Supporting information

Results and discussion

Optimization of the sample preparation and extraction methodology

Visual comparison of the slopes (curve in standard mixture vs MMC curve with identical concentration range) confirmed the presence of signal suppression due to matrix effects and necessitated further use of MMC curves for all three juice matrices and the different types of tomato products. Upon construction of MMC curves, significantly different slopes (non-parallelism of the curves, confirmed by *t*-test[1]) were observed for the majority of target analytes. This revealed the necessity to use matrix specific MMC curves for quantitation purposes (Figure 1).

Method validation

In Tables 1 and 2, regression coefficients (R^2) and experimental *p*-values from lack-of-fit tests for every analyte in each investigated matrix are summarized in Tables 1-2. Additionally, LOD and LOQ values are represented.

Homoscedasticity was assessed as previously described.[2] Briefly, homoscedasticity is evaluated by applying an *F*-test. If the experimental *F*-value is higher than the tabled *F*-value, this is indicative of an heteroscedastic situation, which can be counteracted through weighted least squares linear regression (WLSLR). The optimal weighting factor, $w_{i,}$ is chosen according to a percentage relative error %RE:

$\%RE=([C_{experimental}-C_{assigned}]/C_{assigned})*100$

The effectiveness of a weighting factor is evaluated by calculating $\sum$%RE (the sum of absolute %RE values). In Table 3, $\sum$%RE and accuracy (in terms of bias, %) at three concentration levels obtained by using unweighted (w_i = 1) and weighted (w_i = $1/x^2$) linear regression for all target analytes in tomato juice and tomato sauce are displayed. The weighting factor $1/x^2$ not only produced the least $\sum$%RE for these data sets, but also considerably improved the accuracy for the majority of analytes, particularly at the lowest concentration level of the calibration curve.

Apparent recovery, RSD_r, RSD_R and *U* values for every analyte in each investigated matrix are displayed in Tables 4-5.

***Alternaria* toxins in commercially available foodstuffs**

This study reports the novel detection of modified *Alternaria* toxins (specifically, sulfates of (**1**) alternariol and (**2**) alternariol monomethyl ether) occurring in tomato products. Particularly in tomato concentrate, alternariol-3-sulfate (**8**) and alternariol monomethyl ether (**10**) were detected in 26% and 78% of all samples, in concentrations up to 8.7 and 9.9 µg/kg, respectively.

A Synapt G2-Si mass spectrometer, operated in high resolution MS^E continuum mode (ESI^-), was used to analyse tomato product samples from the survey in which sulfates of **1** and **2** were reported by low resolution tandem mass spectrometry. Accurate masses of both sulfates with an acceptable mass deviation (< 2 mDa) were detected in low energy as well as high energy mode. Component identification was performed by comparing the retention time under identical chromatographic conditions and by matching the high energy fragmentation spectra of the precursor ion from spiked samples to that of naturally contaminated samples (Figure 2). Chromatographic separation was performed using a Waters Acquity UPLC system (Waters, Milford, MA) equipped with a FTN autosampler. A sample volume of 5 µl was injected into an HSS T3 column (1.8 µm, 2.1 x 100 mm) held at 35

°C with a flow rate of 400 µl/min. A gradient elution program with solvent A (ultra-pure water, 1% acetic acid) and solvent B (acetonitrile, 1% acetic acid) was applied as follows: 95% A and 5% B for 0.5 min followed by an increase to 95% B from 0.5 to 16.0 min, 95% B maintained from 16.0 to 17.0 min, ramping back to 95% A from 17.0 to 17.1 min, and maintaining starting conditions from 17.1 to 20 min. Mass spectrometric detection was performed using a SYNAPT G2-Si (Waters, Milford, MA) equipped with an electrospray ionization source operating in negative mode with a capillary voltage of 2.5 kV and a sampling cone voltage of 30 V. The full-scan data were acquired in MS^E continuum high resolution mode within a 50 to 1200 Da mass range with a 0.1 s survey scan time over a 17.5 min run time. In high energy mode, the trap MS collision energy was ramped from 30.0 to 50.0 eV. Desolvation temperature was 500 °C, source temperature 150 °C, cone gas flow 150 L/h and desolvation gas flow 1000 L/h. During acquisition, accurate masses were generated through correction using an external reference (Lock Spray, a 1 ng/µL solution of leucine encephalin infused at a flow rate of 10 µL/min) via a lock spray interface, generating a reference ion of m/z 554.2615 ($[M-H]^-$) in negative ionization mode.

References

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2. Walravens, J.; Mikula, H.; Asam, S.; Rychlik, M.; Njumbe Ediage, E.; Diana Di Mavungu, J.; Van Landschoot, A.; Vanhaecke, L.; De Saeger, S. Development and validation of an ultra-high-performance liquid chromatography tandem mass spectrometric method for the simultaneous determination of free and conjugated Alternaria toxins in cereal-based foodstuffs. *J. Chromatogr. A* **2014**, *1372*, 91-101.

Figure captions

Figure 1. Non-parallelism (confirmed by *t*-test)[1] of the matrix matched calibration (MMC) curves of both [A] **7** and [B] **4** in tomato juice versus tomato concentrate, [C] **1** in apple juice versus grape juice and [D] **8** in grape juice versus carrot juice. Parallelism[1] of the MMC curves of [E] **2** in tomato juice versus tomato concentrate and [F] **3** in tomato juice versus tomato paste due to the application of the corresponding isotope-labelled internal standards $[^{2}H_{4}]$-**2** and $[^{13}C_{6},{}^{15}N]$-**3**.

Figure 2. Extracted ion chromatogram of **10** (m/z 351.0175) in [A] spiked tomato product sample (MS^{E} high energy mode), [B] spiked tomato product sample (MS^{E} low energy mode), [C] naturally contaminated tomato concentrate sample (MS^{E} high energy mode) and [D] naturally contaminated tomato concentrate sample (MS^{E} low energy mode). Comparison of fragmentation spectra (MS^{E} high energy mode) of **10** (m/z 351.0175) in [E] spiked tomato product sample and [F] naturally contaminated tomato concentrate sample.

Tables

Table 1. R^2 values and *p*-values (lack-of-fit test, SPSS) of the matrix-matched calibration curves (range 5-100 µg/kg) in fruit and vegetable juices (apple, carrot and grape juice), supplemented with limits of detection (LOD) and limits of quantitation (LOQ) for all the analytes (µg/kg).

***Alternaria* toxins** [a]	**Apple juice**				**Carrot juice**				**Grape juice**			
	R^2	*p*	**LOD**	**LOQ**	R^2	*p*	**LOD**	**LOQ**	R^2	*p*	**LOD**	**LOQ**
7	0.992	0.981	0.7	2.2	0.997	0.064	1.5	5.0	0.997	0.387	1.2	4.0
8	0.997	0.749	0.4	1.4	0.999	0.098	1.5	4.8	0.996	0.375	1.4	4.5
5	0.995	0.759	1.1	3.6	0.998	0.914	1.5	5.0	0.997	0.770	1.5	5.0
9	0.994	0.833	1.6	5.2	0.998	0.643	1.7	5.6	0.998	0.545	1.6	5.2
3	0.998	0.718	1.3	4.4	0.997	0.986	1.2	4.1	0.998	0.924	1.5	5.0
6	0.993	0.612	1.5	5.0	0.993	0.410	1.7	5.7	0.996	0.157	1.2	4.0
1	0.992	0.647	1.3	4.3	0.997	0.065	1.4	4.8	0.997	0.088	1.4	4.7
4	0.996	0.925	1.0	3.4	0.998	0.141	1.4	4.6	0.997	0.314	1.5	4.9
10	0.994	0.614	1.5	4.8	0.997	0.075	1.2	4.1	0.989	0.163	1.6	5.4
2	0.998	0.945	0.3	1.1	0.998	0.501	0.7	2.2	0.999	0.299	0.8	2.8

[a] **1**: alternariol - **2**: alternariol monomethyl ether - **3**: tenuazonic acid - **4**: tentoxin - **5**: altenuene - **6**: altertoxin-I - **7**: alternariol-3-glucoside - **8**: alternariol-3-sulfate - **9**: alternariol monomethyl ether-3-glucoside **- 10**: alternariol monomethyl ether-3-sulfate.

Table 2. R^2 values and *p*-values (lack-of-fit test, SPSS) of the matrix-matched calibration curves (range 50-1000 µg/kg) in lyophilised tomato products (juice, sauce and concentrate), supplemented with limits of detection (LOD) and limits of quantitation (LOQ) for all the analytes (µg/kg, expressed on fresh weight of the tomato products applying the experimentally determined conversion factor [CF]).

***Alternaria* toxins** [a]	**Tomato juice (CF=0.052)**				**Tomato sauce (CF=0.077)**				**Tomato concentrate (CF=0.216)**			
	R^2	*p*	**LOD**	**LOQ**	R^2	*p*	**LOD**	**LOQ**	R^2	*p*	**LOD**	**LOQ**
7	0.996	0.871	0.5	1.6	0.995	0.717	1.1	3.6	0.991	0.825	1.3	4.3
8	0.996	0.822	0.7	2.4	0.994	0.335	0.5	1.5	0.992	0.733	1.5	5.0
5	0.995	0.546	0.5	1.6	0.992	0.369	1.1	3.6	0.994	0.174	1.6	5.3
9	0.996	0.957	1.0	3.2	0.996	0.824	0.4	1.4	0.991	0.436	1.0	3.5
3	0.994	0.859	0.3	1.1	0.995	0.588	0.4	1.2	0.994	0.779	1.0	3.3
6	0.994	0.170	0.4	1.4	-	-	0.3	1.1	-	-	1.2	3.8
1	0.996	0.547	0.3	0.8	0.993	0.802	0.4	1.4	0.992	0.907	1.1	3.5
4	0.982	0.258	0.2	0.7	0.988	0.781	0.5	1.8	0.991	0.975	1.5	5.0
10	0.991	0.753	0.3	0.9	0.993	0.185	0.3	1.0	0.992	0.969	1.3	4.3
2	0.993	0.990	0.3	0.9	0.997	0.933	0.2	0.8	0.993	0.867	1.4	4.7

[a] **1**: alternariol - **2**: alternariol monomethyl ether - **3**: tenuazonic acid - **4**: tentoxin - **5**: altenuene - **6**: altertoxin-I - **7**: alternariol-3-glucoside - **8**: alternariol-3-sulfate - **9**: alternariol monomethyl ether-3-glucoside **- 10**: alternariol monomethyl ether-3-sulfate.

[b] Because of depletion of the stock solution of **6**, validation experiments for ATX-I in tomato sauce and concentrate were not performed.

Table 3. Sum of the relative errors (∑%RE) and accuracy (Bias, %) at low (50 µg/kg), medium (250 µg/kg) and high (1000 µg/kg) concentration level obtained by using unweighted (w_i = 1) and weighted ($w_i = 1/x^2$) linear regression for all the target analytes in tomato juice and tomato sauce.

***Alternaria* toxins** [a]	**Tomato juice**					**Tomato sauce**				
	w		**Bias (%)**					**Bias (%)**		
	w_i	**∑%RE**	**low**	**medium**	**high**	w_i	**∑%RE**	**low**	**medium**	**high**
7	**1**	630.5	35.5	8.8	0.6	**1**	603.0	6.6	5.5	2.9
	$1/x^2$	**296.8**	**8.2**	**8.6**	**5.1**	$1/x^2$	**309.0**	**9.1**	**4.6**	**1.3**
8	**1**	405.0	-6.5	4.3	4.7	**1**	428.4	33.6	-1.0	-6.6
	$1/x^2$	**261.2**	**4.6**	**4.5**	**3.0**	$1/x^2$	**277.5**	**-0.8**	**-0.5**	**0.5**
5	**1**	376.5	7.6	4.2	5.8	**1**	522.5	14.2	-4.5	-8.6
	$1/x^2$	**297.5**	**-6.8**	**4.9**	**9.4**	$1/x^2$	**382.4**	**1.7**	**-4.4**	**-6.0**
9	**1**	324.7	-2.5	4.4	6.0	**1**	430.4	8.0	-0.4	-8.1
	$1/x^2$	**271.9**	**-2.2**	**4.5**	**6.2**	$1/x^2$	**296.4**	**2.7**	**-0.5**	**-7.3**
3	**1**	461.7	-12.3	0.9	3.6	**1**	455.8	-15.7	0.3	-0.8
	$1/x^2$	**294.3**	**-3.3**	**1.6**	**2.5**	$1/x^2$	**292.5**	**2.5**	**0.4**	**-3.9**
6 [b]	**1**	604.6	-25.1	6.2	5.0	**1**	-	-	-	-
	$1/x^2$	**300.2**	**-1.8**	**5.8**	**0.4**	$1/x^2$	**-**	**-**	**-**	**-**
1	**1**	450.8	-17.6	8.4	8.4	**1**	454.2	-14.9	-1.1	-7.3
	$1/x^2$	**263.5**	**-1.8**	**8.3**	**5.5**	$1/x^2$	**335.5**	**-1.2**	**-1.3**	**-9.6**
4	**1**	1448.8	-40.6	14.8	32.3	**1**	677.0	-18.6	1.6	-8.3
	$1/x^2$	**497.8**	**-1.4**	**10.6**	**8.0**	$1/x^2$	**392.9**	**-5.0**	**1.3**	**-10.6**
10	**1**	600.7	-14.0	5.0	1.9	**1**	532.7	-16.2	-2.2	-5.1
	$1/x^2$	**351.7**	**0.1**	**3.6**	**-1.6**	$1/x^2$	**301.6**	**3.9**	**-2.7**	**-8.8**
2	**1**	631.1	1.5	5.8	0.7	**1**	317.6	15.2	5.7	0.0
	$1/x^2$	**278.0**	**4.9**	**5.6**	**-0.6**	$1/x^2$	**219.1**	**3.1**	**5.5**	**2.0**

[a] **1**: alternariol - **2**: alternariol monomethyl ether - **3**: tenuazonic acid - **4**: tentoxin - **5**: altenuene - **6**: altertoxin-I - **7**: alternariol-3-glucoside - **8**: alternariol-3-sulfate - **9**: alternariol monomethyl ether-3-glucoside **- 10**: alternariol monomethyl ether-3-sulfate.

[b] Because of depletion of the stock solution of **6**, validation experiments for ATX-I in tomato sauce and concentrate were not performed.

Table 4. Repeatability (RSD_r), intermediate precision (RSD_R), apparent recovery (R_A, %) and expanded measurement uncertainty (*U*, %) values for all the analytes at low, medium and high concentration level (μg/kg) in fruit and vegetable juices (apple, carrot and grape juice).

Type of juice	Concentration (μg/kg)	7 [a]				8 [a]				5 [a]				9 [a]				3 [a]			
		RSD_r [b]	RSD_R [b]	R_A [b]	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*
Apple	**5**	12.5	12.5	96.5	48.4	13.7	13.7	99.5	49.4	7.0	13.8	99.3	49.3	15.7	15.7	91.2	54.3	9.1	9.7	104.5	29.1
	50	4.5	4.5	89.1	42.6	3.3	4.0	99.0	36.3	5.1	5.2	95.7	38.4	5.6	5.6	95.9	38.4	3.3	3.3	100.1	9.1
	100	5.6	5.6	93.3	40.0	3.8	4.8	100.0	37.0	6.4	6.4	95.9	38.9	9.5	9.5	93.3	44.0	0.8	3.6	98.8	9.6
Carrot	**5**	3.2	6.6	108.5	42.4	6.7	12.5	96.5	47.3	5.3	12.6	104.7	48.4	15.5	15.5	96.7	53.3	4.0	7.4	101.4	19.4
	50	1.5	2.9	107.2	38.3	2.1	2.4	101.0	35.3	4.7	9.5	105.0	43.7	7.7	7.7	104.7	41.8	3.8	4.2	104.5	15.1
	100	5.9	5.9	100.3	37.5	2.3	3.1	100.0	35.6	6.8	10.0	100.2	43.5	5.7	5.7	101.6	38.4	4.3	5.7	102.8	16.7
Grape	**5**	13.8	13.8	104.2	49.7	6.7	8.5	94.3	42.7	9.2	9.2	100.9	42.9	8.5	11.8	102.1	47.1	4.4	7.1	96.6	19.5
	50	5.0	5.0	105.4	38.4	1.5	3.8	105.6	37.7	5.7	5.7	108.0	41.2	5.6	5.6	103.0	37.8	4.4	4.4	100.6	11.4
	100	3.5	3.5	103.3	49.7	2.5	2.7	105.4	42.7	4.1	4.4	100.5	42.9	5.3	5.6	97.3	47.1	4.0	4.0	98.0	19.5

Type of juice	Concentration (μg/kg)	6 [a]				1 [a]				4 [a]				10 [a]				2 [a]			
		RSD_r [b]	RSD_R [b]	R_A [b]	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*
Apple	**5**	15.0	15.0	97.3	52.7	12.5	13.6	96.4	37.8	12.8	14.7	98.9	40.2	7.9	7.9	99.7	43.7	11.2	11.2	93.0	31.2
	50	3.9	3.9	104.0	37.0	5.4	5.4	94.5	17.3	3.7	3.7	95.2	13.7	4.6	4.6	95.1	37.9	3.3	3.3	95.6	12.7
	100	1.7	6.0	98.8	37.7	10.1	10.1	94.5	26.7	6.8	6.8	96.0	18.8	2.8	5.0	99.0	37.0	4.2	5.9	95.6	17.8
Carrot	**5**	11.8	11.8	87.0	52.5	6.0	6.1	93.5	21.3	7.2	7.2	95.9	21.7	6.7	6.7	96.0	39.4	9.0	9.0	100.5	23.4
	50	6.6	7.3	104.2	41.2	3.2	3.2	105.9	14.5	3.8	3.8	105.1	15.1	2.6	2.6	100.7	35.4	3.5	4.1	97.9	12.0
	100	5.3	5.3	96.0	38.3	6.2	6.2	97.9	16.0	5.7	5.7	98.9	14.7	1.0	1.5	100.4	34.9	2.5	3.4	98.2	9.8
Grape	**5**	8.5	8.5	103.8	41.5	10.7	10.7	96.6	29.9	10.4	10.8	90.8	34.4	11.0	15.3	98.2	53.1	6.8	6.8	103.1	18.1
	50	5.4	5.4	107.2	40.0	4.6	4.6	109.8	23.0	5.7	5.7	108.4	22.3	0.8	1.2	99.7	34.8	3.7	3.7	100.9	10.3
	100	6.4	6.4	96.6	41.5	6.7	6.7	99.4	29.9	4.3	4.3	101.0	34.4	15.3	15.3	108.1	53.1	1.0	2.9	100.2	18.1

[a] **1**: alternariol - **2**: alternariol monomethyl ether - **3**: tenuazonic acid - **4**: tentoxin - **5**: altenuene - **6**: altertoxin-I - **7**: alternariol-3-glucoside - **8**: alternariol-3-sulfate - **9**: alternariol monomethyl ether-3-glucoside **- 10**: alternariol monomethyl ether-3-sulfate.

[b] **RSD_r** and **RSD_R** acceptance criteria: 20 and 25%, respectively; **R_A** imposed guideline ranges: 80-110%.

Table 5. Repeatability (RSD_r), intermediate precision (RSD_R), apparent recovery (R_A, %) and expanded measurement uncertainty (*U*, %) values for all the analytes at low, medium and high concentration level (µg/kg) in lyophilised tomato products (juice, sauce and concentrate).

Tomato product	Concentration (µg/kg)	7 [a]				8 [a]				5 [a]				9 [a]				3 [a]			
		RSD_r [b]	RSD_R [b]	R_A [b]	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*
Juice	**50**	8.1	8.1	108.2	44.3	4.5	10.3	104.6	44.6	14.6	17.9	93.2	60.0	8.5	13.8	97.8	49.8	15.4	15.4	96.7	43.3
	250	6.7	6.7	108.6	42.3	5.0	5.0	104.5	38.0	4.5	4.5	104.9	38.1	6.4	6.4	104.5	39.4	6.0	6.4	101.6	18.5
	1000	2.3	5.6	105.1	38.9	2.0	3.1	103.0	36.1	2.4	2.4	109.4	40.0	3.4	5.2	106.2	39.4	6.4	6.4	102.5	17.6
Sauce	**50**	8.9	12.4	109.1	52.0	7.8	13.1	99.2	48.4	3.1	11.0	101.7	44.4	6.7	10.5	102.7	44.7	9.3	12.8	102.5	34.8
	250	4.3	6.0	104.6	39.4	5.5	8.5	99.5	41.2	8.9	8.9	95.6	43.2	6.6	6.6	99.5	38.6	5.1	5.5	100.4	15.6
	1000	4.6	6.3	101.3	38.6	6.4	8.1	100.5	40.9	3.4	12.3	94.0	47.1	5.8	6.3	92.7	41.2	7.9	7.9	96.1	22.2
Concentrate	**50**	8.5	8.5	93.6	43.2	3.6	9.9	105.5	44.4	6.5	6.5	96.2	38.9	9.5	11.4	100.5	46.5	7.7	12.5	106.1	35.6
	250	7.5	9.8	101.3	43.7	4.4	10.0	99.1	42.9	1.1	7.5	98.5	39.3	4.8	6.4	100.2	38.7	3.4	7.8	105.0	22.7
	1000	5.2	7.4	99.7	39.8	6.2	6.2	92.7	41.2	4.0	5.8	97.9	38.0	3.5	11.0	93.4	45.6	5.5	7.4	95.6	21.4

Tomato product	Concentration (µg/kg)	6 [a,c]				1 [a]				4 [a]				10 [a]				2 [a]			
		RSD_r [b]	RSD_R [b]	R_A [b]	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*	RSD_r	RSD_R	R_A	*U*
Juice	**50**	8.2	11.2	98.2	45.6	5.8	5.8	98.2	16.7	11.1	11.1	98.6	29.1	9.9	10.1	100.1	44.9	6.6	6.6	104.9	20.5
	250	9.8	9.8	105.8	44.7	8.0	8.0	108.4	26.4	15.6	15.6	110.6	48.6	8.5	8.5	103.6	41.3	2.0	4.6	105.6	16.5
	1000	5.6	5.6	100.4	37.6	3.7	3.7	105.5	14.7	3.4	4.1	108.0	19.8	4.8	4.8	98.4	43.2	5.4	7.6	99.4	20.2
Sauce	**50**	-	-	-	-	5.8	5.8	98.8	25.8	8.5	12.2	95.0	33.2	9.4	9.4	103.9	43.5	5.7	11.0	103.1	29.3
	250	-	-	-	-	8.0	8.0	98.7	23.8	6.4	6.4	101.3	17.0	6.0	6.8	97.27	39.6	5.3	5.3	105.5	17.4
	1000	-	-	-	-	3.7	3.7	90.4	24.9	2.8	10.3	89.4	32.3	9.3	9.3	91.2	46.4	5.4	5.4	102.0	14.3
Concentrate	**50**	-	-	-	-	9.5	10.8	93.7	31.5	10.0	10.0	89.3	33.9	9.1	11.1	98.4	45.9	4.8	9.5	90.7	29.9
	250	-	-	-	-	4.7	10.0	98.9	25.5	5.0	9.9	95.8	26.2	5.1	9.1	96.0	42.3	5.6	5.6	93.8	18.6
	1000	-	-	-	-	6.6	6.6	92.3	23.2	7.2	8.4	91.3	28.3	7.2	8.6	93.5	43.4	3.7	10.1	95.3	26.6

[a] **1**: alternariol - **2**: alternariol monomethyl ether - **3**: tenuazonic acid - **4**: tentoxin - **5**: altenuene - **6**: altertoxin-I - **7**: alternariol-3-glucoside - **8**: alternariol-3-sulfate - **9**: alternariol monomethyl ether-3-glucoside - **10**: alternariol monomethyl ether-3-sulfate.

[b] **RSD_r** and **RSD_R** acceptance criteria: 20 and 25%, respectively; **R_A** imposed guideline ranges: 80-110%.

[c] Because of depletion of the ATX-I stock solution, validation experiments for ATX-I in tomato sauce and concentrate were not performed.

Figure graphics

Figure 1

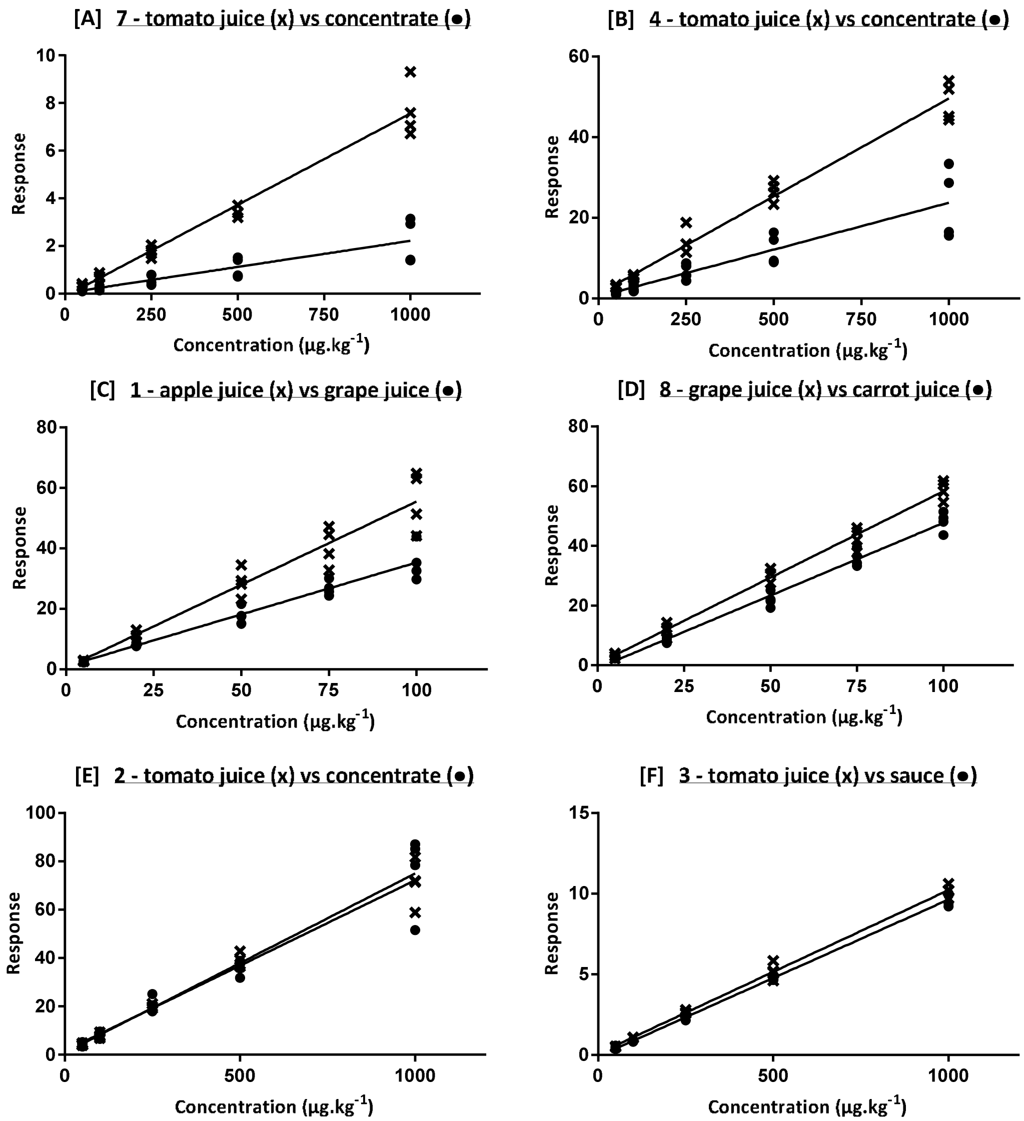
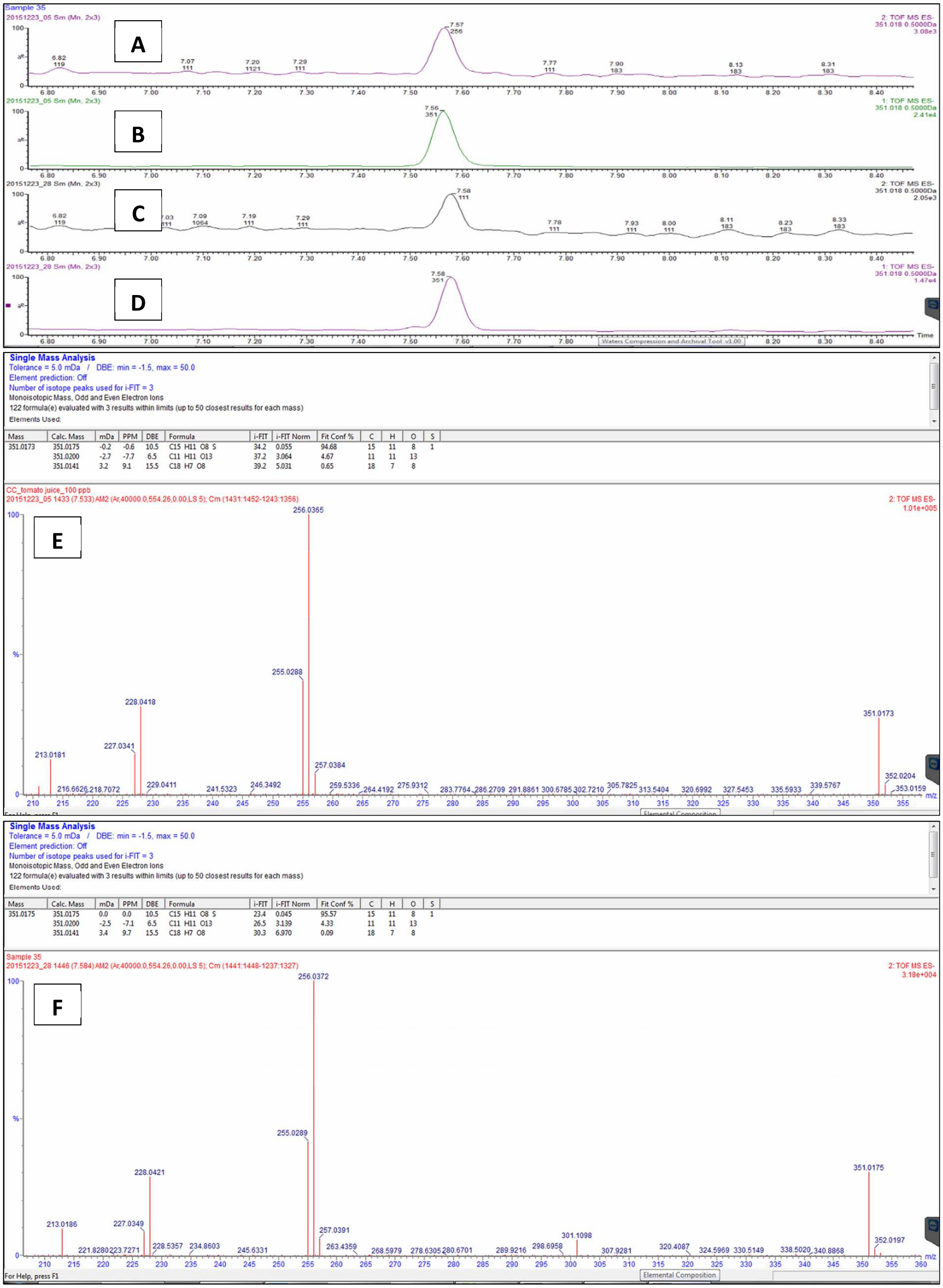


Figure 2



A
B
C
D
E
F
Sample 35
20151223_05 Sm (Mn, 2x3)
2: TOF MS ES- 351.018 0.5000Da 3.08e3
1: TOF MS ES- 351.018 0.5000Da 2.41e4
20151223_28 Sm (Mn, 2x3)
2: TOF MS ES- 351.018 0.5000Da 2.05e3
1: TOF MS ES- 351.018 0.5000Da 1.47e4
Time
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Odd and Even Electron Ions
122 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O | S
351.0173 | 351.0175 | -0.2 | -0.6 | 10.5 | C15 H11 O8 S | 34.2 | 0.055 | 94.68 | 15 | 11 | 8 | 1
351.0200 | -2.7 | -7.7 | 6.5 | C11 H11 O13 | 37.2 | 3.064 | 4.67 | 11 | 11 | 13
351.0141 | 3.2 | 9.1 | 15.5 | C18 H7 O8 | 39.2 | 5.031 | 0.65 | 18 | 7 | 8
CC_tomato juice_100 ppb
20151223_05 1433 (7.533) AM2 (Ar,40000.0,554.26,0.00,LS 5); Cm (1431:1452-1243:1356)
2: TOF MS ES- 1.01e+005
256.0365
255.0288
228.0418
227.0341
213.0181
351.0173
257.0384
352.0204
353.0159
m/z
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Odd and Even Electron Ions
122 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O | S
351.0175 | 351.0175 | 0.0 | 0.0 | 10.5 | C15 H11 O8 S | 23.4 | 0.045 | 95.57 | 15 | 11 | 8 | 1
351.0200 | -2.5 | -7.1 | 6.5 | C11 H11 O13 | 26.5 | 3.139 | 4.33 | 11 | 11 | 13
351.0141 | 3.4 | 9.7 | 15.5 | C18 H7 O8 | 30.3 | 6.970 | 0.09 | 18 | 7 | 8
Sample 35
20151223_28 1446 (7.584) AM2 (Ar,40000.0,554.26,0.00,LS 5); Cm (1441:1448-1237:1327)
2: TOF MS ES- 3.18e+004
256.0372
255.0289
228.0421
227.0349
213.0186
351.0175
257.0391
301.1098
352.0197
Elemental Composition
For Help, press F1