxin B_1	$[M + H]^+$	313.07066	100	100	-	-	100			100		
	$[M + 1 + H]^+$	314.07402	18.4	19.2	2.6	4.3	18.2	1.1	-1.2	18.6	1.9	3.0
	$[M + 2 + H]^+$	315.07737	1.6	2.5	4.0	55.8	2.2	1.0	40.3	2.3	1.2	43.9
Aflatoxin B_2	$[M + H]^+$	315.08631	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	316.08967	18.4	18.4	3.6	-0.1	19.0	1.1	3.3	18.4	1.4	0.5
	$[M + 2 + H]^+$	317.09302	1.6	2.5	3.5	56.1	2.3	1.0	42.4	2.3	1.2	46.7
Aflatoxin G_1	$[M + H]^+$	329.06558	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	330.06893	18.4	18.4	1.4	0.3	18.6	0.7	1.4	18.5	0.8	0.0
	$[M + 2 + H]^+$	331.07229	1.6	2.8	9.1	78.2	2.5	2.6	56.2	2.5	2.8	53.0
Aflatoxin G_2	$[M + H]^+$	331.08123	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	332.08458	18.4	18.6	5.0	1.4	18.5	2.2	0.6	18.7	0.2	1.8
	$[M + 2 + H]^+$	333.08794	1.6	2.8	3.2	79.0	2.4	0.6	53.7	2.6	2.8	63.4
Beauvreicin	$[M + NH_4]^+$	801.44331	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + NH_4]^+$	802.44666	48.7	55.6	10.5	14.3	51.8	1.2	6.5	51.2	1.0	4.1
	$[M + 2 + NH_4]^+$	803.45002	11.6	16.6	10.6	43.1	14.7	3.8	27.0	14.4	0.6	23.7
Citrinin	$[M + H]^+$	251.09140	100	100			100	-	-	100	-	-
	$[M + 1 + H]^+$	252.09475	14.1	14.0	2.3	-0.6	14.5	1.7	2.9	14.4	0.7	3.3
	$[M + 2 + H]^+$	253.09565	1.0	1.2	12.6	11.8	2.3	85.6	127.5	1.2	1.3	20.8
Deoxynivalenol	$[M + H]^+$	297.13326	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	298.13662	16.2	ND	-	-	17.0	3.7	5.1	17.2	4.9	3.9
	$[M + 2 + H]^+$	299.13751	1.2	ND	-	-	ND	-	-	2.0	14.6	67.2
Diacetoxyscirpenol	$[M + H]^+$	384.20168	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	385.20503	20.6	21.7	5.8	5.4	21.1	0.9	2.7	21.3	2.0	3.4
	$[M + 2 + H]^+$	386.20839	2.0	3.4	30.6	69.0	3.2	3.8	61.1	3.3	6.7	56.1
Ergocornine	$[M + H]^+$	562.30240	100	100	-	-	100	-	-	100	-	-

Compound	Adduct	Theoretical Mass	Theoretical Abundance	1 ng/mL			10 ng/mL			100 ng/mL		
				Average Abundance	% RSD	% Difference	Average Abundance	% RSD	% Difference	Average Abundance	% RSD	% Difference
	$[M + 1 + H]^+$	563.30575	33.5	35.1	1.5	4.7	34.7	2.6	3.6	34.4	0.6	3.0
	$[M + 2 + H]^+$	564.30911	5.4	7.0	5.6	28.3	6.7	5.2	24.0	6.7	0.6	24.9
Ergocristine	$[M + H]^+$	610.30239	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	611.30575	37.9	39.2	4.7	3.4	38.9	2.1	2.6	39.3	1.0	4.0
	$[M + 2 + H]^+$	612.30911	7.0	9.6	4.1	38.0	8.5	3.5	22.4	8.5	2.0	24.0
Ergocryptine	$[M + H]^+$	576.31805	100	100			100	-	-	100	-	-
	$[M + 1 + H]^+$	577.32140	34.6	36.4	4.6	5.0	36.7	1.1	6.1	36.5	1.9	7.0
	$[M + 2 + H]^+$	578.32476	5.8	9.7	23.5	66.9	7.5	2.8	29.2	7.4	1.5	29.8
Ergometrine	$[M + H]^+$	326.18630	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	327.18966	20.6	21.4	1.3	4.3	20.1	1.0	-2.4	20.4	1.3	0.0
	$[M + 2 + H]^+$	328.19301	2.0	ND	-	-	2.3	6.2	12.6	2.1	3.2	3.0
Ergosine	$[M + H]^+$	548.28675	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	549.29010	32.5	33.9	5.3	4.5	34.0	0.7	4.7	33.7	0.4	3.6
	$[M + 2 + H]^+$	550.29346	5.1	7.4	6.4	45.3	6.4	3.0	25.9	6.4	1.2	24.6
Ergotamine	$[M + H]^+$	582.27110	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	583.27445	35.7	39.2	5.5	9.9	37.6	2.5	5.3	36.8	1.0	2.1
	$[M + 2 + H]^+$	584.27781	6.2	9.4	5.8	51.8	7.7	1.2	24.1	7.6	1.3	23.4
Fumonisin B_1	$[M + H]^+$	722.39575	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	723.39910	36.8	38.8	5.0	5.4	39.1	2.0	6.4	38.7	2.4	6.8
	$[M + 2 + H]^+$	724.40246	6.6	11.7	21.7	78.8	10.4	2.0	58.5	10.0	1.5	49.2
Fumonisin B_2	$[M + H]^+$	706.40083	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	707.40419	36.8	40.6	5.1	10.5	38.8	2.5	5.6	39.4	0.7	6.5
	$[M + 2 + H]^+$	708.40754	6.6	12.0	13.7	82.5	10.0	4.8	52.8	10.0	1.3	49.9
Fusarenon-X	$[M + H]^+$	355.13874	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	356.14210	18.4	ND	-	-	20.0	2.9	9.0	18.7	4.1	-3.2
	$[M + 2 + H]^+$	357.14299	1.6	ND	-	-	3.6	13.5	120.0	3.0	8.3	68.8
HT-2	$[M + NH_4]^+$	442.24354	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + NH_4]^+$	443.24690	23.8	27.8	8.0	16.8	25.9	4.0	8.7	24.9	0.5	5.3
	$[M + 2 + NH_4]^+$	444.25025	2.7	ND	-	-	4.6	5.5	72.0	4.4	1.5	65.0
Neosolaniol	$[M + H]^+$	400.19659	100	ND	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	401.19995	20.6	ND	-	-	21.8	4.6	6.0	21.6	1.3	4.8
	$[M + 2 + H]^+$	402.20330	2.0	ND	-	-	3.9	5.2	97.2	3.5	2.7	79.4
Ochratoxin A	$[M + H]^+$	404.08954	100	100	-	-	100	-	-	100	-	-

Compound	Adduct	Theoretical Mass	Theoretical Abundance	1 ng/mL			10 ng/mL			100 ng/mL		
				Average Abundance	% RSD	% Difference	Average Abundance	% RSD	% Difference	Average Abundance	% RSD	% Difference
	$[M + 1 + H]^+$	405.09290	21.6	23.9	5.5	10.7	22.1	3.5	2.3	22.3	0.5	2.9
	$[M + 2 + H]^+$	406.08659	32.0	32.2	5.0	0.9	30.8	1.6	-3.7	30.9	0.3	-2.9
	$[M + 3 + H]^+$	407.08995	6.9	6.9	8.4	0.2	7.1	2.5	2.9	6.9	1.2	0.5
Ochratoxin B	$[M + H]^+$	370.12851	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	371.13187	21.6	23.2	2.4	7.1	21.9	2.5	1.1	22.0	0.3	1.2
	$[M + 2 + H]^+$	372.13522	2.2	3.6	4.2	61.1	3.0	0.4	35.2	3.1	3.4	42.6
Sterigmatocystin	$[M + H]^+$	325.07066	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	326.07402	19.5	20.4	9.4	4.9	19.8	0.8	1.8	19.9	0.4	2.7
	$[M + 2 + H]^+$	327.07737	1.8	ND	-	-	2.9	15.8	63.3	2.6	2.8	51.7
T-2	$[M + NH_4]^+$	484.25411	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + NH_4]^+$	485.25746	26.0	28.7	5.5	10.5	27.6	3.3	6.3	27.1	1.6	6.0
	$[M + 2 + NH_4]^+$	486.26082	3.2	6.1	28.5	88.9	5.2	3.6	62.2	5.1	2.8	61.8
Verrucarin A	$[M + NH_4]^+$	520.25411	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + NH_4]^+$	521.25746	29.2	30.2	2.1	3.5	30.1	0.7	3.0	30.5	0.6	4.8
	$[M + 2 + NH_4]^+$	522.26082	4.1	6.3	4.7	52.5	5.9	1.6	43.5	5.9	2.7	45.8
Zearalenone	$[M + H]^+$	319.15400	100	100	-	-	100	-	-	100	-	-
	$[M + 1 + H]^+$	320.15736	19.5	20.5	5.1	5.3	20.1	1.4	3.3	20.0	1.1	2.5
	$[M + 2 + H]^+$	321.16071	1.8	3.7	45.8	104.3	2.4	0.6	34.6	2.4	4.2	29.2

Supporting Table S6. Mycotoxin concentrations (average ± standard deviation, n = 3) found in finished cereal and nut products. (-) indicates none of the mycotoxins were detected with the Q-Orbitrap method. Numerical values labeled in red (avg ± SD) are LC-MS/MS results obtained from J. Agric. Food Chem. 2013, 61, 4771-4782.

		Mycotoxin concentration (µg/kg, Average ± standard deviation, *n*=3)																		
		AFB_1	AFB_2	AFG_1	BEA	DON	ERGCN	ERGCR	ERGCT	ERGM	ERGS	ERGT	FB_1	FB_2	NEO	OTA	OTB	ST	T-2	ZEN
Rice																				
	Rice flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.6±0.5 (3.3±0.3)	-	0.8±0.2 (0.9±0.2)	-	-
	Rice flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Rice flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Rice flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Rice	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Rice	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Wheat																				
	Wheat flour	-	-	-	-	-	1.8±0.5 (2.4±0.4)	7.3±1.5 (6.4±1.3)	7.4±1.8 (7.7±1.3)	3.4±0.6 (3.1±0.6)	1.1±0.3 (1.4±0.5)	9.0±2.6 (8.3±1.6)	-	-	-	-	-	-	-	-
	Wheat flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.5±0.3 (1.7±0.1)	-	1.4±0.4 (1.1±0.2)	1.1±0.4 (1.6±0.7)	-
	Wheat flour	-	-	-	1.6±0.2 (1.8±0.3)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Wheat flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.2±0.2 (1.5±0.1)	-	-	-	-
	Spaghetti	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.9±0.5 (2.2±0.3)	-	-	-	-
	Spaghetti	-	-	-	-	90±15 (88±10)	3.7±0.6 (3.8±0.3)	5.3±1.4 (5.6±1.0)	8.9±1.5 (8.8±1.2)	-	1.5±0.3 (1.5±0.3)	12.8±2.9 (10.7±2.1)	-	-	-	-	-	-	-	-
	Spaghetti	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.7±0.3 (1.9±0.3)	-	-	-	-
	Wheat elbow	-	-	-	-	50±13 (63±17)	-	-	-	-	-	-	-	-	-	2.2±0.7 (2.7±0.3)	-	-	-	-
	Wheat flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Wheat flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Wheat flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Spaghetti	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Spaghetti	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Spaghetti	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

		Mycotoxin concentration (μg/kg, Average ± standard deviation, *n*=3)																		
		AFB_1	AFB_2	AFG_1	BEA	DON	ERGCN	ERGCR	ERGCT	ERGM	ERGS	ERGT	FB_1	FB_2	NEO	OTA	OTB	ST	T-2	ZEN
	Wheat penne	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Wheat penne	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Corn																				
	Corn flour	-	-	-	0.8±0.2 (1.0±0.2)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Corn flour	-	-	-	-	115±26 (134±21)	-	-	-	-	-	-	64±16 (71±19)	42±11 (54±18)	-	2.4±0.6 (3.1±0.3)	-	-	-	-
	Corn flour	-	-	-	2.9±0.6 (2.6±0.4)	-	-	-	-	-	-	-	50±9 (58±12)	27±8 (33±16)	-	-	-	-	-	-
	Corn flour	-	-	-	0.8±0.3 (1.1±0.4)	61±11 (78±13)	-	-	-	-	-	-	65±23 (52±19)	40±12 (34±11)	-	-	-	-	-	246±43 (284±66)
	Corn flour	-	-	-	7.0±3.2 (9.0±6.0)	-	-	-	-	-	-	-	50±7 (46±2)	-	-	-	-	-	-	-
	Corn flour	-	-	-	108±16 (130±10)	-	-	-	-	-	-	-	510±83 (426±72)	365±46 (418±56)	-	-	-	-	-	279±21 (339±16)
	Corn flour	-	-	-	1.5±0.4 (1.8±0.3)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Corn flour	-	-	-	2.7±0.5 (2.2±0.3)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Corn flour	-	-	-	-	-	-	-	-	-	-	-	1175±182 (1143±87)	750±84 (937±46)	-	-	-	-	-	205±18 (233±32)
	Corn meal	-	-	-	0.9±0.1 (0.6±0.1)	-	-	-	-	-	-	-	205±26 (149±23)	96±17 (80±22)	-	-	-	-	-	-
	Corn meal	-	-	-	1.7±0.4 (1.6±0.4)	80±21 (90±25)	-	-	-	-	-	-			-	-	-	-	1.0±0.3 (1.2±0.4)	102±14 (115±32)
	Corn meal	-	-	-	1.0±0.2 (1.0±0.2)	-	-	-	-	-	-	-	70±12 (78±16)	32±10 (35±18)	-	-	-	-	-	-
	Corn meal	-	-	-	1.7±0.4 (1.7±0.4)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Corn meal	-	-	-	5.5±1.7 (5.8±2.4)	-	-	-	-	-	-	-	50±5 (41±5)	-	-	-	-	-	-	-
	Corn meal	-	-	-	37±8 (48±6)	-	-	-	-	-	-	-	50±9 (41±5)	28±8 (25±4)	-	-	-	-	-	-
	Corn meal	-	-	-	35±9 (44±6)	-	-	-	-	-	-	-	84±13 (68±7)	-	-	-	-	-	-	-
	Corn flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Corn grit	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

		Mycotoxin concentration (μg/kg, Average ± standard deviation, *n*=3)																		
		AFB_1	AFB_2	AFG_1	BEA	DON	ERGCN	ERGCR	ERGCT	ERGM	ERGS	ERGT	FB_1	FB_2	NEO	OTA	OTB	ST	T-2	ZEN
Peanut																				
	Peanut flour	0.4±0.1 (0.3±0.1)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut butter	0.6±0.1 (0.6±0.1)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut butter	0.6±0.1 (0.6±0.1)	-	-	4.5±1.1 (5.0±0.7)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut butter	0.3±0.1 (0.3±0.1)	-	-	0.8±0.2 (0.9±0.4)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut butter	0.4±0.1 (0.4±0.1)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut butter	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut butter	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut butter	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut butter	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Peanut candy	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Pistachio																				
	Roasted pistachio	-	-	-	1.9±0.6 (1.4±0.5)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Pistachio flour	1.2±0.1 (1.4±0.1)	0.9±0.2 (0.6±0.1)	0.5±0.1 (0.4±0.1)	-	-	-	-	-	-	-	-	-	-	-	6.6±0.7 (7.1±0.3)	2.3±0.4 (2.8±0.3)	-	-	-
	Pistachio butter	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.1±0.3 (1.1±0.2)	-	-	-	-
	Pistachio butter	0.5±0.1 (0.7±0.3)	-	-	-	-	-	-	-	-	-	-	-	-	46±8 (58±2)	1.0±0.1 (1.1±0.1)	0.5±0.1 (0.6±0.1)	-	-	-
	Roasted pistachio	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Roasted pistachio	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Roasted pistachio	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Roasted pistachio	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Roasted pistachio	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Pistachio butter	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

		Mycotoxin concentration (µg/kg, Average ± standard deviation, *n*=3)																		
		AFB_1	AFB_2	AFG_1	BEA	DON	ERGCN	ERGCR	ERGCT	ERGM	ERGS	ERGT	FB_1	FB_2	NEO	OTA	OTB	ST	T-2	ZEN
Almond																				
	Almond flour	0.3±0.1 (0.3±0.2)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Almond flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Almond flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Almond flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Almond flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Almond flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Almond flour	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Almond butter	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Almond butter	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Mycotoxin abbreviations used: Aflatoxin B1 (AFB1), Aflatoxin B2 (AFB2), Aflatoxin G1 (AFG1), Beauvericin (BEA), Deoxynivalenol (DON), Ergocornine (ERGCN), Ergocryptin (ERGCR), Ergocristine (ERGCT), Ergometrine (ERGM), Ergosine (ERGS), Ergotamine (ERGT), Fumonisin B1 (FB1), Fumonisin B2 (FB2), Neosolaniol (NEO), Ochratoxin A (OTA), Ochratoxin B (OTB), Sterigmatocystin (ST), T-2 Toxin (T2), Zearalenone (ZEN)

Supporting Table S7. Experimental Masses and Mass Accuracies of Ions used in the Identification of Mycotoxins in Solvent (50:50 Acetonitrile:Water Mixture).

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 ng/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
Aflatoxin B_1	$[C_{17}H_{12}O_6 + H]^+$	313.07066	313.07065	1.04	-0.03	0.33	313.07065	1.04	0.35	-0.22	313.07060	6.24	-0.19	0.20
	$C_{16}H_{13}O_5^+$	285.07575	285.07562	1.04	-0.46	0.36	285.07564	8.66	-0.04	-0.56	285.07560	4.58	-0.53	0.16
	$C_{15}H_{10}O_5^+$	270.05227	270.05210	1.02	-0.64	0.38	270.05220	1.27	-0.20	-0.80	270.05219	9.50	-0.33	0.35
	$C_{15}H_{13}O_4^+$	257.08084	257.08103	2.78	0.77	1.08	257.08093	3.00	0.48	0.37	257.08094	9.64	0.41	0.38
Aflatoxin B_2	$[C_{17}H_{14}O_6 + H]^+$	315.08631	315.08625	1.40	-0.18	0.45	315.08621	1.08	0.06	-0.41	315.08623	9.17	-0.25	0.29
	$C_{16}H_{15}O_5^+$	287.09140	287.09137	1.08	-0.10	0.38	287.09140	7.94	0.31	-0.10	287.09139	1.14	-0.03	0.40
	$C_{14}H_{11}O_5^+$	259.06000	259.06021	1.31	0.81	0.50	259.06017	1.14	1.16	0.46	259.06017	4.58	0.66	0.18
Aflatoxin G_1	$[C_{17}H_{12}O_7 + H]^+$	329.06558	329.06558	1.08	0.00	0.33	329.06538	3.46	-0.55	-0.73	329.06542	4.58	-0.49	0.14
	$C_{17}H_{11}O_6^+$	311.05501	311.05504	1.21	0.08	0.39	311.05485	3.46	-0.46	-0.66	311.05487	6.00	-0.46	0.19
	$C_{16}H_{11}O_5^+$	283.06001	283.06023	8.66	0.78	0.31	283.05995	6.93	-0.35	-0.35	283.05999	7.55	-0.07	0.27
	$C_{14}H_{11}O_4^+$	243.06519	243.06529	6.43	0.45	0.26	243.06517	3.00	0.06	-0.19	243.06520	2.52	0.05	0.10
Aflatoxin G_2	$[C_{17}H_{14}O_7 + H]^+$	331.08123	331.08116	1.29	-0.22	0.39	331.08111	1.73	-0.33	-0.42	331.08116	1.56	-0.22	0.47
	$C_{17}H_{13}O_6^+$	313.07066	313.07060	1.25	-0.21	0.40	313.07063	1.73	-0.05	-0.14	313.07065	1.08	-0.05	0.35
	$C_{16}H_{13}O_5^+$	285.07575	285.07570	2.30	-0.16	0.81	285.07564	2.23	0.53	-0.88	285.07575	2.89	0.01	1.01
Beauvreicin	$C_9H_{12}N^+$	134.09643	134.09654	4.58	0.85	0.34	134.09654	3.06	0.78	0.63	134.09655	9.07	0.90	0.68
	$C_{20}H_{28}NO_5^+$	362.19620	362.19631	6.24	0.31	0.17	362.19620	2.22	0.17	-0.69	362.19611	1.85	-0.26	0.51
	$C_{15}H_{20}NO_3^+$	262.14377	262.14387	6.93	0.38	0.26	262.14388	6.24	0.34	0.23	262.14389	1.97	0.46	0.75
	$C_{15}H_{18}NO_2^+$	244.13321	244.13333	1.03	0.50	0.42	244.13331	5.86	0.35	0.27	244.13333	1.66	0.50	0.68
Citrinin	$C_{13}H_{13}O_4^+$	233.08084	233.08096	5.51	0.52	0.24	233.08095	6.43	0.28	0.79	233.08095	5.20	0.49	0.22
	$[C_{13}H_{14}O_5 + H]^+$	251.09140	251.09146	2.89	0.25	0.11	251.09150	5.86	0.12	0.48	251.09150	5.86	0.38	0.23
Deoxynivalenol	$C_{13}H_{15}O_2^+$	203.10666	-	-	-	-	203.10666	1.29	-0.42	0.76	203.10683	2.65	0.86	0.13
	$C_{14}H_{17}O_4^+$	249.11214	-	-	-	-	249.11211	4.65	-2.19	0.42	249.11215	2.01	0.06	0.81
	$C_{14}H_{15}O_3^+$	231.10157	-	-	-	-	231.10175	2.44	1.55	1.16	231.10160	1.39	0.13	0.60
	$C_{11}H_{11}O_2^+$	175.07536	-	-	-	-	175.07562	1.70	1.45	2.48	175.07548	1.17	0.73	0.67
	$C_8H_9O_2^+$	137.05971	-	-	-	-	137.05984	5.86	1.27	1.12	137.05982	4.36	0.83	0.32
Diacetoxyscirpenol	$C_8H_9^+$	105.06988	105.07029	5.03	3.96	0.48	105.07031	2.31	4.03	4.03	105.07037	3.06	4.66	0.29
	$C_{12}H_{13}^+$	157.10118	157.10150	2.69	2.06	1.71	157.10136	2.52	0.97	1.16	157.10143	8.74	1.63	0.56
	$C_{14}H_{15}^+$	183.11683	183.11706	5.00	1.25	2.73	183.11695	7.64	0.23	1.05	183.11709	9.17	1.44	0.50
	$C_{14}H_{15}O^+$	199.11174	199.11195	1.44	1.05	0.72	199.11185	1.42	0.14	0.09	199.11192	6.66	0.91	0.33

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 ng/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
	$C_{15}H_{15}O^+$	211.11174	-	-	-	-	211.11188	3.79	0.51	0.84	211.11200	1.46	1.21	0.69
	$C_{15}H_{17}O_2^+$	229.12231	229.12258	4.27	1.21	1.86	229.12236	1.03	-0.25	0.37	229.12249	6.11	0.79	0.27
	$C_{15}H_{19}O_3^+$	247.13287	-	-	-	-	247.13295	2.12	-0.65	0.56	247.13304	2.90	0.68	1.17
	$C_{15}H_{21}O_4^+$	265.14344	-	-	-	-	-	-	-	-	265.14350	8.34	0.26	3.15
Ergocornine	$C_{15}H_{15}N_2^+$	223.12298	223.12307	6.35	0.41	0.28	223.12309	8.08	0.74	0.11	223.12306	7.94	0.38	0.36
	$C_{19}H_{17}O_2N_2^+$	305.12845	305.12845	1.67	-0.01	0.55	305.12849	1.51	0.18	-0.41	305.12858	1.15	0.42	0.38
	$C_{16}H_{18}N_3O^+$	268.14444	268.14447	5.20	0.12	0.19	268.14448	8.66	0.34	-0.22	268.14446	9.17	0.08	0.34
	$C_{14}H_{10}NO^+$	208.07569	208.07584	8.96	0.70	0.43	208.07584	8.50	0.86	0.24	208.07583	5.03	0.65	0.24
Ergocristine	$C_{15}H_{15}N_2^+$	223.12298	223.12308	7.37	0.49	0.33	223.12309	9.17	0.87	0.07	223.12300	8.14	0.10	0.37
	$C_{19}H_{17}O_2N_2^+$	305.12845	305.12853	1.83	0.25	0.60	305.12855	1.42	0.67	-0.21	305.12841	1.96	-0.14	0.64
	$C_{16}H_{18}N_3O^+$	268.14444	268.14444	7.94	0.00	0.30	268.14449	1.21	0.68	-0.22	268.14434	3.46	-0.37	0.13
	$C_{14}H_{10}NO^+$	208.07569	208.07581	7.55	0.57	0.36	208.07583	8.62	1.05	0.24	208.07577	6.08	0.38	0.29
Ergocryptine	$C_{15}H_{15}N_2^+$	223.12298	223.12308	3.46	0.47	0.16	223.12306	1.01	0.65	-0.16	223.12307	8.74	0.41	0.39
	$C_{16}H_{18}N_3O^+$	268.14444	268.14449	6.24	0.19	0.23	268.14445	1.39	0.34	-0.55	268.14446	7.55	0.08	0.28
	$C_{14}H_{10}NO^+$	208.07569	208.07584	5.51	0.73	0.26	208.07580	1.04	0.86	-0.05	208.07583	8.08	0.65	0.39
Ergometrine	$C_{15}H_{15}N_2^+$	223.12298	223.12324	3.21	1.17	0.14	223.12314	6.66	1.05	0.47	223.12302	7.37	0.22	0.33
	$C_{19}H_{24}N_3O_2^+$	326.18630	326.18627	1.65	-0.10	0.51	326.18626	7.55	0.11	-0.35	326.18620	1.14	-0.32	0.35
	$C_{14}H_{10}NO^+$	208.07569	208.07599	4.51	1.42	0.22	208.07599	1.28	2.11	0.91	208.07594	6.24	1.20	0.30
Ergosine	$C_{15}H_{15}N_2^+$	223.12298	223.12309	4.93	0.50	0.22	223.12311	1.04	1.14	0.34	223.12306	4.62	0.37	0.21
	$C_{14}H_{19}N_2O_3^+$	263.13902	263.13912	1.21	0.38	0.46	263.13920	9.64	1.11	0.54	263.13906	6.24	0.16	0.24
	$C_{14}H_{10}NO^+$	208.07569	208.07608	1.20	1.86	0.58	208.07595	6.35	1.58	1.05	208.07583	4.04	0.65	0.19
Ergotamine	$C_{15}H_{15}N_2^+$	223.12298	223.12310	7.64	0.55	0.34	223.12309	4.16	0.74	0.47	223.12307	1.05	0.43	0.47
	$C_{17}H_{17}N_2O_3^+$	297.12337	297.12353	8.08	0.53	0.27	297.12344	8.50	0.58	0.14	297.12344	1.85	0.25	0.62
	$C_{17}H_{13}N_2O_2^+$	277.09715	277.09726	1.50	0.38	0.54	277.09727	6.93	0.71	0.27	277.09722	1.05	0.24	0.38
	$C_{14}H_{10}NO^+$	208.07569	208.07591	1.46	1.07	0.70	208.07596	5.69	1.58	1.05	208.07592	8.66	1.10	0.42
Fumonisin B_1	$C_{22}H_{40}NO^+$	334.31044	334.31051	3.23	0.19	0.96	334.31047	6.81	0.23	0.15	334.31043	1.59	-0.02	0.48
	$C_{22}H_{42}NO_2^+$	352.32101	352.32157	4.74	1.61	1.35	352.32105	2.62	-0.67	0.21	352.32104	1.43	0.11	0.41
	$C_{22}H_{38}N^+$	316.29988	-	-	-	-	316.29979	5.03	-0.12	-0.24	316.29999	1.37	0.36	0.43
Fumonisin B_2	$C_{22}H_{42}NO^+$	336.32609	336.32610	1.83	0.03	0.55	336.32624	1.40	0.89	0.06	336.32611	1.08	0.06	0.32
	$C_{22}H_{44}NO_2^+$	-	-	-	-	-	-	-	-	-	354.33680	1.73	0.41	0.05
	$C_{22}H_{40}N^+$	318.31553	318.31569	1.58	0.52	0.50	318.31594	1.42	1.14	1.80	318.31564	9.00	0.36	0.28

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 ng/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
Fusarenon-X	$C_{14}H_{13}O_3^+$	229.08592	229.08592	4.49	-0.02	1.96	229.08592	4.49	-0.88	-1.40	229.08606	1.25	0.62	0.55
	$C_{14}H_{15}O_4^+$	247.09649	247.09672	2.50	0.95	1.01	247.09672	2.50	1.76	-0.18	247.09662	2.29	0.56	0.92
	$C_{13}H_{13}O_2^+$	201.09101	201.09106	4.02	0.25	2.00	201.09106	4.02	2.56	-0.83	201.09112	4.04	0.55	0.20
	$C_{11}H_{11}O_2^+$	175.07536	175.07547	1.33	0.63	0.76	175.07547	1.33	0.82	-0.21	175.07547	5.00	0.65	0.29
	$C_8H_9O_2^+$	137.05971	137.05977	7.09	0.44	0.52	137.05977	7.09	0.90	-0.12	137.05981	5.69	0.78	0.41
HT-2	$C_{14}H_{15}O_4^+$	169.10118	169.10135	1.06	1.02	0.63	169.10135	1.06	1.50	1.26	169.10130	1.14	0.71	0.67
	$C_{15}H_{19}O_4^+$	263.12779	-	-	-	-	-	-	-	-	263.12788	3.85	0.36	1.46
	$C_{14}H_{15}O_4^+$	215.10666	215.10710	3.84	2.06	1.79	215.10710	3.84	0.81	4.11	215.10710	1.15	2.05	0.53
	$C_{14}H_{13}O^+$	197.09609	197.09634	1.13	1.26	0.57	197.09634	1.13	1.92	0.91	197.09629	7.55	1.01	0.38
	$C_{13}H_{13}O^+$	185.09609	185.09635	1.73	1.40	0.09	185.09635	1.73	1.45	1.45	185.09628	1.44	1.04	0.78
	$C_{12}H_{13}^+$	157.10118	157.10136	1.25	1.16	0.80	157.10136	1.25	1.10	0.40	157.10151	5.86	2.10	0.37
	$C_{11}H_{13}^+$	145.10118	145.10136	8.89	1.26	0.61	145.10136	8.89	1.95	1.05	145.10133	8.50	1.03	0.59
Ochratoxin A	$C_{11}H_{10}ClO_5^+$	257.02111	257.02115	6.00	0.14	0.23	257.02115	6.00	0.14	0.38	257.02104	9.17	-0.28	0.36
	$C_{19}H_{14}ClO_4^+$	341.05751	341.05758	4.58	0.20	0.13	341.05758	4.58	0.05	0.31	341.05732	1.51	-0.57	0.44
	$C_{11}H_8ClO_4^+$	239.01056	239.01064	7.00	0.32	0.29	239.01064	7.00	0.32	0.62	239.01052	7.64	-0.17	0.32
	$C_8H_{10}N^+$	120.08078	120.08102	3.00	2.03	0.25	120.08102	3.00	2.03	2.28	120.08098	3.00	1.70	0.25
Ochratoxin B	$C_{11}H_{11}O_5^+$	223.06010	223.06012	5.51	0.08	0.25	223.06012	5.51	0.31	0.09	223.06016	5.13	0.25	0.23
	$C_{11}H_9O_4^+$	205.04954	205.04957	4.04	0.15	0.20	205.04957	4.04	0.36	0.12	205.04961	4.51	0.35	0.22
	$C_8H_{10}N^+$	120.08078	120.08101	2.31	1.92	0.19	120.08101	2.31	2.03	2.03	120.08105	3.79	2.25	0.32
Sterigmatocystin	$[C_{18}H_{12}O_6 + H]^+$	325.07066	325.07056	1.08	-0.32	0.33	325.07058	8.66	-0.41	-0.41	325.07068	5.20	0.05	0.16
	$C_{17}H_{10}O_6^+$	310.04719	310.04704	9.64	-0.48	0.31	310.04706	7.94	-0.61	-0.51	310.04716	6.24	-0.10	0.20
	$C_{17}H_{13}O_5^+$	297.07575	297.07582	9.24	0.22	0.31	297.07581	1.10	0.40	-0.24	-	-	-	-
	$C_{16}H_9O_6^+$	281.04445	281.04438	6.24	-0.25	0.22	281.04437	5.20	-0.50	-0.18	281.04431	1.37	-0.50	0.49
T-2	$C_{13}H_{13}O^+$	185.09609	185.09628	4.93	1.00	0.27	185.09626	8.39	1.13	0.37	185.09624	1.10	0.82	0.59
	$C_{14}H_{15}O_2^+$	215.10666	215.10686	9.64	0.95	0.45	215.10687	7.94	1.13	0.58	215.10685	8.74	0.92	0.41
	$C_{14}H_{13}O^+$	197.09609	197.09632	6.11	1.18	0.31	197.09632	7.02	1.11	0.80	197.09628	1.03	0.94	0.52
	$C_{13}H_{13}^+$	169.10118	169.10132	8.08	0.83	0.48	169.10134	5.03	0.90	0.67	169.10132	9.85	0.85	0.58
Verrucarin A	$C_{15}H_{19}O_2^+$	231.13796	231.13801	1.48	0.23	0.64	231.13805	1.21	0.97	0.32	231.13809	6.03	0.56	0.26
	$C_{15}H_{21}O_3^+$	249.14852	249.14856	1.51	0.16	0.61	249.14861	7.51	0.64	0.04	249.14863	1.44	0.44	0.58
	$C_{12}H_{17}O_2^+$	193.12231	193.12233	1.27	0.14	0.66	193.12233	1.27	0.85	0.02	193.12244	5.77	0.71	0.30
	$C_{10}H_{13}^+$	133.10118	133.10128	6.81	0.75	0.51	133.10128	6.81	1.15	0.92	133.10131	4.04	0.97	0.30

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 ng/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
Zearalenone	$C_8H_9^+$	105.06988	105.07025	6.81	3.58	0.65	-	-	-	-	105.07029	4.16	3.90	0.40
	$C_{12}H_{11}O_2^+$	187.07536	187.07480	1.31	-2.97	0.70	187.07507	6.24	-1.26	-1.42	187.07538	8.14	0.15	0.44
	$C_{18}H_{19}O_3^+$	283.13287	-	-	-	-	283.13338	2.27	0.88	2.15	283.13298	1.47	0.37	0.52
	$C_{12}H_{11}O_3^+$	203.07027	-	-	-	-	203.07025	7.09	0.29	-0.40	203.07031	9.61	0.21	0.47
	$C_{13}H_{11}O_4^+$	231.06546	231.06546	9.85	0.00	0.43	231.06542	1.00	0.26	-0.22	231.06534	8.14	-0.50	0.35

Supporting Table S8. Experimental Masses and Mass Accuracies of Ions used in the Identification of Mycotoxins in Peanut Matrix extracted with 50:50 Acetonitrile:Water Mixture.

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 mg/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
Aflatoxin B_1	$[C_{17}H_{12}O_6 + H]^+$	313.07066	313.07064	1.65	-0.06	0.53	313.07075	1.65	0.29	0.53	313.07062	5.20	-0.13	0.17
	$C_{16}H_{13}O_5^+$	285.07575	285.07560	1.51	-0.53	0.53	285.07570	1.71	-0.19	0.60	285.07561	6.93	-0.49	0.24
	$C_{15}H_{10}O_5^+$	270.05227	270.05223	1.71	-0.15	0.63	270.05227	1.26	-0.03	0.47	270.05220	4.04	-0.29	0.15
	$C_{15}H_{13}O_4^+$	257.08084	257.08089	1.14	0.21	0.44	257.08111	1.31	1.06	0.51	257.08102	1.93	0.73	0.75
Aflatoxin B_2	$[C_{17}H_{14}O_6 + H]^+$	315.08631	315.08611	3.46	-0.63	0.11	315.08623	1.73	-0.25	0.05	315.08628	4.58	-0.10	0.15
	$C_{16}H_{15}O_5^+$	287.09140	287.09126	1.14	-0.49	0.40	287.09138	1.73	-0.07	0.06	287.09145	3.46	0.17	0.12
	$C_{14}H_{11}O_5^+$	259.06000	259.06013	9.17	0.50	0.35	259.06014	6.93	0.54	0.27	259.06032	1.05	1.24	0.41
Aflatoxin G_1	$[C_{17}H_{12}O_7 + H]^+$	329.06558	329.06557	9.17	-0.03	0.28	329.06566	1.10	0.25	0.33	329.06561	1.39	0.09	0.42
	$C_{17}H_{11}O_6^+$	311.05501	311.05505	7.94	0.11	0.26	311.05515	3.51	0.42	0.11	311.05512	1.10	0.33	0.35
	$C_{16}H_{11}O_5^+$	283.06001	283.06017	8.66	0.57	0.31	-	-	-	-	283.06017	1.14	0.57	0.40
	$C_{14}H_{11}O_4^+$	243.06519	243.06529	1.33	0.45	0.55	243.06528	3.08	0.39	1.27	243.06545	1.25	1.10	0.51
Aflatoxin G_2	$[C_{17}H_{14}O_7 + H]^+$	331.08123	331.08102	1.10	-0.62	0.33	331.08115	5.77	-0.25	0.17	331.08122	3.46	-0.03	0.10
	$C_{17}H_{13}O_6^+$	313.07066	313.07058	1.05	-0.27	0.34	313.07066	4.04	-0.03	0.13	313.07073	6.93	0.21	0.22
	$C_{16}H_{13}O_5^+$	285.07575	285.07572	1.37	-0.12	0.48	285.07583	1.54	0.27	0.54	285.07572	1.10	-0.12	0.38
Beauvreicin	$C_9H_{12}N^+$	134.09643	134.09653	6.93	0.78	0.52	134.09653	1.53	0.75	0.11	134.09654	5.20	0.85	0.39
	$C_{20}H_{28}NO_5^+$	362.19620	362.19628	1.21	0.22	0.33	362.19622	9.64	0.06	0.27	362.19622	1.21	0.06	0.33
	$C_{15}H_{20}NO_3^+$	262.14377	262.14385	1.25	0.31	0.48	262.14386	3.00	0.34	0.11	262.14389	1.04	0.46	0.40
	$C_{15}H_{18}NO_2^+$	244.13321	244.13330	1.23	0.39	0.50	244.13331	2.08	0.42	0.09	244.13334	1.15	0.57	0.47
Citrinin	$C_{13}H_{13}O_4^+$	233.08084	233.08095	8.33	0.51	0.36	233.08093	1.53	0.42	0.07	233.08095	4.16	0.48	0.18
	$[C_{13}H_{14}O_5 + H]^+$	251.09140	251.09150	7.23	0.41	0.29	251.09149	4.04	0.35	0.16	251.09149	3.79	0.37	0.15
Deoxynivalenol	$C_{13}H_{15}O_2^+$	203.10666	-	-	-	-	203.10661	1.11	-0.21	0.54	203.10677	6.24	0.56	0.31
	$C_{14}H_{17}O_4^+$	249.11214	-	-	-	-	249.11327	5.29	4.55	0.21	249.11224	1.12	0.41	0.45
	$C_{14}H_{15}O_3^+$	231.10157	-	-	-	-	231.10227	3.55	3.04	1.54	231.10144	3.18	-0.57	1.38
	$C_{11}H_{11}O_2^+$	175.07536	175.07548	5.17	0.73	2.95	175.07550	2.15	0.80	1.23	175.07552	6.11	0.96	0.35
	$C_8H_9O_2^+$	137.05971	-	-	-	-	137.05978	6.51	0.56	0.47	137.05981	5.69	0.78	0.41
Diacetoxyscirpenol	$C_8H_9^+$	105.06988	-	-	-	-	105.07036	3.51	4.57	0.33	105.07037	5.86	4.66	0.56
	$C_{12}H_{13}^+$	157.10118	157.10130	4.51	0.80	0.29	157.10141	9.85	1.48	0.63	157.10146	1.47	1.80	0.94
	$C_{14}H_{15}^+$	183.11683	183.11701	4.31	1.00	2.36	183.11706	1.73	1.27	0.09	183.11708	4.93	1.36	0.27

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 mg/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
	$C_{14}H_{15}O^+$	199.11174	199.11196	1.05	1.10	0.53	199.11193	6.35	0.96	0.32	199.11194	1.31	1.00	0.66
	$C_{15}H_{15}O^+$	211.11174	-	-	-	-	211.11191	1.23	0.78	0.58	211.11196	9.17	1.03	0.43
	$C_{15}H_{17}O_2^+$	229.12231	229.12251	4.25	0.90	1.85	229.12248	1.12	0.74	0.49	229.12254	1.19	1.01	0.52
	$C_{15}H_{19}O_3^+$	247.13287	-	-	-	-	247.13300	9.17	0.52	0.37	247.13311	1.59	0.95	0.65
	$C_{15}H_{21}O_4^+$	265.14344	-	-	-	-	265.14367	6.72	0.87	2.54	265.14381	8.41	1.41	3.17
Ergocornine	$C_{15}H_{15}N_2^+$	223.12298	223.12309	2.89	0.53	0.13	223.12305	5.13	0.32	0.23	223.12310	6.35	0.55	0.28
	$C_{19}H_{17}O_2N_2^+$	305.12845	305.12858	8.66	0.41	0.28	305.12852	9.64	0.22	0.32	305.12856	9.17	0.35	0.30
	$C_{16}H_{18}N_3O^+$	268.14444	268.14450	3.00	0.23	0.11	268.14443	5.13	-0.04	0.19	268.14450	3.00	0.23	0.11
	$C_{14}H_{10}NO^+$	208.07569	208.07585	5.69	0.78	0.27	208.07579	7.37	0.49	0.35	208.07586	4.04	0.83	0.19
Ergocristine	$C_{15}H_{15}N_2^+$	223.12298	223.12301	1.15	0.14	0.05	223.12309	6.00	0.52	0.27	223.12311	9.61	0.59	0.43
	$C_{19}H_{17}O_2N_2^+$	305.12845	305.12851	7.94	0.18	0.26	305.12850	1.14	0.15	0.37	305.12855	1.76	0.31	0.58
	$C_{16}H_{18}N_3O^+$	268.14444	268.14448	1.73	0.15	0.06	268.14447	6.00	0.12	0.22	268.14453	1.20	0.34	0.45
	$C_{14}H_{10}NO^+$	208.07569	208.07577	3.46	0.38	0.17	208.07585	5.13	0.78	0.25	208.07586	1.00	0.80	0.48
Ergocryptine	$C_{15}H_{15}N_2^+$	223.12298	223.12309	1.21	0.52	0.54	223.12305	3.79	0.32	0.17	223.12310	3.21	0.55	0.14
	$C_{16}H_{18}N_3O^+$	268.14444	268.14448	1.21	0.15	0.45	268.14444	3.00	0.00	0.11	268.14450	3.00	0.23	0.11
	$C_{14}H_{10}NO^+$	208.07569	208.07588	9.50	0.89	0.46	208.07580	4.04	0.51	0.19	208.07585	4.93	0.75	0.24
Ergometrine	$C_{15}H_{15}N_2^+$	223.12298	223.12318	8.02	0.93	0.36	223.12305	9.50	0.35	0.43	223.12300	1.61	0.11	0.72
	$C_{19}H_{24}N_3O_2^+$	326.18630	326.18581	1.50	-1.52	0.46	326.18629	1.21	-0.03	0.37	326.18625	1.91	-0.17	0.59
	$C_{14}H_{10}NO^+$	208.07569	208.07609	8.50	1.94	0.41	208.07594	1.01	1.20	0.49	208.07589	1.36	0.97	0.65
Ergosine	$C_{15}H_{15}N_2^+$	223.12298	223.12310	4.73	0.58	0.21	223.12312	3.79	0.66	0.17	223.12313	8.66	0.69	0.39
	$C_{14}H_{19}N_2O_3^+$	263.13902	263.13925	7.94	0.88	0.30	263.13919	3.00	0.65	0.11	263.13916	1.08	0.54	0.41
	$C_{14}H_{10}NO^+$	208.07569	208.07595	2.08	1.23	0.10	208.07596	3.00	1.30	0.14	208.07590	6.66	0.99	0.32
Ergotamine	$C_{15}H_{15}N_2^+$	223.12298	223.12309	1.32	0.50	0.59	223.12319	1.15	0.96	0.52	223.12313	7.55	0.69	0.34
	$C_{17}H_{17}N_2O_3^+$	297.12337	297.12343	1.86	0.22	0.63	297.12360	1.72	0.77	0.58	297.12350	1.25	0.45	0.42
	$C_{17}H_{13}N_2O_2^+$	277.09715	277.09710	1.02	-0.21	0.37	277.09738	1.37	0.81	0.50	277.09728	1.05	0.45	0.38
	$C_{14}H_{10}NO^+$	208.07569	208.07582	1.92	0.64	0.92	208.07603	1.31	1.62	0.63	208.07600	7.51	1.50	0.36
Fumonisin B_1	$C_{22}H_{40}NO^+$	334.31044	334.31036	1.37	-0.23	0.41	334.31047	1.96	0.10	0.59	334.31052	5.20	0.23	0.16
	$C_{22}H_{42}NO_2^+$	352.32101	352.32116	3.88	0.43	1.10	352.32112	1.58	0.31	0.45	352.32118	4.58	0.49	0.13
	$C_{22}H_{38}N^+$	316.29988	316.29968	5.196	-0.62	0.16	316.30000	2.59	0.38	0.82	316.30008	7.94	0.64	0.25
Fumonisin B_2	$C_{22}H_{42}NO^+$	336.32609	336.32609	6.24	0.00	0.19	336.32615	2.30	0.18	0.68	336.32612	1.25	0.08	0.37
	$C_{22}H_{44}NO_2^+$	354.33666	354.33652	0.00027 93	-0.39	0.79	354.33671	3.88	0.16	1.09	354.33683	1.27	0.50	0.36

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 mg/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
	$C_{22}H_{40}N^+$	318.31553	318.31567	1.25	0.46	0.39	318.31562	2.31	0.30	0.73	318.31565	1.11	0.40	0.35
Fusarenon-X	$C_{14}H_{13}O_3^+$	229.08592	-	-	-	-	229.08603	1.08	0.48	0.47	229.08613	4.04	0.93	0.18
	$C_{14}H_{15}O_4^+$	247.09649	-	-	-	-	-	-	-	-	247.09670	5.13	0.88	0.21
	$C_{13}H_{13}O_2^+$	201.09101	-	-	-	-	201.09136	3.46	1.74	1.72	201.09116	1.73	0.76	0.09
	$C_{11}H_{11}O_2^+$	175.07536	-	-	-	-	175.07558	5.69	1.26	0.32	175.07553	2.31	1.01	0.13
	$C_8H_9O_2^+$	137.05971	-	-	-	-	137.05991	4.58	1.49	0.33	137.05985	1.15	1.07	0.08
HT-2	$C_{14}H_{15}O_4^+$	169.10118	-	-	-	-	169.10134	1.10	0.94	0.65	169.10141	9.71	1.36	0.57
	$C_{15}H_{19}O_4^+$	263.12779	-	-	-	-	-	-	-	-	263.12797	3.40	0.70	1.29
	$C_{14}H_{15}O_4^+$	215.10666	-	-	-	-	215.10676	8.88	0.48	0.41	215.10703	1.77	1.75	0.82
	$C_{14}H_{13}O^+$	197.09609	-	-	-	-	197.09650	1.65	2.06	0.84	197.09630	7.57	1.07	0.38
	$C_{13}H_{13}O^+$	185.09609	-	-	-	-	185.09622	4.37	0.68	2.36	185.09645	3.59	1.92	1.94
	$C_{12}H_{13}^+$	157.10118	-	-	-	-	157.10138	1.56	1.29	0.99	157.10151	1.59	2.10	1.02
	$C_{11}H_{13}^+$	145.10118	-	-	-	-	145.10135	1.59	1.19	1.09	145.10138	1.15	1.42	0.79
Ochratoxin A	$C_{11}H_{10}ClO_5^+$	257.02111	257.02111	1.05	-0.01	0.41	257.02110	7.55	-0.05	0.29	257.02117	6.24	0.22	0.24
	$C_{19}H_{14}ClO_4^+$	341.05751	341.05768	6.42	0.49	1.88	341.05749	2.02	-0.06	0.59	341.05746	1.14	-0.15	0.33
	$C_{11}H_8ClO_4^+$	239.01056	239.01054	7.57	-0.11	0.32	239.01058	7.55	0.07	0.32	239.01064	5.69	0.31	0.24
	$C_8H_{10}N^+$	120.08078	120.08106	1.27	2.34	1.05	120.08101	5.29	1.95	0.44	120.08104	2.08	2.23	0.17
Ochratoxin B	$C_{11}H_{11}O_5^+$	223.06010	223.06017	9.29	0.30	0.42	223.06019	3.21	0.39	0.14	223.06027	3.51	0.75	0.16
	$C_{11}H_9O_4^+$	205.04954	205.04960	8.08	0.33	0.39	205.04963	3.21	0.48	0.16	205.04972	4.04	0.88	0.20
	$C_8H_{10}N^+$	120.08078	120.08092	3.51	1.17	0.29	120.08106	1.00	2.37	0.08	120.08111	1.53	2.75	0.13
Sterigmatocystin	$[C_{18}H_{12}O_6 + H]^+$	325.07066	325.07066	3.46	-0.01	0.11	325.07065	1.04	-0.04	0.32	325.07052	1.56	-0.46	0.48
	$C_{17}H_{10}O_6^+$	310.04719	310.04715	3.00	-0.13	0.10	310.04713	1.48	-0.19	0.48	310.04703	1.37	-0.51	0.44
	$C_{17}H_{13}O_5^+$	297.07575	297.07580	1.26	0.16	0.42	297.07591	1.56	0.53	0.53	297.07571	1.72	-0.12	0.58
	$C_{16}H_9O_6^+$	281.04445	281.04439	1.25	-0.21	0.44	281.04430	7.55	-0.53	0.27	281.04431	1.67	-0.50	0.59
T-2	$C_{13}H_{13}O^+$	185.09609	185.09622	5.77E-06	0.68	0.03	185.09626	7.23	0.89	0.39	185.09631	6.03	1.16	0.33
	$C_{14}H_{15}O_2^+$	215.10666	215.10693	5.51	1.26	0.26	215.10685	9.24	0.92	0.43	215.10692	7.51	1.21	0.35
	$C_{14}H_{13}O^+$	197.09609	197.09616	1.45	0.33	0.74	197.09626	8.74	0.87	0.44	197.09630	5.51	1.07	0.28
	$C_{13}H_{13}^+$	169.10118	169.10124	1.15	0.35	0.68	169.10133	8.50	0.92	0.50	169.10135	5.51	1.04	0.33
Verrucarin A	$C_{15}H_{19}O_2^+$	231.13796	231.13810	6.24	0.62	0.27	231.13820	5.69	1.04	0.25	231.13812	8.96	0.72	0.39
	$C_{15}H_{21}O_3^+$	249.14852	249.14872	5.03	0.81	0.20	249.14872	8.39	0.79	0.34	249.14859	2.52	0.26	0.10
	$C_{12}H_{17}O_2^+$	193.12231	193.12238	2.89	0.36	0.15	193.12256	1.15	1.31	0.60	193.12246	7.23	0.81	0.37
	$C_{10}H_{13}^+$	133.10118	133.10131	2.08	0.97	0.16	133.10137	5.57	1.45	0.42	133.10131	4.04	0.97	0.30

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 mg/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
Zearalenone	$C_8H_9^+$	105.06988	105.07029	2.65	3.93	0.25	105.07036	4.73	4.57	0.45	105.07031	1.15	4.15	0.11
	$C_{12}H_{11}O_2^+$	187.07536	187.07510	5.42	-1.39	2.90	187.07515	5.51	-1.12	0.29	187.07550	2.31	0.79	0.12
	$C_{18}H_{19}O_3^+$	283.13287	-	-	-	-	-	-	-	-	283.13304	3.46	0.60	0.12
	$C_{12}H_{11}O_3^+$	203.07027	-	-	-	-	203.07024	4.51	-0.17	0.22	203.07041	1.15	0.67	0.06
	$C_{13}H_{11}O_4^+$	231.06546	231.06522	1.65	-1.05	0.71	231.06536	2.08	-0.45	0.09	231.06547	7.09	0.06	0.31

Supporting Table S9. Experimental Masses and Mass Accuracies of Ions used in the Identification of Mycotoxins in Wheat Matrix extracted with 50:50 Acetonitrile:Water Mixture.

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 mg/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
Aflatoxin B_1	$[C_{17}H_{12}O_6 + H]^+$	313.07066	313.07063	2.00	-0.11	0.64	313.07059	1.08	-0.13	0.35	313.07055	9.17	-0.33	0.29
	$C_{16}H_{13}O_5^+$	285.07575	285.07558	2.16	-0.58	0.76	285.07567	1.29	-0.39	0.45	285.07546	1.35	-1.03	0.47
	$C_{15}H_{10}O_5^+$	270.05227	270.05246	5.54	0.67	2.05	270.05212	5.20	-0.61	0.19	270.05215	1.37	-0.37	0.51
	$C_{15}H_{13}O_4^+$	257.08084	257.08085	2.31	0.07	0.90	257.08086	2.04	-0.11	0.79	257.08075	7.94	-0.29	0.31
Aflatoxin B_2	$[C_{17}H_{14}O_6 + H]^+$	315.08631	315.08624	6.00	-0.22	0.19	315.08618	1.31	-0.48	0.42	315.08614	4.58	-0.55	0.15
	$C_{16}H_{15}O_5^+$	287.09140	287.09144	7.55	0.14	0.26	287.09134	1.04	-0.28	0.36	287.09131	0.00E+00	-0.31	0.00
	$C_{14}H_{11}O_5^+$	259.06000	259.06035	1.56	1.36	0.60	259.06020	1.25	0.64	0.48	259.06043	0.000461194	2.06	1.78
Aflatoxin G_1	$[C_{17}H_{12}O_7 + H]^+$	329.06558	329.06561	7.94	0.09	0.24	329.06540	1.08	-0.58	0.33	329.06574	5.13	0.54	0.16
	$C_{17}H_{11}O_6^+$	311.05501	311.05504	7.55	0.08	0.24	311.05486	1.35	-0.51	0.43	311.05498	4.58	-0.06	0.15
	$C_{16}H_{11}O_5^+$	283.06001	283.06020	7.55	0.67	0.27	283.05998	1.40	-0.11	0.50	283.06395	4.56	14.24	1.61
	$C_{14}H_{11}O_4^+$	243.06519	243.06529	6.00	0.43	0.25	243.06527	5.03	0.44	0.21	243.06532	1.53	0.59	0.06
Aflatoxin G_2	$[C_{17}H_{14}O_7 + H]^+$	331.08123	331.08119	1.05	-0.12	0.32	331.08112	5.20	-0.30	0.16	331.08109	3.51	-0.46	0.11
	$C_{17}H_{13}O_6^+$	313.07066	313.07094	5.54	0.88	1.77	313.07051	8.02	-0.59	0.26	313.07061	3.46	-0.22	0.11
	$C_{16}H_{13}O_5^+$	285.07575	285.07797	1.46	7.80	5.14	285.07664	2.24	0.11	7.86	285.07567	6.93	-0.19	0.24
Beauvreicin	$C_9H_{12}N^+$	134.09643	134.09654	1.53	0.87	0.11	134.09650	3.06	0.66	0.23	134.09649	3.21	0.56	0.24
	$C_{20}H_{28}NO_5^+$	362.19620	362.19622	6.10	0.06	1.68	362.19615	9.71	-0.05	0.27	362.19606	1.27	-0.50	0.35
	$C_{15}H_{20}NO_3^+$	262.14377	262.14386	1.08	0.34	0.41	262.14377	5.20	0.08	0.20	262.14378	7.55	0.13	0.29
	$C_{15}H_{18}NO_2^+$	244.13321	244.13331	4.58	0.43	0.19	244.13326	5.77	0.30	0.24	244.13322	6.56	0.14	0.27
Citrinin	$C_{13}H_{13}O_4^+$	233.08084	233.08086	7.37	0.12	0.32	233.08090	7.37	0.15	0.32	233.08085	9.24	0.20	0.40
	$[C_{13}H_{14}O_5 + H]^+$	251.09140	251.09140	6.81	-0.01	0.27	251.09142	8.39	-0.04	0.33	251.09150	9.64	0.25	0.38
Deoxynivalenol	$C_{13}H_{15}O_2^+$	203.10666	-	-	-	-	203.10672	1.71	0.05	0.84	203.10668	1.62	-0.17	0.80
	$C_{14}H_{17}O_4^+$	249.11214	-	-	-	-	249.11517	3.76	12.57	1.51	249.11204	3.46	-0.91	1.39
	$C_{14}H_{15}O_3^+$	231.10157	-	-	-	-	231.10352	1.91	6.54	8.28	231.10166	7.55	0.29	0.33
	$C_{11}H_{11}O_2^+$	175.07536	-	-	-	-	175.07531	2.27	-0.60	1.30	175.07546	4.04	0.49	0.23
	$C_8H_9O_2^+$	137.05971	-	-	-	-	137.06063	7.52	5.24	5.48	137.05980	1.36	0.29	0.99
Diacetoxyscirpenol	$C_8H_9^+$	105.06988	105.07035	7.00	4.50	0.67	105.07032	5.03	4.02	0.48	105.07030	1.53	4.07	0.15
	$C_{12}H_{13}^+$	157.10118	157.10138	5.00	1.29	0.32	157.10134	1.15	0.92	0.74	157.10127	3.51	0.65	0.22
	$C_{14}H_{15}^+$	183.11683	183.11703	2.67	1.13	1.46	183.11692	6.24	0.42	0.34	183.11696	7.09	0.85	0.39

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 mg/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
	$C_{14}H_{15}O^+$	199.11174	199.11192	1.25	0.90	0.63	199.11184	6.24	0.41	0.31	199.11178	1.73	0.21	0.09
	$C_{15}H_{15}O^+$	211.11174	-	-	-	-	211.11180	1.80	0.27	0.85	211.11191	6.24	0.83	0.30
	$C_{15}H_{17}O_2^+$	229.12231	229.12240	2.04	0.39	0.89	229.12244	9.45	0.52	0.41	229.12231	9.07	0.05	0.40
	$C_{15}H_{19}O_3^+$	247.13287	-	-	-	-	247.13299	2.75	0.09	1.11	247.13292	1.82	0.48	0.74
	$C_{15}H_{21}O_4^+$	265.14344	-	-	-	-	265.14440	2.47	4.60	9.31	265.14664	2.66	11.88	1.00
Ergocornine	$C_{15}H_{15}N_2^+$	223.12298	223.12312	8.33	0.63	0.37	223.12302	7.09	0.09	0.32	223.12301	1.15	0.15	0.05
	$C_{19}H_{17}O_2N_2^+$	305.12845	305.12863	6.00	0.58	0.20	305.12842	7.94	-0.15	0.26	305.12841	4.51	-0.20	0.15
	$C_{16}H_{18}N_3O^+$	268.14444	268.14451	9.64	0.27	0.36	268.14439	9.17	-0.28	0.34	268.14438	3.00	-0.18	0.11
	$C_{14}H_{10}NO^+$	208.07569	208.07589	8.39	0.97	0.40	208.07577	5.69	0.32	0.27	208.07579	3.00	0.48	0.14
Ergocristine	$C_{15}H_{15}N_2^+$	223.12298	223.12310	7.64	0.55	0.34	223.12304	8.02	0.30	0.36	223.12306	6.03	0.27	0.27
	$C_{19}H_{17}O_2N_2^+$	305.12845	305.12846	4.58	0.02	0.15	305.12842	1.31	-0.18	0.43	305.12846	1.21	-0.10	0.40
	$C_{16}H_{18}N_3O^+$	268.14444	268.14444	6.00	0.00	0.22	268.14446	1.05	0.07	0.39	268.14447	6.00	0.04	0.22
	$C_{14}H_{10}NO^+$	208.07569	208.07584	7.94	0.72	0.38	208.07580	8.08	0.49	0.39	208.07583	4.73	0.57	0.23
Ergocryptine	$C_{15}H_{15}N_2^+$	223.12298	223.12308	5.69	0.46	0.25	223.12301	3.21	0.19	0.14	223.12298	1.08	-0.08	0.48
	$C_{16}H_{18}N_3O^+$	268.14444	268.14448	6.93	0.15	0.26	268.14440	1.73	-0.16	0.06	268.14434	1.25	-0.49	0.47
	$C_{14}H_{10}NO^+$	208.07569	208.07585	4.58	0.77	0.22	208.07578	1.53	0.41	0.07	208.07575	1.01	0.12	0.48
Ergometrine	$C_{15}H_{15}N_2^+$	223.12298	223.12312	1.33	0.63	0.60	223.12294	9.85	-0.04	0.44	223.12302	1.99	0.12	0.89
	$C_{19}H_{24}N_3O_2^+$	326.18630	326.18602	2.57	-0.87	0.79	326.18612	1.75	-0.42	0.54	326.18625	2.46	-0.23	0.75
	$C_{14}H_{10}NO^+$	208.07569	-	-	-	-	208.07585	1.35	0.94	0.65	208.07592	2.12	0.97	1.02
Ergosine	$C_{15}H_{15}N_2^+$	223.12298	223.12310	4.04	0.55	0.18	223.12302	4.93	0.13	0.22	223.12309	5.77E-06	0.51	0.03
	$C_{14}H_{19}N_2O_3^+$	263.13902	263.13914	1.83	0.46	0.70	263.13904	7.94	-0.03	0.30	263.13908	6.24	0.21	0.24
	$C_{14}H_{10}NO^+$	208.07569	208.07586	6.93	0.81	0.33	208.07583	6.24	0.56	0.30	208.07584	1.53	0.73	0.07
Ergotamine	$C_{15}H_{15}N_2^+$	223.12298	223.12310	2.08	0.58	0.09	223.12306	5.13	0.31	0.23	223.12303	6.66	0.15	0.30
	$C_{17}H_{17}N_2O_3^+$	297.12337	297.12365	1.73	0.95	0.06	297.12343	6.24	0.13	0.21	297.12338	9.00	-0.06	0.30
	$C_{17}H_{13}N_2O_2^+$	277.09715	277.09790	2.26	2.69	0.82	277.09721	9.64	0.07	0.35	277.09717	5.20	-0.02	0.19
	$C_{14}H_{10}NO^+$	208.07569	208.07579	5.03	0.46	0.24	208.07592	1.30	0.86	0.62	208.07590	6.00	0.91	0.29
Fumonisin B_1	$C_{22}H_{40}NO^+$	334.31044	334.31037	1.31	-0.20	0.39	334.31045	1.72	0.19	0.52	334.31044	1.99	0.15	0.59
	$C_{22}H_{42}NO_2^+$	352.32101	352.32093	5.28	-0.21	1.50	352.32112	3.46	0.36	0.10	352.32115	1.96	0.53	0.56
	$C_{22}H_{38}N^+$	316.29988	316.30009	1.06	0.67	3.34	316.29992	1.86	0.31	0.59	316.30005	1.97	0.74	0.62
Fumonisin B_2	$C_{22}H_{42}NO^+$	336.32609	336.32601	1.35	-0.24	0.40	336.32603	3.46	-0.20	0.10	336.32604	4.58	-0.19	0.14
	$C_{22}H_{44}NO_2^+$	354.33666	-	-	-	-	354.33666	4.58	0.00	0.13	354.33668	6.24	0.05	0.18
	$C_{22}H_{40}N^+$	318.31553	318.31552	6.00	-0.02	0.19	318.31554	3.46	0.06	0.11	318.31552	3.00	-0.02	0.09

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 mg/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
Fusarenon-X	$C_{14}H_{13}O_3^+$	229.08592	-	-	-	-	229.08615	1.07	1.16	0.47	229.08606	5.03	0.61	0.22
	$C_{14}H_{15}O_4^+$	247.09649	-	-	-	-					247.09662	1.45	0.36	0.59
	$C_{13}H_{13}O_2^+$	201.09101	-	-	-	-	201.09227	1.24	3.94	6.16	201.09109	1.00	0.42	0.50
	$C_{11}H_{11}O_2^+$	175.07536	-	-	-	-	175.07544	1.08	0.41	0.62	175.07546	6.56	0.57	0.37
	$C_8H_9O_2^+$	137.05971	-	-	-	-	137.05982	5.57	0.95	0.41	137.05978	3.51	0.51	0.26
HT-2	$C_{14}H_{15}O_4^+$	169.10118	-	-	-	-								
	$C_{15}H_{19}O_4^+$	263.12779	-	-	-	-								
	$C_{14}H_{15}O_4^+$	215.10666	-	-	-	-	215.10763	7.16	3.90	3.33	215.10931	3.86	13.04	1.79
	$C_{14}H_{13}O^+$	197.09609	-	-	-	-	197.09766	1.14	7.66	5.80	197.09817	2.45	10.95	1.24
	$C_{13}H_{13}O^+$	185.09609	-	-	-	-	185.09686	6.74	3.02	3.64	185.09790	4.74	10.23	2.56
	$C_{12}H_{13}^+$	157.10118	-	-	-	-	-	-	-	-	-	-	-	-
	$C_{11}H_{13}^+$	145.10118	-	-	-	-	-	-	-	-	-	-	-	-
Ochratoxin A	$C_{11}H_{10}ClO_5^+$	257.02111	257.02117	1.05	0.22	0.41	257.02114	1.14	-0.06	0.44	257.02111	6.24	-0.10	0.24
	$C_{19}H_{14}ClO_4^+$	341.05751	341.05749	5.74	-0.08	1.68	341.05750	1.43	-0.17	0.42	341.05752	1.40	-0.12	0.41
	$C_{11}H_8ClO_4^+$	239.01056	239.01063	4.58	0.28	0.19	239.01063	9.64	0.13	0.40	239.01058	5.29	-0.01	0.22
	$C_8H_{10}N^+$	120.08078	120.08109	5.51	2.64	0.46	120.08105	5.77	2.13	0.48	120.08104	3.46	2.09	0.29
Ochratoxin B	$C_{11}H_{11}O_5^+$	223.06010	223.06022	1.11	0.52	0.50	223.06015	4.36	0.30	0.20	223.06021	1.40	0.28	0.63
	$C_{11}H_9O_4^+$	205.04954	205.04966	8.02	0.62	0.39	205.04959	2.89	0.34	0.14	205.04965	1.20	0.34	0.59
	$C_8H_{10}N^+$	120.08078	120.08109	6.36	2.60	0.53	120.08107	1.53	2.41	0.13	120.08107	9.07	2.19	0.76
Sterigmatocystin	$[C_{18}H_{12}O_6 + H]^+$	325.07066	325.07075	2.44	0.26	0.75	325.07069	9.17	0.18	0.28	325.07063	1.05	0.00	0.32
	$C_{17}H_{10}O_6^+$	310.04719	310.04721	2.08	0.07	0.67	310.04716	4.58	-0.08	0.15	310.04710	1.05	-0.18	0.34
	$C_{17}H_{13}O_5^+$	297.07575	297.07499	1.39	-2.55	4.70	297.07545	5.34	-1.51	1.80	297.07591	2.55	0.85	0.86
	$C_{16}H_9O_6^+$	281.04445	-	-	-	-	281.04411	6.84	-1.83	2.43	281.04420	1.14	-0.73	0.40
T-2	$C_{13}H_{13}O^+$	185.09609	185.09619	9.02	0.51	0.49	185.09619	2.52	0.47	0.14	185.09627	5.51	1.10	0.30
	$C_{14}H_{15}O_2^+$	215.10666	215.10688	5.86	1.02	0.27	215.10678	2.52	0.52	0.12	215.10689	7.09	1.19	0.33
	$C_{14}H_{13}O^+$	197.09609	197.09627	1.04	0.91	0.53	197.09624	3.00	0.70	0.15	197.09628	7.57	1.09	0.38
	$C_{13}H_{13}^+$	169.10118	169.10120	4.16	0.12	0.25	169.10125	1.15	0.43	0.07	169.10134	3.46	1.04	0.20
Verrucarin A	$C_{15}H_{19}O_2^+$	231.13796	231.13819	1.19	1.03	0.52	231.13808	4.58	0.48	0.20	231.13816	7.64	0.89	0.33
	$C_{15}H_{21}O_3^+$	249.14852	249.14860	1.48	0.33	0.60	249.14856	1.15	0.01	0.46	249.14935	1.50	1.01	6.02
	$C_{12}H_{17}O_2^+$	193.12231	193.12244	4.93	0.71	0.26	193.12239	3.00	0.38	0.16	193.12295	9.47	1.45	4.90
	$C_{10}H_{13}^+$	133.10118	133.10133	3.51	1.12	0.26	133.10128	4.04	0.64	0.30	133.10133	4.62	1.19	0.35
	$C_8H_9^+$	105.06988	105.07030	2.52	4.06	0.24	105.07029	1.00	3.93	0.10	105.07033	3.00	4.31	0.29

Compound	Molecular Formula	Theoretical Mass (Dalton)	1 ng/mL				10 ng/mL				100 mg/mL			
			Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)		Experimental Mass		Accuracy (ppm)	
			Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD	Average (Dalton)	SD (ppm)	Average	SD
Zearalenone	$C_{12}H_{11}O_2^+$	187.07536	187.07485	1.10	-2.72	0.59	187.07506	3.00	-1.58	0.16	187.07540	1.21	0.11	0.65
	$C_{18}H_{19}O_3^+$	283.13287	-	-	-	-	283.13285	1.14	0.08	0.40	283.13298	1.99	0.20	0.70
	$C_{12}H_{11}O_3^+$	203.07027	-	-	-	-	203.07017	3.61	-0.45	0.18	203.07033	1.46	0.17	0.72
	$C_{13}H_{11}O_4^+$	231.06546	231.06547	2.57	0.03	1.11	231.06530	7.02	-0.70	0.30	231.06537	1.56	-0.52	0.67

Supporting Table S10. Experimental Masses and Mass Accuracies of Ions used in the Identification of Isotope-labeled Mycotoxins in Solvent (50:50 Acetonitrile:Water) and Peanut and Wheat Matrices extracted with 50:50 Acetonitrile:Water Mixture.

Compound	Molecular Formula	Theoretical Mass	Solvent (n = 9)				Peanut (n = 9)				Wheat (n = 9)			
			Experimental Mass	SD	RSD, %	Average δ_M, ppm	Experimental Mass	SD	RSD, %	Average δ_M, ppm	Experimental Mass	SD	RSD, %	Average δ_M, ppm
			Dalton				Dalton				Dalton			
($^{13}C_{17}$)-Aflatoxin B_1	$[^{13}C_{17}H_{12}O_6 + H]^+$	330.12770	330.12766	1.38E-04	0.004	-0.12	330.12769	1.06E-04	0.003	-0.04	330.12764	1.19E-04	0.004	-0.19
	$^{13}C_{16}H_{13}O_5^+$	301.12943	301.12947	1.26E-04	0.004	0.15	301.12949	9.56E-05	0.003	0.21	301.12944	1.21E-04	0.004	0.03
($^{13}C_{34}$)-Fumonisin B_1	$^{13}C_{22}H_{40}NO^+$	356.38425	356.38431	1.20E-04	0.003	0.16	356.38435	1.27E-04	0.004	0.29	356.38430	1.40E-04	0.004	0.15
	$^{13}C_{22}H_{42}NO_2^+$	374.39481	374.39491	1.90E-04	0.005	0.27	374.39496	2.21E-04	0.006	0.40	374.39494	1.75E-04	0.005	0.33
	$^{13}C_{22}H_{38}N^+$	338.37368	338.37370	2.21E-04	0.007	0.07	338.37386	1.58E-04	0.005	0.53	338.37378	1.94E-04	0.006	0.28
($^{13}C_{20}$)-Ochratoxin A	$^{13}C_{11}H_{10}ClO_5^+$	268.05803	268.05804	6.25E-05	0.002	0.02	268.05805	8.84E-05	0.003	0.07	268.05803	1.22E-04	0.005	0.00
	$^{13}C_{19}H_{14}ClO_4^+$	360.12084	360.12117	1.26E-04	0.003	0.92	360.12108	1.73E-04	0.005	0.65	360.12110	1.42E-04	0.004	0.73
	$^{13}C_{11}H_8ClO_4^+$	250.04747	250.04759	4.25E-05	0.002	0.51	250.04760	8.01E-05	0.003	0.54	250.04758	1.04E-04	0.004	0.47
	$^{13}C_8H_{10}N^+$	128.10761	128.10781	5.12E-05	0.004	1.53	128.10781	5.59E-05	0.004	1.56	128.10780	6.25E-05	0.005	1.44
($^{13}C_{24}$)-T-2	$^{13}C_{13}H_{13}O^+$	198.13970	198.13989	7.13E-05	0.004	0.94	198.13992	9.42E-05	0.005	1.09	198.13991	4.50E-05	0.002	1.02
	$^{13}C_{14}H_{15}O_2^+$	229.15384	229.15385	9.72E-05	0.004	0.02	229.15392	9.12E-05	0.004	0.33	229.15386	8.47E-05	0.004	0.11
	$^{13}C_{14}H_{13}O^+$	211.14306	211.14320	9.11E-05	0.004	0.69	211.14327	9.32E-05	0.004	1.01	211.14324	9.01E-05	0.004	0.85
	$^{13}C_{13}H_{13}^+$	182.14479	182.14498	7.68E-05	0.004	1.02	182.14502	7.30E-05	0.004	1.28	182.14498	3.67E-05	0.002	1.06
($^{13}C_{18}$)-Zearalenone	$^{13}C_{12}H_{11}O_2^+$	199.11561	199.11572	3.91E-05	0.002	0.55	199.11575	1.18E-04	0.006	0.70	199.11571	8.42E-05	0.004	0.47
	$^{13}C_{18}H_{19}O_3^+$	301.19326	301.19332	1.05E-04	0.003	0.21	301.19338	1.85E-04	0.006	0.41	301.19324	1.33E-04	0.004	-0.05
	$^{13}C_{13}H_{11}O_4^+$	215.11053	215.11067	3.13E-05	0.001	0.68	215.11069	1.23E-04	0.006	0.77	215.11064	9.22E-05	0.004	0.50
	$^{13}C_{12}H_{11}O_3^+$	244.10880	244.10896	2.57E-05	0.001	0.67	244.10899	1.69E-04	0.007	0.79	244.10901	1.89E-04	0.008	0.87

Supporting Table S11. Molecular ions and % ion ratios used to identify mycotoxins, including proposed molecular formulae and theoretical masses. Average ion ratios (% Avg) and relative standard deviations (RSD) based on triplicate results each of the mycotoxins fortified in solvent (acetonitrile:water) and acetonitrile:water extracts from peanut and wheat matrices at 1, 10 and 100 ng/mL. The % ion ratio was determined by the ratio of the ion signal responses extracted of the ion to the response with the signal of the molecular or fragment ion (indicated in bold) of the highest signal intensity.

Compound	Molecular Formula	Theoretical Mass	1 ng/mL					10 ng/mL					100 ng/mL				
			Solvent	Peanut	Wheat	Average	RSD	Solvent	Peanut	Wheat	Average	RSD	Solvent	Peanut	Wheat	Average	RSD
Aflatoxin B_1	$[C_{17}H_{12}O_6 + H]^+$	313.07066	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{16}H_{13}O_5^+$	285.07575	29	29	29	29	0.7	29	30	29	29	1.9	31	30	30	30	2.6
	$C_{15}H_{10}O_5^+$	270.05227	6	5	5	6	6.0	5	6	6	6	3.2	6	5	6	6	2.1
	$C_{15}H_{13}O_4^+$	257.08084	4	4	4	4	5.1	4	4	4	4	2.2	5	4	4	4	9.7
($^{13}C_{17}$)-Aflatoxin B_1	$[^{13}C_{17}H_{12}O_6 + H]^+$	330.12770	-	-	-	-	-	100	100	100	-	-	-	-	-	-	-
	$^{13}C_{16}H_{13}O_5^+$	301.12943	-	-	-	-	-	31	30	30	30	1.8	-	-	-	-	-
Aflatoxin B_2	$[C_{17}H_{14}O_6 + H]^+$	315.08631	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{16}H_{15}O_5^+$	287.09140	10	9	10	10	3.3	10	10	10	10	0.9	10	9	10	10	0.1
	$C_{14}H_{11}O_5^+$	259.06000	5	4	5	5	3.5	4	4	4	4	0.6	5	4	4	5	2.8
Aflatoxin G_1	$[C_{17}H_{12}O_7 + H]^+$	329.06558	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{17}H_{11}O_6^+$	311.05501	31	30	31	31	3.3	31	28	31	30	6.3	31	31	37	34	10.8
	$C_{16}H_{11}O_5^+$	283.06001	12	12	12	12	1.9	12	6	13	11	33.6	13	13	10	11	15.1
	$[C_{14}H_{11}O_4^+$	243.06519	20	20	21	20	1.3	20	18	20	19	5.2	21	21	20	20	5.0
Aflatoxin G_2	$[C_{17}H_{14}O_7 + H]^+$	331.08123	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{17}H_{13}O_6^+$	313.07066	15	15	9	13	24.8	16	15	12	14	14.8	16	15	16	16	0.1
	$C_{16}H_{13}O_5^+$	285.07575	3	3	3	3	13.5	3	3	3	3	9.4	3	3	3	3	0.4
Beauvreicin	$C_9H_{12}N^+$	134.09643	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{20}H_{28}NO_5^+$	362.19620	8	8	8	8	4.4	8	8	8	8	2.9	8	8	8	8	0.1
	$C_{15}H_{20}NO_3^+$	262.14377	25	25	25	25	0.6	26	26	26	26	1.3	27	26	26	27	1.6
	$C_{15}H_{18}NO_2^+$	244.13321	64	66	64	65	1.4	66	65	65	65	1.1	67	62	66	67	1.5
Citrinin	$C_{13}H_{13}O_4^+$	233.08084	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{13}H_{15}O_5^+$	251.09140	225	225	170	207	15.2	213	101	44	119	71.7	36	47	41	41	13.5
Deoxynivalenol	$C_{13}H_{15}O_2^+$	203.10666	-	-	-	-	-	100	100	199	133	43	100	100	100	100	0.0
	$C_{14}H_{17}O_4^+$	249.11214	-	-	-	-	-	32	32	32	32	0.5	34	35	35	35	1.3
	$C_{14}H_{15}O_3^+$	231.10157	-	-	-	-	-	58	45	55	52	13.0	58	53	56	56	4.4
	$C_{11}H_{11}O_2^+$	175.07536	-	-	-	-	-	86	74	76	79	8.5	80	74	80	78	4.2
	$C_8H_9O_2^+$	137.05971	-	-	-	-	-	64	50	54	56	13.1	51	54	50	52	4.1

Diacetoxyscirpenol	$C_8H_9^+$	105.06988	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{12}H_{13}^+$	157.10118	57	51	52	53	5.8	51	50	53	51	2.5	51	53	51	52	2.9
	$C_{14}H_{15}^+$	183.11683	41	41	45	42	4.5	46	42	43	44	5.4	44	47	42	44	4.9
	$C_{14}H_{15}O^+$	199.11174	66	67	60	64	6.1	70	65	69	68	4.4	71	70	69	70	1.0
	$C_{15}H_{15}O^+$	211.11174	28	23	22	24	15.0	26	25	24	25	3.0	26	27	24	26	5.6
	$C_{15}H_{17}O_2^+$	229.12231	42	40	39	40	3.9	42	43	45	43	3.8	41	45	42	43	3.8
	$C_{15}H_{19}O_3^+$	247.13287	26	24	23	25	5.9	27	28	26	27	3.3	30	29	27	29	4.5
	$C_{15}H_{21}O_4^+$	265.14344	-	-	-	-	-	6	7	7	7	14.2	8	7	7	7	8.0
	$C_{17}H_{23}O_5^+$	307.15400	8	3	5	6	40.4	8	8	6	7	10.2	7	8	7	7	12.6
Ergocornine	$C_{15}H_{15}N_2^+$	223.12298	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{19}H_{17}O_2N_2^+$	305.12845	26	24	26	25	3.4	24	25	25	24	2.2	26	25	19	22	21.5
	$C_{16}H_{18}N_3O^+$	268.14444	63	63	60	62	2.9	64	61	57	61	7.5	57	57	54	56	4.3
	$C_{14}H_{10}NO^+$	208.07569	65	66	62	64	3.2	65	64	60	62	5.6	60	60	57	59	3.8
Ergocristine	$C_{15}H_{15}N_2^+$	223.12298	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{19}H_{17}O_2N_2^+$	305.12845	27	27	26	27	1.7	25	25	26	26	2.0	27	27	27	27	1.5
	$C_{16}H_{18}N_3O^+$	268.14444		36	32	34	7.9	37	36	35	36	3.2	37	35	33	35	7.3
	$C_{14}H_{10}NO^+$	208.07569	61	57	56	58	4.6	59	58	57	58	2.5	59	60	57	58	2.5
Ergocryptine	$C_{15}H_{15}N_2^+$	223.12298	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{16}H_{18}N_3O^+$	268.14444		54	49	52	7.1	53	53	49	51	5.1	52	51	50	51	2.2
	$C_{14}H_{10}NO^+$	208.07569	67	64	62	64	3.4	66	66	63	65	3.0	66	65	63	65	2.8
Ergometrine	$C_{15}H_{15}N_2^+$	223.12298	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{19}H_{24}N_3O_2^+$	326.18630	58	60	62	60	3.1	57	58	58	58	0.3	58	57	58	58	0.2
	$C_{14}H_{10}NO^+$	208.07569	42	40	39	40	2.9	44	41	42	43	4.3	41	38	41	41	0.6
Ergosine	$C_{15}H_{15}N_2^+$	223.12298	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{14}H_{19}N_2O_3^+$	263.13902	18	19	17	18	3.2	18	18	18	18	0.6	10	10	10	10	0.6
	$C_{14}H_{10}NO^+$	208.07569	13	15	14	14	5.6	14	14	13	13	2.4	62	66	64	63	1.8
Ergotamine	$C_{15}H_{15}N_2^+$	223.12298	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{17}H_{17}N_2O_3^+$	297.12337	22	21	21	21	2.2	21	21	21	21	0.3	21	21	21	21	1.0
	$C_{17}H_{13}N_2O_2^+$	277.09715	14	15	15	15	2.7	15	15	15	15	0.6	15	14	14	14	0.8
	$C_{14}H_{10}NO^+$	208.07569	13	13	12	13	7.0	13	13	13	13	2.5	12	12	12	12	3.7
Fumonisin B_1	$C_{22}H_{40}NO^+$	334.31044	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{22}H_{42}NO_2^+$	352.32101	57	59	63	60	5.4	60	58	59	60	2.0	61	61	63	62	1.5
	$C_{22}H_{38}N^+$	316.29988	24	27	26	26	5.9	24	25	26	25	3.1	26	24	27	27	2.1
($^{13}C_{34}$)-Fumonisin B_1	$^{13}C_{22}H_{40}NO^+$	356.38425	-	-	-	-	-	100	100	100	-	-	-	-	-	-	-
	$^{13}C_{22}H_{42}NO_2^+$	374.39481	-	-	-	-	-	58	56	55	57	3.2	-	-	-	-	-
	$^{13}C_{22}H_{38}N^+$	356.38425	-	-	-	-	-	24	24	26	25	5.2	-	-	-	-	-
Fumonisin B_2	$C_{22}H_{42}NO^+$	336.32609	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-

	$C_{22}H_{44}NO_2^+$	354.33666	15	20	20	18	15.7	22	20	20	21	6.5	21	20	19	20	7.2
	$C_{22}H_{40}N^+$	318.31553	67	64	66	65	2.4	70	66	70	70	0.0	71	69	67	69	4.1
Fusarenon-X	$C_{14}H_{13}O_3^+$	229.08592	-	-	-	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{14}H_{15}O_4^+$	247.09649	-	-	-	-	-	39	47	44	44	9.0	44	47	46	45	3.5
	$C_{13}H_{13}O_2^+$	201.09101	-	-	-	-	-	68	79	68	72	9.1	75	79	75	76	3.3
	$C_{11}H_{11}O_2^+$	175.07536	-	-	-	-	-	116	128	120	121	5.4	120	126	128	125	3.3
	$C_8H_9O_2^+$	137.05971	-	-	-	-	-	128	119	151	132	12.4	133	129	133	132	1.7
HT-2	$C_{14}H_{15}O_4^+$	169.10118	-	-	-	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{15}H_{19}O_4^+$	263.12779	-	-	-	-	-	39	38	16	28	57.9	38	38	29	33	17.8
	$C_{14}H_{15}O_4^+$	215.10666	-	-	-	-	-	53	44	40	47	19.8	48	47	29	39	34.4
	$C_{14}H_{13}O^+$	197.09609	-	-	-	-	-	61	71	71	66	11.1	73	76	64	69	9.7
	$C_{13}H_{13}O^+$	185.09609	-	-	-	-	-	60	52	55	57	5.8	58	54	32	45	39.5
	$C_{12}H_{13}^+$	157.10118	-	-	-	-	-	86	91	116	101	20.6	90	91	118	104	19.0
	$C_{11}H_{13}^+$	145.10118	-	-	-	-	-	82	103	129	105	31.4	87	87	141	114	33.0
Ochratoxin A	$C_{11}H_{10}ClO_5^+$	257.02111	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{19}H_{14}ClO_4^+$	341.05751	5	5	6	5	5.7	6	6	7	7	3.6	8	8	8	8	4.2
	$C_{11}H_8ClO_4^+$	239.01056	22	25	24	24	4.7	44	37	47	46	6.0	83	87	98	91	11.7
	$C_8H_{10}N^+$	120.08078	5	5	5	5	3.2	6	6	6	6	1.1	8	8	8	8	3.7
($^{13}C_{20}$)-Ochratoxin A	$^{13}C_{11}H_{10}ClO_5^+$	268.05803	-	-	-	-	-	100	100	100	-	-	-	-	-	-	-
	$^{13}C_{19}H_{14}ClO_4^+$	360.12084	-	-	-	-	-	6	6	6	6	0.7	-	-	-	-	-
	$^{13}C_{11}H_8ClO_4^+$	250.04747	-	-	-	-	-	31	29	27	29	7.6	-	-	-	-	-
	$^{13}C_8H_{10}N^+$	128.10761	-	-	-	-	-	6	5	6	6	0.8	-	-	-	-	-
Ochratoxin B	$C_{11}H_{11}O_5^+$	223.06010	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{11}H_9O_4^+$	205.04954	37	39	40	38	4.1	109	129	123	116	8.7	189	196	200	195	4.0
	$C_8H_{10}N^+$	120.08078	2	2	2	2	10.7	4	4	4	4	6.0	5	5	5	5	4.2
Sterigmatocystin	$C_{18}H_{13}O_6^+$	325.07066	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{17}H_{10}O_6^+$	310.04719	72	72	71	72	1.0	71	71	75	73	4.2	73	72	73	73	0.4
	$C_{17}H_{13}O_5^+$	297.07575	7	7	5	6	22.5	7	6	7	7	1.5	6	7	7	7	2.4
	$C_{16}H_9O_6^+$	281.04445	9	8	6	8	18.1	8	8	10	9	9.2	9	9	8	9	4.8
T-2	$C_{13}H_{13}O^+$	185.09609	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{14}H_{15}O_2^+$	215.10666	72	79	83	78	7.1	78	77	77	77	0.8	75	75	76	76	0.4
	$C_{14}H_{13}O^+$	197.09609	47	46	48	47	2.1	47	47	48	47	1.4	46	46	48	47	2.6
	$C_{13}H_{13}^+$	169.10118	62	67	71	67	6.7	62	63	61	62	1.2	60	59	62	61	2.0
($^{13}C_{24}$)-T-2	$^{13}C_{13}H_{13}O^+$	198.13970	-	-	-	-	-	100	100	100			-	-	-	-	-
	$^{13}C_{14}H_{15}O_2^+$	229.15384	-	-	-	-	-	72	77	75	74	2.3	-	-	-	-	-
	$^{13}C_{14}H_{13}O^+$	211.14306	-	-	-	-	-	45	50	46	45	2.3	-	-	-	-	-
	$^{13}C_{13}H_{13}^+$	182.14479	-	-	-	-	-	60	63	62	61	1.7	-	-	-	-	-

Verrucarin A	$C_{15}H_{19}O_2^+$	231.13796	100	100	100	-	-	100	100	100	-	-	100	100	100	-	-
	$C_{15}H_{21}O_3^+$	249.14852	45	42	44	43	5.7	48	46	40	45	9.3	44	43	36	41	10.6
	$C_{12}H_{17}O_2^+$	193.12231	55	53	51	54	1.9	59	57	57	58	2.0	57	58	40	52	19.6
	$C_{10}H_{13}^+$	133.10118	49	57	63	53	11.3	64	60	61	62	3.4	60	60	51	57	9.1
	$C_8H_9^+$	105.06988	66	65	71	66	1.9	69	69	68	69	0.8	67	66	77	70	8.7
	$C_5H_9O^+$	85.06479	121	125	129	125	3.3	130	132	126	129	2.4	124	127	120	124	2.8
Zearalenone	$C_{12}H_{11}O_2^+$	187.07536	100	100	100	-	-	100	100	100	-	-	100	100	100		
	$C_{18}H_{19}O_3^+$	283.13287	59	57	61	59	3.1	50	51	49	50	2.1	46	48	49	48	2.6
	$C_{12}H_{11}O_3^+$	203.07027	83	72	78	78	6.6	65	68	64	66	2.7	64	66	66	65	1.3
	$C_{13}H_{11}O_4^+$	231.06546	49	44	51	48	8.1	37	38	47	40	14.7	36	37	37	37	1.4
($^{13}C_{18}$)-Zearalenone	$^{13}C_{12}H_{11}O_2^+$	199.11561	-	-	-	-	-	100	100	100	-	-	-	-	-	-	-
	$^{13}C_{18}H_{19}O_3^+$	301.19326	-	-	-	-	-	44	44	43	43	1.2	-	-	-	-	-
	$^{13}C_{13}H_{11}O_4^+$	215.11053	-	-	-	-	-	64	65	62	63	1.6	-	-	-	-	-
	$^{13}C_{12}H_{11}O_3^+$	244.10880	-	-	-	-	-	33	32	31	32	2.7	-	-	-	-	-