

# 1 **Supporting Information**

## 2 **A chemometric strategy for accurately identifying illegal additive** 3 **compounds in health food by using ultra-high-performance liquid** 4 **chromatography coupled to high resolution mass spectrometry**

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21 **Table S1.** Parameter optimization of AntDAS2, XCMS, MZmine2 and MS-DIAL

Method	Parameter optimization
MZmine2	<p><b>Feature detection:</b> Polarity: Positive, Spectrum type: Centroided, Mass list name: masses</p> <p><b>ADAP chromatogram builder:</b> Group intensity threshold = 1.0E2, Min highest intensity = 1.0E2, m.z tolerance = 0.01 m/z or 10.0 ppm, Suffix = Chromatograms-adap</p> <p><b>Deconvolution:</b> Algorithm: Wavelets, m/z center calculation: MEDIAN</p> <p><b>Remove of isotopes:</b> m/z tolerance:0.01 m/z or 10.0 ppm, Retention time tolerance:0.05 min</p> <p><b>Time correction:</b> m/z tolerance:0.01 m/z or 20.0 ppm, Retention time tolerance: 1.0 min, Minimum standard intensity: 1.0E2</p> <p><b>Peak alignment :</b> RANSAC aligner, m/z tolerance=0.01 Da or 20.0 ppm, RT tolerance after correction=0.1 absolute (min), Minimum number of points=20.0%</p> <p><b>Peak filling :</b> m/z tolerance: 0.001, m/z or 5.0 ppm</p> <p><b>Normalized :</b> m/z tolerance: 0.01 m/z or 20.0 ppm, Retention time tolerance: 1.0 min, Minimum standard intensity: 1.0E02</p>
XCMS	default
MS-DIAL	<p><b>Feature detection:</b> MS1 tolerance = 0.01 Da, Mass slice width = 0.1 Da, Retention time tolerance = 0.5 min, Mass slice width: 0.1 Da</p> <p><b>Feature detection:</b> default</p> <p><b>Adduct:</b> MS1 tolerance = 0.01 Da, Retention time tolerance = 0.5 min, Adducts=[M+H]<sup>+</sup>, [M+NH<sub>4</sub>]<sup>+</sup>, [M+Na]<sup>+</sup>, [M+CH<sub>3</sub>OH+H]<sup>+</sup>, [M+K]<sup>+</sup>, [M+ACN+H]<sup>+</sup>, [M+H-H<sub>2</sub>O]<sup>+</sup>, [M+H-2H<sub>2</sub>O]<sup>+</sup>, [M+2Na-H]<sup>+</sup>, [M+ACN+Na]<sup>+</sup>, [M+2K-H]<sup>+</sup>, [M+2ACN+H]<sup>+</sup></p>
AntDAS2	default

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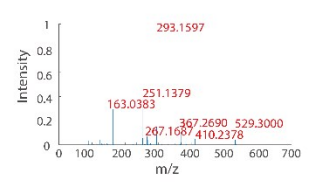
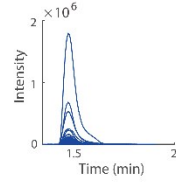
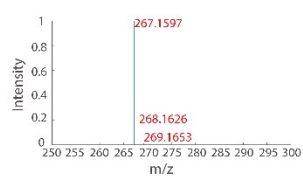
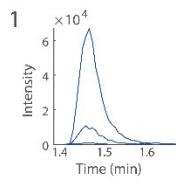
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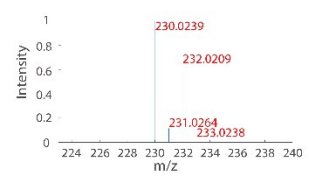
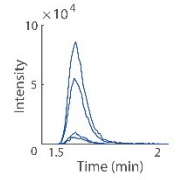
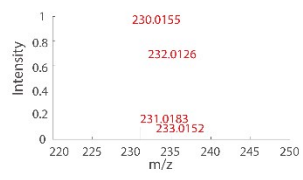
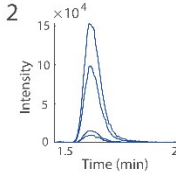
25 **Table S2.** The finally screened 70 features from the developed strategy

RT (min)	m/z	RT (min)	m/z	RT (min)	m/z
1.053	247.1864	7.497	239.0807	10.443	303.1945
1.450	127.1223	7.497	254.1039	10.448	405.2619
1.462	384.2471	7.494	271.1068	10.445	450.3200
1.472	267.1685	7.491	315.0968	10.705	482.3451
1.666	230.0241	7.494	345.1066	10.705	317.2097
1.665	234.0180	7.491	347.1228	10.967	207.0904
2.053	206.1394	7.494	378.1651	10.959	441.1654
2.902	268.1903	7.491	385.0783	10.963	455.1806
3.182	384.1656	7.491	392.1806	10.958	469.1968
3.340	358.1215	7.612	268.0965	10.959	567.2317
5.882	609.2771	7.613	284.0910	10.965	611.2592
5.906	211.0746	7.890	110.0958	11.144	199.1475
5.908	305.1750	7.889	125.1066	11.136	303.1943
5.909	515.2427	7.888	153.1017	11.137	464.3361
6.243	607.2620	7.886	324.1370	11.425	473.2849
6.759	321.1003	7.893	362.0921	11.424	496.3609
6.763	347.0795	9.735	510.3397	11.439	464.3355
6.759	446.1839	9.766	382.0597	11.454	510.3400
6.944	91.0541	9.791	338.0335	11.548	455.2379
6.947	172.0421	9.788	352.0490	11.546	478.3141
6.945	271.1105	9.791	429.1320	12.098	524.3558
7.305	230.1896	9.838	528.2133	12.195	492.3296
7.305	453.2740	9.842	573.2708		
7.491	195.0911	10.447	199.1474		

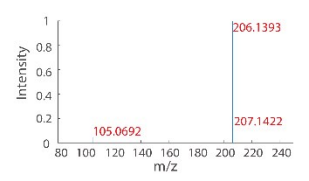
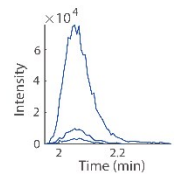
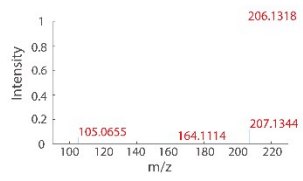
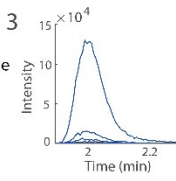
Compound Name:  
Atenolol



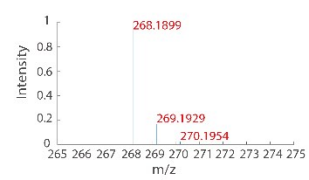
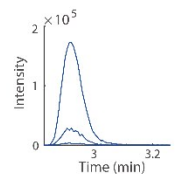
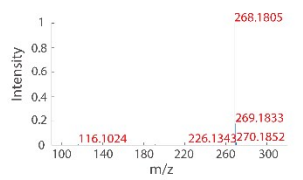
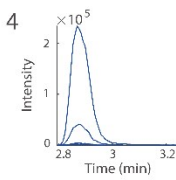
Compound Name:  
Clonidine hydrochloride



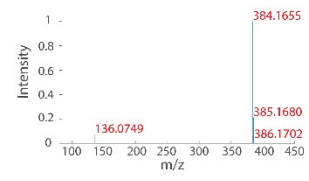
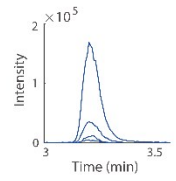
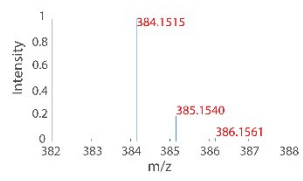
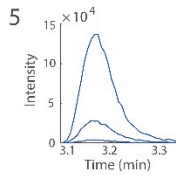
Compound Name:  
Phenformin hydrochloride



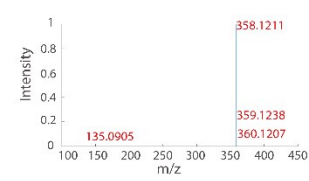
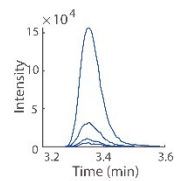
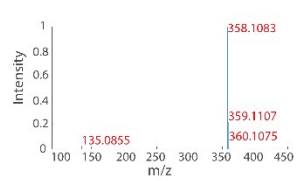
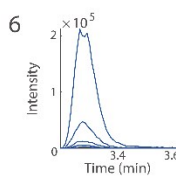
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Metoprolol-tartrate salt



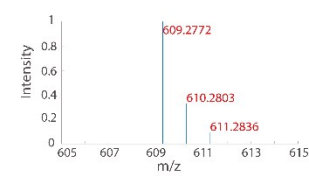
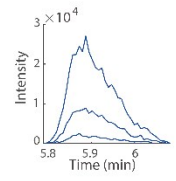
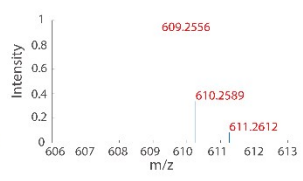
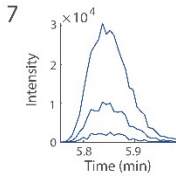
Compound Name:  
Prazosin hydrochloride



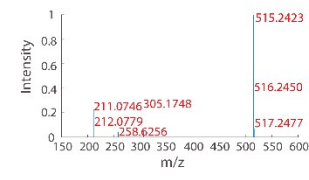
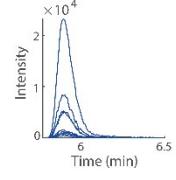
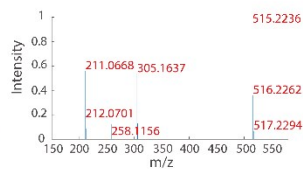
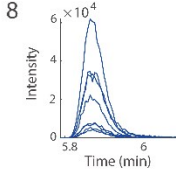
Compound Name:  
Rosiglitazone maleate



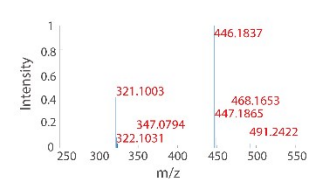
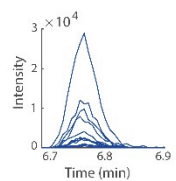
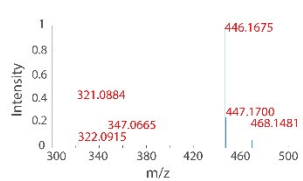
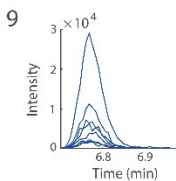
Compound Name:  
Reserpine



Compound Name:  
Telmisartan

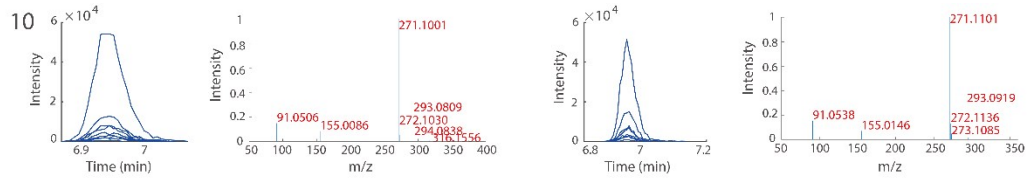


Compound Name:  
Glipizide

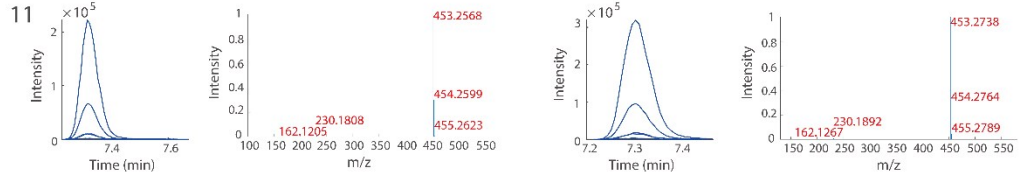


28 **Figure S1.** EICs and mass spectra of 18 standards in mixture (left two columns) and *Goujiya*  
29 Tea matrix.  
30

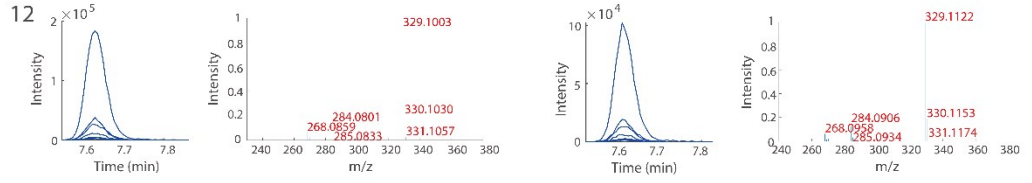
Compound Name:  
Tolbutamide



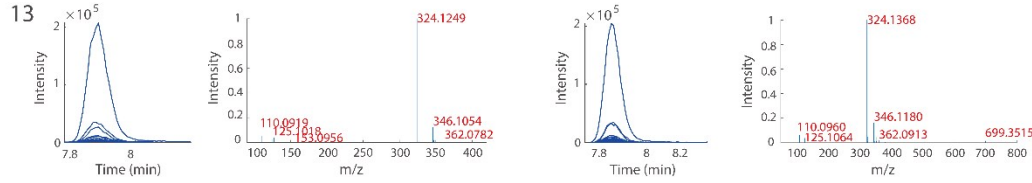
Compound Name:  
Repaglinide



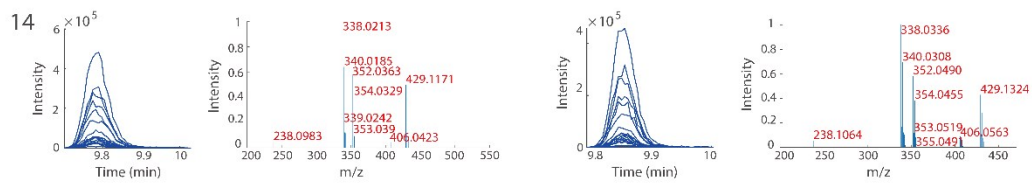
Compound Name:  
Nifedipine



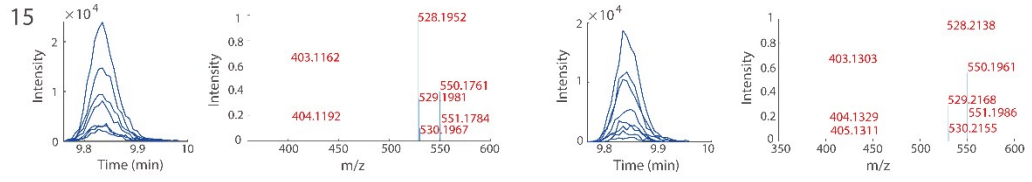
Compound Name:  
Gliclazide



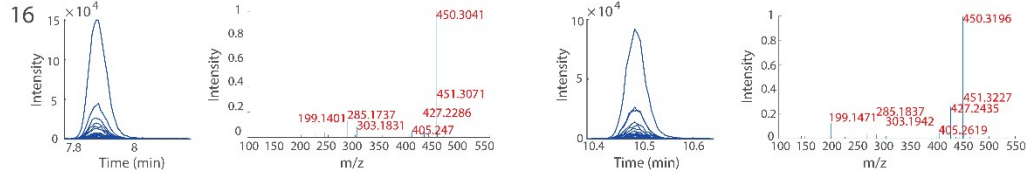
Compound Name:  
Felodipine



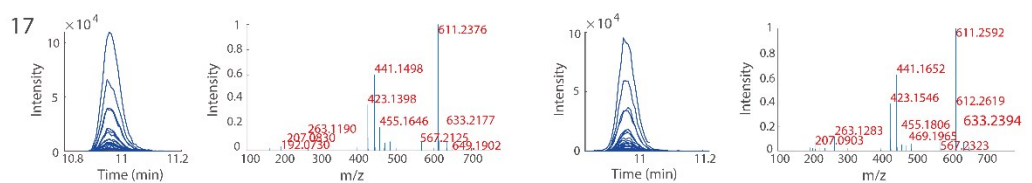
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Gliquidone



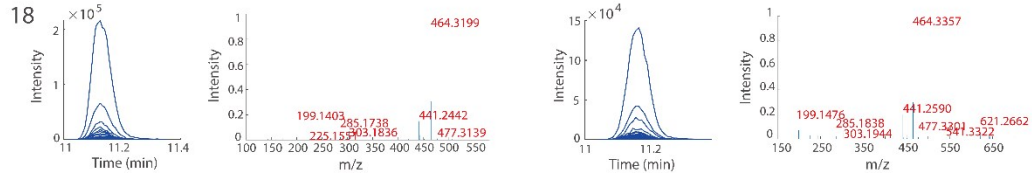
Compound Name:  
Lovastatin



Compound Name:  
Candesartan Cilexetil

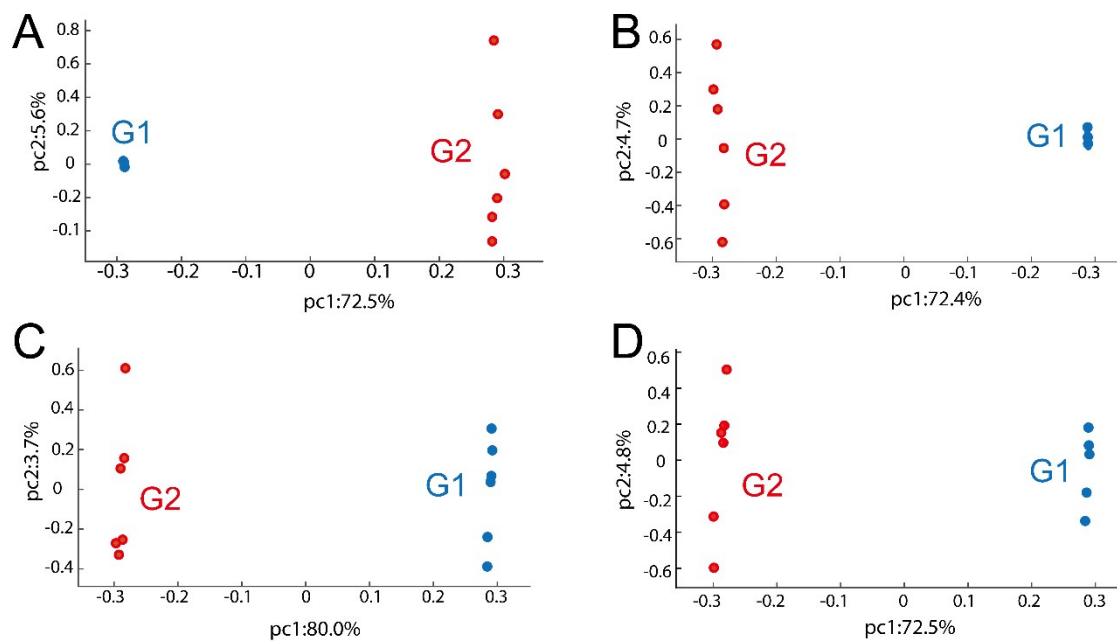


Compound Name:  
Simvastatin



31

32 Figure S1 continued.



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34 **Figure S2.** PCA analysis results based on screened features. (A) Mzmine2, (B) XCMS, (C)  
 35 MS-DIAL, and (D) AntDAS2. ‘G1’ and ‘G2’ represent the reference and illegal additive  
 36 groups, respectively.

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