Electronic Supplementary Material (ESI) for Food & Function.

Evaluation of the bitter components of bamboo shoots using a metabolomics approach

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Supplementary information

The MRM parameters of the target compounds

Analyte	Precursor	Product	Fragmentor (V)	CE/V	Retention Time (min)	Retention Window (min)	Polarity
L-Ornithine	133.1	70.0	75	18	0.7	1.0	Positive
Cytidine	244.1	112.0	70	7	1.3	1.2	Positive
Deoxycytidine	228.1	112.0	60	5	1.6	1.4	Positive
Adenine	136.1	119.0	110	23	23	1.2	Positive
Uridine	245.1	113.0	50	3	2.6	1.4	Positive
Thymine	125.0	42.2	70	11	3.3	1.3	Negative
L-Phenylalanine	166.1	120.0	70	10	5.1	1.6	Positive
Guanosine	284.1	152.0	80	7	5.3	1.5	Positive
Deoxyguanosine	268.1	152.0	50	5	5.8	1.2	Positive
Adenosine	268.1	136.0	90	18	6.0	1.2	Positive
Deoxyadenosine	252.1	136.0	70	10	6.2	1.2	Positive
Thymidine	241.1	42.0	120	13	6.4	1.1	Negative
L-Tryptophan	205.1	187.9	70	6	6.9	1.2	Positive
4-Hydroxybenzoic acid	137.0	93.0	70	16	7.8	1.2	Negative

Quantitative parameters of the target compounds

Analyte	LLOD (nmol/L)	LLOQ (nmol/L)	Calibration Curve	R^2
L-Ornithine	0.6	2.4	y = 0.004124x + 0.068207	0.9959
Cytidine	0.6	2.4	y = 0.020108x + 0.054362	0.9996
Deoxycytidine	0.6	1.2	y = 0.012964x + 0.050614	0.9998
Adenine	1.2	4.9	y = 0.005702x + 0.081530	0.9960
Uridine	6.1	12.2	y = 0.001864x + 0.047844	0.9996
Thymine	6.1	12.2	y = 0.000159x + 0.000686	0.9943
^{L}-Phenylalanine	0.2	2.0	y = 0.013478x + 0.258212	0.9997
Guanosine	0.6	1.2	y = 0.015587x + 0.083880	0.9997
Deoxyguanosine	0.6	1.2	y = 0.014647x + 0.040103	0.9993
Adenosine	0.6	1.2	y = 0.015622x + 0.055392	0.9982
Deoxyadenosine	0.1	0.5	y = 0.036048x + 0.036428	0.9992
Thymidine	6.1	12.2	y = 0.000108x + 0.002637	0.9998
^{L}-Tryptophan	1.2	4.9	y = 0.011205x + 0.068946	0.9992
4-Hydroxybenzoic acid	3.1	12.2	y = 0.001146x + 0.064647	0.9987

The recovery and standard deviation of the target compounds in the QC sample (n = 5)

Analyte	Concentration	Recovery	RSD
L-Ornithine	312.5 nmol/L	108.8%	2.9%
Cytidine	312.5 nmol/L	104.4%	2.2%
Deoxycytidine	312.5 nmol/L	114.8%	2.6%
Adenine	312.5 nmol/L	107.0%	4.1%
Uridine	1562.5 nmol/L	111.5%	3.1%
Thymine	1562.5 nmol/L	111.1%	3.2%
L-Phenylalanine	62.5 nmol/L	94.9%	6.4%
Guanosine	312.5 nmol/L	103.9%	1.8%
Deoxyguanosine	312.5 nmol/L	104.3%	1.8%
Adenosine	312.5 nmol/L	104.3%	1.7%
Deoxyadenosine	62.5 nmol/L	102.3%	1.8%
Thymidine	1562.5 nmol/L	104.2%	2.8%
L-Tryptophan	312.5 nmol/L	105.2%	1.9%
4-Hydroxybenzoic acid	1562.5 nmol/L	100.2%	2.1%

The quantification results

Sample	Final Conc. (nmol/g)																	
Name	*L*-Ornithine	Cytidine	Deoxycytidine	Adenine	Tranexamic acid	Uridine	Thymine	*L*-Phenylalanine	4-Hydroxyphenylacetic acid	Guanosine	Deoxyguanosine	Adenosine	Deoxyadenosine	Thymidine	*L*-Tryptophan	4-Hydroxybenzoic acid	Isovanillic acid	Isovitexin
KZ-1	1787.908	11.233	0.129	306.047	N.D.	647.313	Detected	2403.346	N.D.	76.264	0.280	0.118	0.026	0.740	862.197	0.443	N.D.	Detected
KZ-2	2755.575	13.724	0.736	313.607	Detected	830.057	0.154	4521.616	N.D.	92.831	0.295	0.046	0.010	2.099	526.935	1.611	N.D.	Detected
KZ-3	1568.576	9.252	0.103	270.468	Detected	678.449	N.D.	2136.360	N.D.	68.246	0.172	0.034	0.008	1.354	670.186	0.474	N.D.	Detected
KZ-4	1957.983	8.963	0.195	288.548	Detected	818.784	N.D.	3487.149	N.D.	83.172	0.262	0.037	Detected	2.283	551.329	0.470	N.D.	Detected
KZ-5	1781.587	10.154	0.248	331.025	N.D.	791.834	N.D.	3522.962	N.D.	83.748	0.247	Detected	0.005	1.773	683.306	0.545	N.D.	Detected
KZ-6	2334.533	11.148	0.502	306.143	N.D.	740.065	N.D.	3494.816	N.D.	76.615	0.356	0.045	Detected	3.157	458.854	3.516	N.D.	Detected
MMZ-1	1140.120	2.008	0.029	190.763	Detected	42.543	N.D.	982.741	0.887	13.513	0.152	11.859	0.127	0.258	265.343	1.792	N.D.	Detected
MMZ-2	113.817	1.588	0.067	20.030	Detected	30.024	N.D.	98.886	1.325	9.169	0.252	25.115	0.262	0.152	157.591	1.936	N.D.	Detected
MMZ-3	2053.327	4.735	0.084	82.946	Detected	91.551	N.D.	2168.620	2.812	24.056	0.152	77.749	0.168	0.184	1322.998	3.339	N.D.	Detected
MMZ-4	472.959	1.757	0.078	12.556	N.D.	21.268	N.D.	266.256	2.212	8.232	0.229	25.895	0.210	0.185	223.313	1.298	N.D.	Detected
MMZ-5	2454.083	12.171	0.166	279.620	Detected	194.093	Detected	2453.469	3.054	105.297	1.709	45.139	1.473	0.810	1155.972	3.406	N.D.	Detected
MMZ-6	208.908	5.156	0.066	70.081	Detected	82.680	N.D.	324.437	0.307	21.742	0.267	1.264	0.069	0.198	196.882	1.634	N.D.	Detected
MZ-1	298.974	1.955	0.014	8.150	N.D.	30.467	N.D.	503.531	8.942	9.449	0.050	34.500	0.051	Detected	102.942	37.901	N.D.	Detected
MZ-2	607.207	2.307	Detected	8.625	Detected	29.346	N.D.	901.291	7.536	11.049	0.018	33.074	0.035	Detected	182.709	17.512	N.D.	Detected
MZ-3	577.700	2.485	Detected	7.993	Detected	36.099	N.D.	828.964	7.963	9.160	0.026	44.715	0.056	Detected	205.832	25.236	N.D.	Detected
MZ-4	426.177	4.027	0.050	16.733	N.D.	56.209	N.D.	610.742	6.832	13.472	0.083	50.992	0.081	Detected	161.890	40.808	N.D.	Detected
MZ-5	283.481	1.920	Detected	15.765	Detected	31.594	N.D.	454.213	8.557	12.203	0.052	16.435	0.055	Detected	107.575	48.557	N.D.	Detected

MZ-6	282.981	2.235	Detected	8.798	Detected	38.343	N.D.	458.776	9.538	12.712	0.043	39.908	0.064	Detected	89.262	53.130	N.D.	Detected
TLZ-1	1108.342	9.248	Detected	62.249	Detected	106.196	N.D.	694.917	N.D.	17.661	0.043	9.600	0.120	0.355	173.603	12.387	N.D.	Detected
TLZ-2	1451.942	17.688	0.047	113.705	N.D.	176.846	N.D.	1010.683	N.D.	32.651	0.119	13.586	0.311	0.749	220.294	24.349	N.D.	Detected
TLZ-3	1267.972	13.682	0.031	52.177	Detected	130.507	N.D.	672.546	N.D.	26.518	0.096	59.315	0.295	0.560	127.128	13.350	N.D.	Detected
TLZ-4	1573.181	13.075	0.014	67.037	0.112	160.618	N.D.	715.923	N.D.	24.093	0.056	29.622	0.248	0.455	136.467	14.559	N.D.	Detected
TLZ-5	1862.999	25.115	0.075	158.805	Detected	409.371	N.D.	990.296	N.D.	37.628	0.276	4.346	0.282	1.514	208.556	8.685	N.D.	Detected
TLZ-6	588.953	7.635	0.034	37.095	Detected	122.164	N.D.	176.846	N.D.	21.205	0.130	63.041	0.152	0.290	38.303	8.192	N.D.	Detected

Note: KZ = Bamboo shoots of *Pleioblastus amarus*; MMZ = Bamboo shoots of *Bambusa rutila*; MZ = Bamboo shoots of *Dendrocalamus latiflorus*; TLZ = Bamboo shoots of *Dendrocalamus brandisii.*

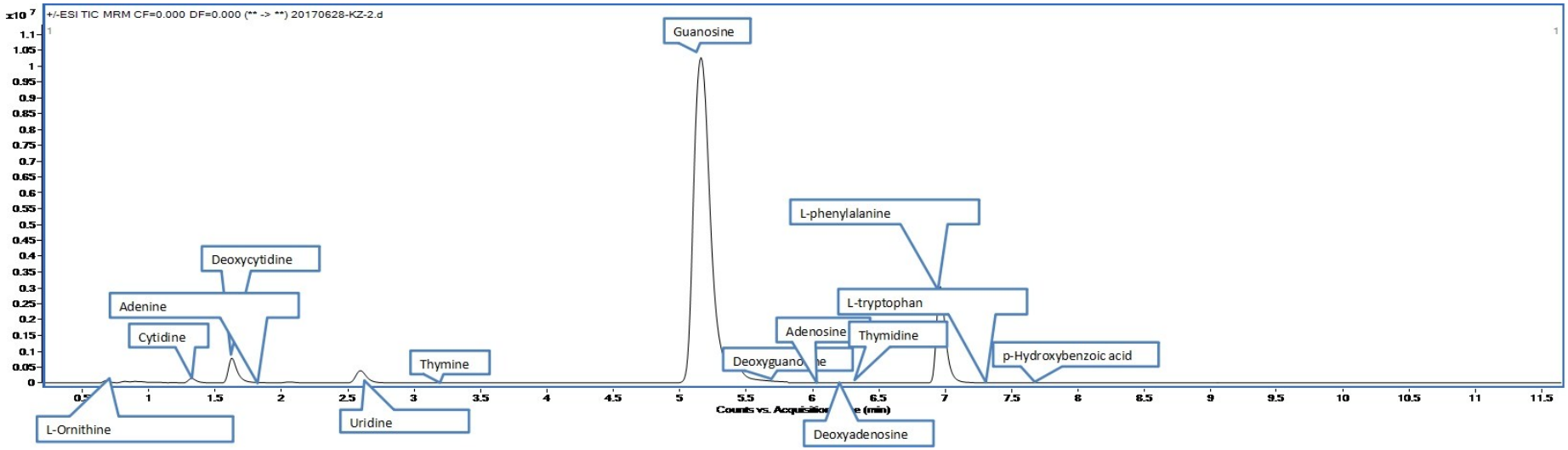
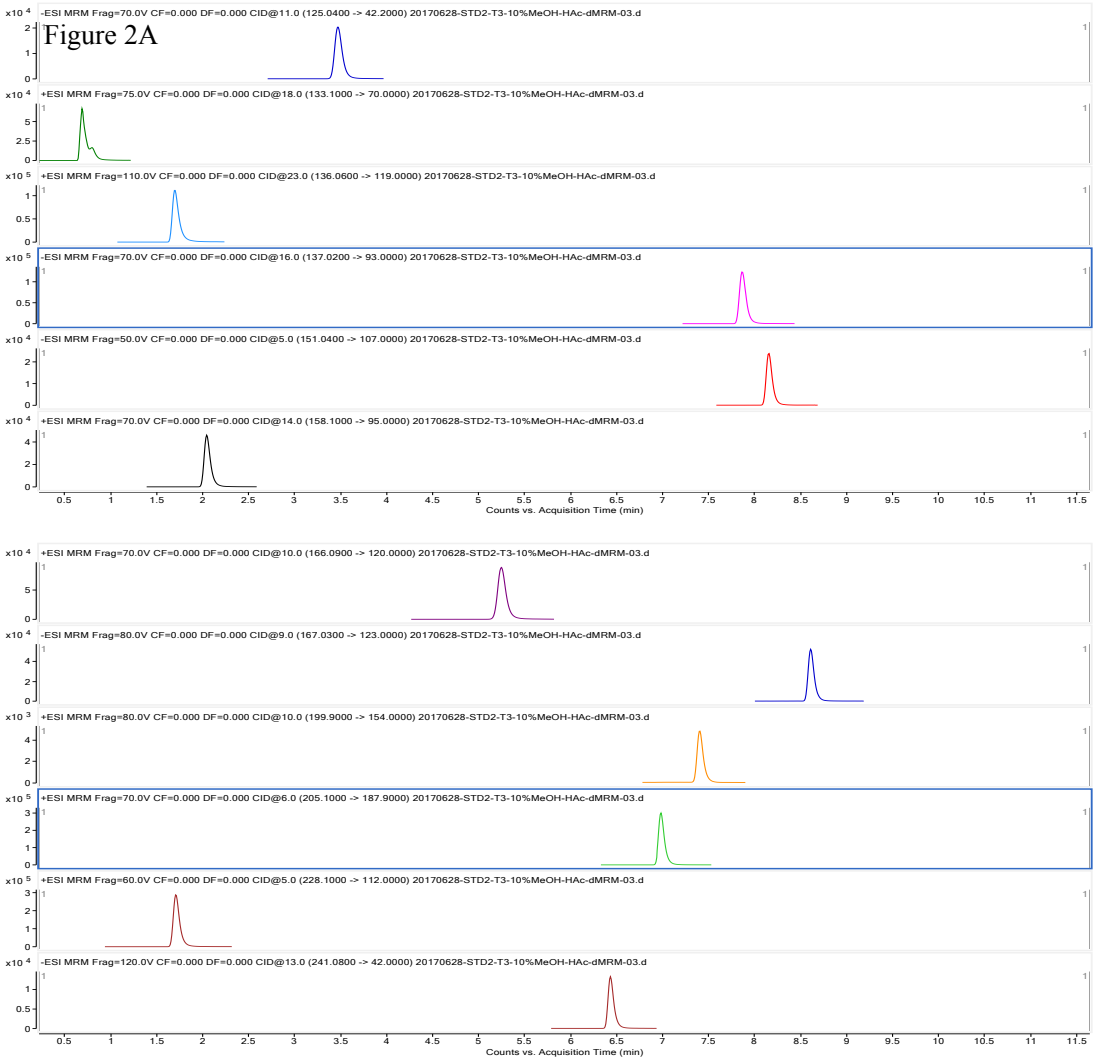


Figure 1: The LC-MS spectrum of bamboo shoots (*Pleioblastus amarus*)

Figure 2A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+ESI MRM Frag=70.0V CF=0.000 DF=0.000 CID@14.0 (158.1000 -> 95.0000) 20170628-STD2-T3-10%MeOH-HAc-dMRM-03.d
Counts vs. Acquisition Time (min)

+ESI MRM Frag=70.0V CF=0.000 DF=0.000 CID@10.0 (166.0900 -> 120.0000) 20170628-STD2-T3-10%MeOH-HAc-dMRM-03.d
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+ESI MRM Frag=80.0V CF=0.000 DF=0.000 CID@10.0 (199.9000 -> 154.0000) 20170628-STD2-T3-10%MeOH-HAc-dMRM-03.d
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+ESI MRM Frag=60.0V CF=0.000 DF=0.000 CID@5.0 (228.1000 -> 112.0000) 20170628-STD2-T3-10%MeOH-HAc-dMRM-03.d
-ESI MRM Frag=120.0V CF=0.000 DF=0.000 CID@13.0 (241.0800 -> 42.0000) 20170628-STD2-T3-10%MeOH-HAc-dMRM-03.d
Counts vs. Acquisition Time (min)

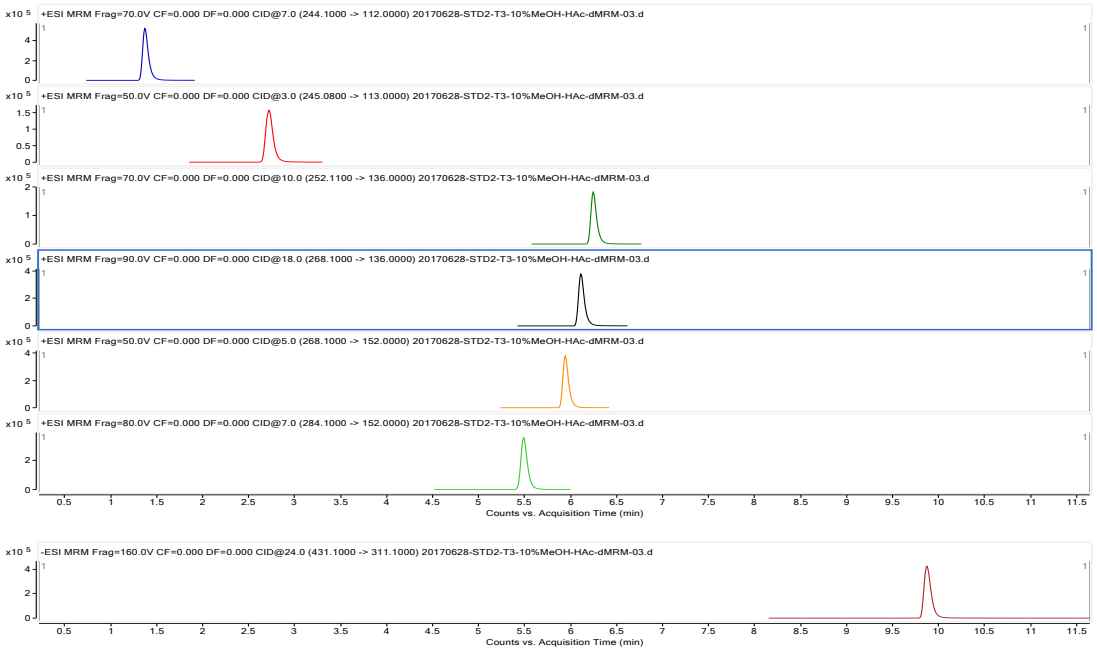
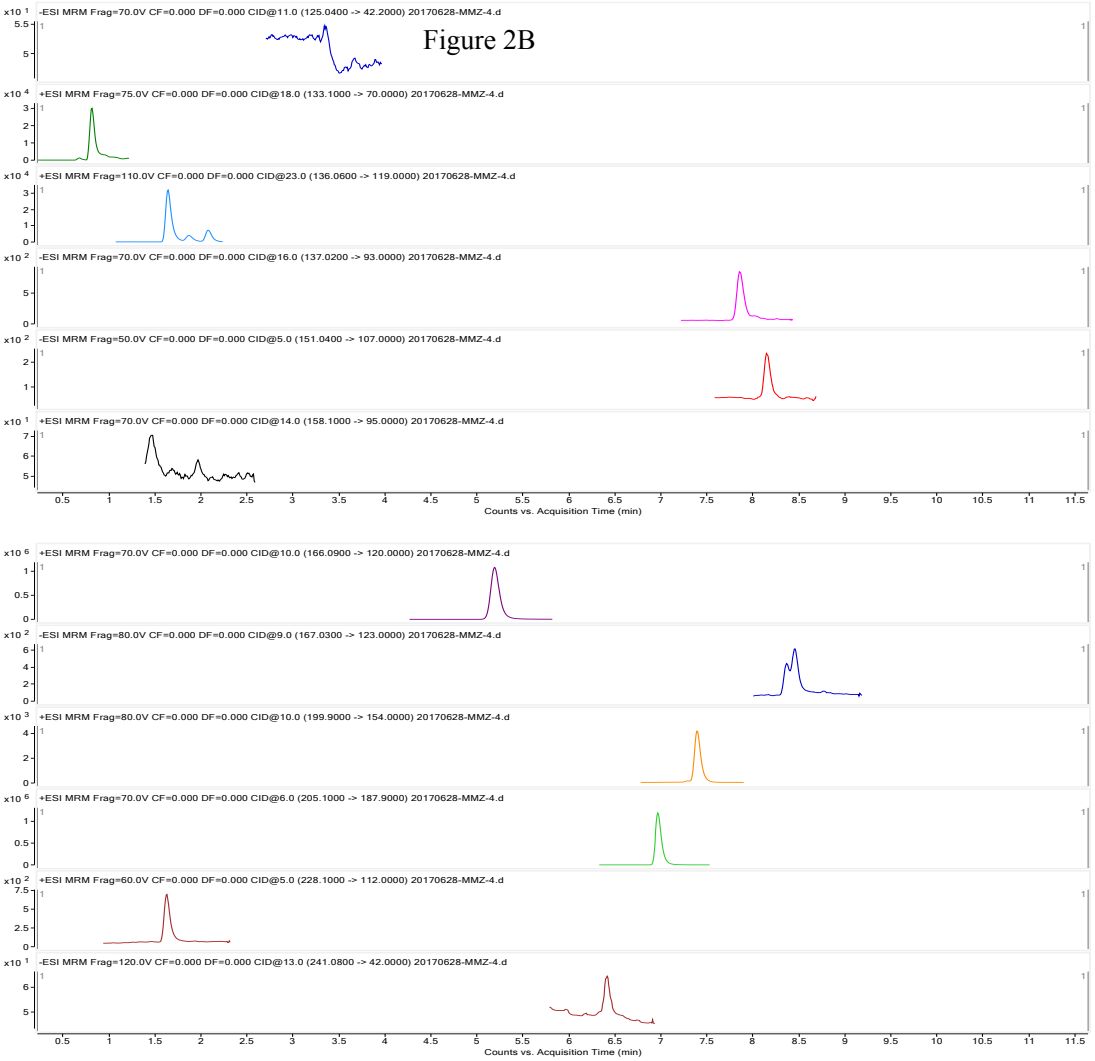


Figure 2A: The extracted ion chromatographs (EICs) from a standard solution

Figure 2B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-ESI MRM Frag=70.0V CF=0.000 DF=0.000 CID@16.0 (137.0200 -> 93.0000) 20170628-MMZ-4.d
-ESI MRM Frag=50.0V CF=0.000 DF=0.000 CID@5.0 (151.0400 -> 107.0000) 20170628-MMZ-4.d
+ESI MRM Frag=70.0V CF=0.000 DF=0.000 CID@14.0 (158.1000 -> 95.0000) 20170628-MMZ-4.d
Counts vs. Acquisition Time (min)
+ESI MRM Frag=70.0V CF=0.000 DF=0.000 CID@10.0 (166.0900 -> 120.0000) 20170628-MMZ-4.d
-ESI MRM Frag=80.0V CF=0.000 DF=0.000 CID@9.0 (167.0300 -> 123.0000) 20170628-MMZ-4.d
+ESI MRM Frag=80.0V CF=0.000 DF=0.000 CID@10.0 (199.9000 -> 154.0000) 20170628-MMZ-4.d
+ESI MRM Frag=70.0V CF=0.000 DF=0.000 CID@6.0 (205.1000 -> 187.9000) 20170628-MMZ-4.d
+ESI MRM Frag=60.0V CF=0.000 DF=0.000 CID@5.0 (228.1000 -> 112.0000) 20170628-MMZ-4.d
-ESI MRM Frag=120.0V CF=0.000 DF=0.000 CID@13.0 (241.0800 -> 42.0000) 20170628-MMZ-4.d
Counts vs. Acquisition Time (min)

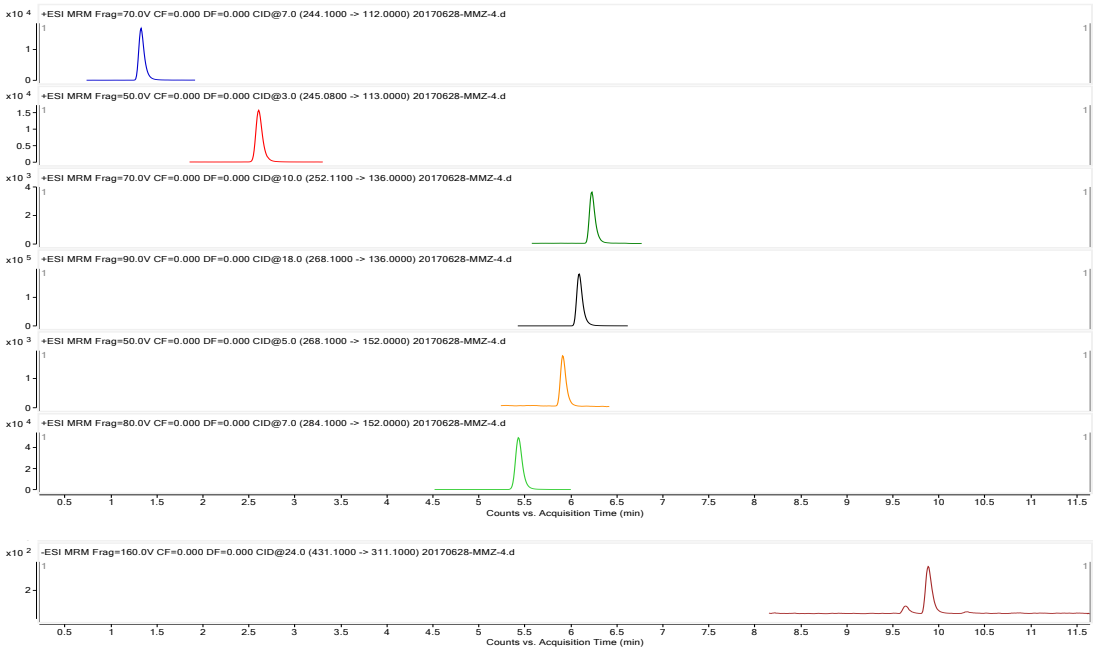

Figure2B: The extracted ion chromatographs (EICs) from a spiked sample