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Screening for Plant Toxins in Honey and Herbal Beverage by Ultrahigh-Performance Liquid Chromatography-Ion Mobility-Quadrupole Time of Flight Mass Spectrometry

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Abstract

The standards of plant toxins were separated by a C18 column with gradient elution with 0.1% formic acid/water (V/V) and 0.1% formic acid/acetonitrile (V/V) as mobile phase and acquired by ion mobility-quadrupole time of flight mass spectrometry (IM-QTOF MS) in positive ion mode. A database of 308 plant toxins including retention time, collision cross-section (CCS) and its fragment ions was established. Honey dissolved in water or herbal beverage was extracted by acetonitrile and purified with PSA sorbent, and then acquired by ultrahigh-performance liquid chromatography IM-QTOFMS. The acquired data were processed by comparing with the database we established to confirm the target compounds. The average recoveries for samples at two levels ranged from 60.6% - 120.1%, with relative standard deviation (n = 6) less than 25%. The limit of quantitation for plant toxins ranged from 1 - 20 μg/kg. The developed screening method was used in determination of honey, herbal beverage and honey flavored tea beverage samples. The results showed that berberine was detected in one honey with 1 μg/kg and caffeine was present in some beverages with the concentration from 200 and 5500 μg/kg. This method could meet the requirement for rapid screening of plant toxins in honey and herbal beverage. It can be used for the quality control of honey and herbal beverage in enterprises or quality inspection departments. It also can be used in the rapid screening of food poisoning.

Keywords

Screening, Plant Toxins, Honey, Herbal Beverage, Ultrahigh-Performance Liquid Chromatography ion Mobility-Quadrupole time of Flight Mass

Spectrometry

1. Introduction

Honey and herbal beverage are the favorite functional foods due to natural to meet consumer wish for green, containing "organic and bioactive" components [1] [2]. The consumption of honey was 0.24 kg/person in 2018, and herbal beverage accounts for 13% of beverage consumption in China. For honey and beverage safety risk, one of the key topics related to public health issues, can originate from various factors, such as chemicals used in the production, or contaminants in raw materials [3]. The European Food Safety Authority (EFSA) reported that a tremendously high number of herbal products such as herbal teas, contain significant amounts of toxic alkaloids, such as nicotine, pyrrolizidine, or tropane alkaloids [4] [5].

Plant toxins exist in natural plant and are widely found in roots and fruits of plants. Some poisonous plant flowers are collected by bees and lead to phytotoxins in honey. Poisoning occurred due to eating honey containing Tripterygium wilfordii phytotoxins [6]. There was also report of poisoning due to eating honey contaminated with tutin, a plant-derived neurotoxin [7]. Some poisonous plants are easy to be confused with wild vegetables or Chinese herbal medicine, which makes human beings intake this kind of wild plant accidentally and causes undesirable poisoning. For example, *Datura stramonium Linn,* also known as *Datura metel L*, is easily misused as agricultural weed for animals, transferring it into milk and causing tropane alkaloids poisoning [8]. Literatures [9] [10] had shown that tea, honey and traditional medicine contain pyrrolizidine alkaloids (PAs) which are highly toxic to animal, human and infants [11].

Most plant toxins displayed neurotoxicity [12] and developmental toxicity [13] which can cause minor liver damage [9] to the consumers, including chills, sweating, sleepy and other symptoms. Their high toxicity poses a serious health risk for the consumers. Now most of the countries in the world have limit standard for contaminants or pesticide residues in honey and beverages, but there is still no limit standard for detecting plant toxins. Fortunately, the safety of honey and beverages has attracted public attention in recent years.

At present, many methods [9] [14]-[22] were used for the detection of plant toxins. Dawidowicz [14] described a method detecting thujone in alcoholic beverages using gas chromatography combined with solid phase microextraction. Bodi [15] developed liquid chromatography tandem mass spectrometry (LC-MS/MS) with C18 or SCX SPE clean-up detecting PAs in 274 tea and 87 honey samples, suggesting that PA in tea samples are most likely a contamination caused by co-harvesting of PA-producing plants. Hövelmann [21] identified N-caprylhistamine-β-glucoside from tomato and screened for imidazole alkaloids using LC-MS/MS. Lee [20] analyzed of six toxic alkaloids including methyllycaconi-

tine, deltaline, lupanine, anagyrine 5, 6-dehydrolupanine and zygaxine from goats and cows by LC high-resolution MS (LC-HR-MS). In recent years, time-of-flight MS (TOF MS), ion-orbit MS and other HR MS have been applied in the field of hazard chemicals analysis with their high quality accuracy, high throughput and high scanning speed [19] [23]. In this study, UPLC-ion mobility-QTOF MS was used to establish for plant toxins database and an extraction and purification method for plant toxins in honey and beverage was optimization. The established method and database were used for screening the real samples.

2. Materials and Methods

2.1. Chemicals and Reagents

The plant toxin standards were from Enzo life science, Dr. Ehrenstorfer GmbH (Augsburg, Germany) and Sigma-Aldrich (St. Louis, MO, USA). The stock solutions were prepared by acetonitrile (ACN) with the concentration of 1000 μg/mL and stored at −20˚C. The 1 μg/mL working standard solutions were diluted by ACN/H_2O (1/9, v/v). Honey and herbal beverage are commercially available. HPLC-MS-grade methanol, ACN and H_2O were purchased from J. T. Baker (Deventer, The Netherlands) and Honeywell (Augsburg, Germany). Leucine enkephalin (LE) and formic acid (purity > 99%) were from Sigma-Aldrich (St. Louis, MO, USA). Sodium chloride (NaCl) and magnesium sulfate ($MgSO_4$) of analytical purity were got from the Beijing Chemical Reagent Company (Beijing, China). The Discovery ®DSC-18, primary-secondary amine (PSA), graphitized carbon black (GCB), EMR, Zsep, Zsep+, and Zsep/C18 sorbent were from Supelco (Bellefonte, PA, USA). PSA 50 mg/$MgSO_4$ 150 mg was from Dikma. Solid phase extraction (SPE) prime HLB and lipid EMR were got from Waters Corp. and Agilent Corp., respectively.

2.2. UPLC-IM-QTOF MS Conditions

Waters ACQUITY™ UPLC-IM-QTOF MS (Vion, Milford, USA) was used in this experiment. Chromatographic separation was conducted on a BEH C18 column (2.1 mm × 100 mm; 1.7 μm; Waters) at 50˚C. The gradient conditions are shown in Table 1 with the phase A was 0.1% formic acid/ACN (V/V), and phase B was 0.1% formic acid/H_2O (V/V). The flow rate was 0.45 mL/min, and

Table 1. The condition of liquid chromatography for plant toxins.

Time (min)	%A	%B
0.0	2	98
0.25	2	98
20	99	1
24	99	1
25	2	98
30	2	98

the injection volume was 5 μL.

A QTOF mass spectrometer (Waters Corp., Milford, MA, U.S.A.) equipped with an ESI source was used. The MS parameters were set as follows: capillary voltage, 1.0 kV; source temperature, 120˚C; desolvation temperature, 500˚C; desolvation gas rate, 800 L/h. The m/z range was 50 - 2000 Da. The acquisition mode was $HDMS^E$ with a low energy of 6 eV and elevated energy ramping from 15 to 45 eV to obtain the protonated or deprotonated molecule and the fragments ions for the compound in one injection. To ensure the accuracy of mass, the real-time calibration of LE (50 ng/mL, positive ion mode: 556.2771) was carried out. The plant toxins standard was acquired by UPLC-IM-TOF MS with ESI positive mode. The data was processed by UNIFI 1.7 software (Waters Corp.).

2.3. Sample Preparation

Approximately 1.0 g (±0.01 g) of the homogeneous herbal beverage or honey was weighed into a 10 mL polypropylene centrifuge tube. After the honey dissolved in 1 mL water, 5 mL of ACN was added to the herbal beverage or honey and the mixtures were vortexed for 1 min. Added 1.0 g NaCl, then the sample was vortexed for 1 min and centrifuged at 9000 rpm for 5 min. Later, the supernatant was transferred into another tube which containing 50 mg PSA, vortexed for 1 min and centrifuged at 9000 rpm for 5 min. The supernatant was evaporated to near dryness under a gentle stream of nitrogen at 50˚C, and the residues were dissolved with 0.5 mL ACN/H_2O (5/95, v/v) before analyzed by UPLC-IM-QTOFMS.

3. Results and Discussion

3.1. Self-Build Database

There are many commercial libraries for searching the information of the chemical compounds, such as the toxin and the target (T3DB) [24], spectral library for organic compounds (SDBS), MassBank [25], NIST mass spectral library and chemistry library. As for searching plant toxins, little information was obtained from those above libraries. To date, there is no commercial library used on LC-MS system. The main drawback is considered to be the variability of the spectra obtained using LC-MS equipment from different manufacturers. The spectrums of LC-MS are greatly affected by ion source or transfer optics. Thus, UPLC-IM-QTOF MS database for plant toxins was established in our laboratory.

The plant toxin standard was acquired by UPLC-IM-TOF MS with ESI positive mode using 2.2 conditions. By entering the.mol file of the compound (loading from www.chemspider.com), UNIFI software processed the data. The retention time (RT), collision cross-section (CCS) and fragment ions generated from the compound were collected in our database. CCS is the characteristic of the compound. The RT changes with the change of different chromatographic conditions and matrix, but CCS and mass charge ratio parameters are not affected by the different instruments, which can ensure the accuracy of analyte identifi-

cation and obtain the structural state information of samples. The literature [26] displayed compared with retention time (RT)+MS/MS, RT + MS/MS + CCS can reduce candidate substances 80% effectively when screening. Therefore, CCS can provide additional information to confirm the substances analyzed except RT and fragment ions in this study. In the database of 308 compounds for screening, the CCS results of these 308 compounds were confirmed. Through model test, the relationship between CCS and $[M + H]^+$ was obtained, and the fitting degree R^2 reaches 0.9287 (**Figure 1**) demonstrated that there is a linear relationship between CCS and molecular weight.

The detail information of the database was shown in **Table S1**. Take aconitine as an example, the chromatography spectrum of aconitine was shown in **Figure 2(a)**. The RT (7.77 min) of aconitine was obtained. **Figure 2(b)** was the mass spectrum with a low and ramped high energy of collision energy, respectively. We obtained the m/z of the $[M + H]^+$ of aconitine is 646.3211 and the fragment ions are 586.2999, 526.2799, 554.2748, 368.1829. The CCS for $[M + H]^+$ of aconitine is 238.58 Å. The self-build database established in our laboratory contained over 300 compounds (**Table S1**) including aconitines, pyrrolidines, solanines, colchicine, tripterygium wilfordii toxins. Quality control (QC) and LE also were used to investigate the sensitivity and accuracy of the instrument in the whole experiment.

3.2. Sample Preparation Optimization

In order to extract more compounds from the matrix, the experiment selected 80 representative compounds (**Table S2**) to optimize the preparation method. The

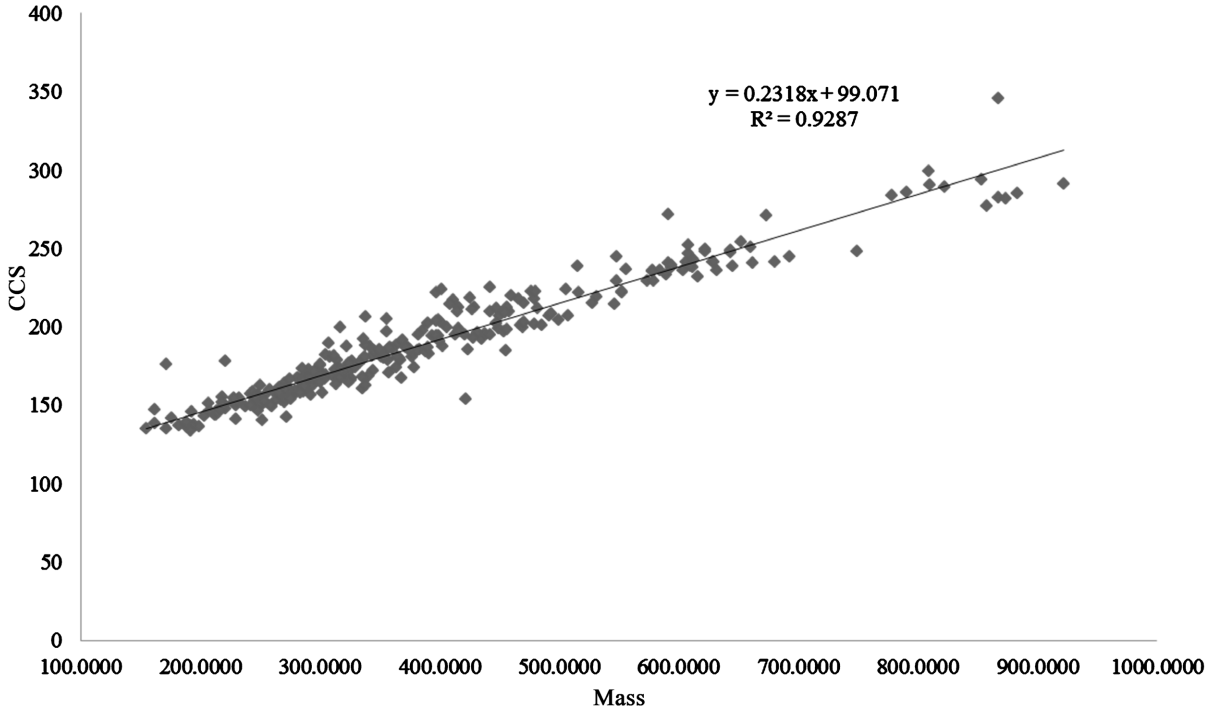
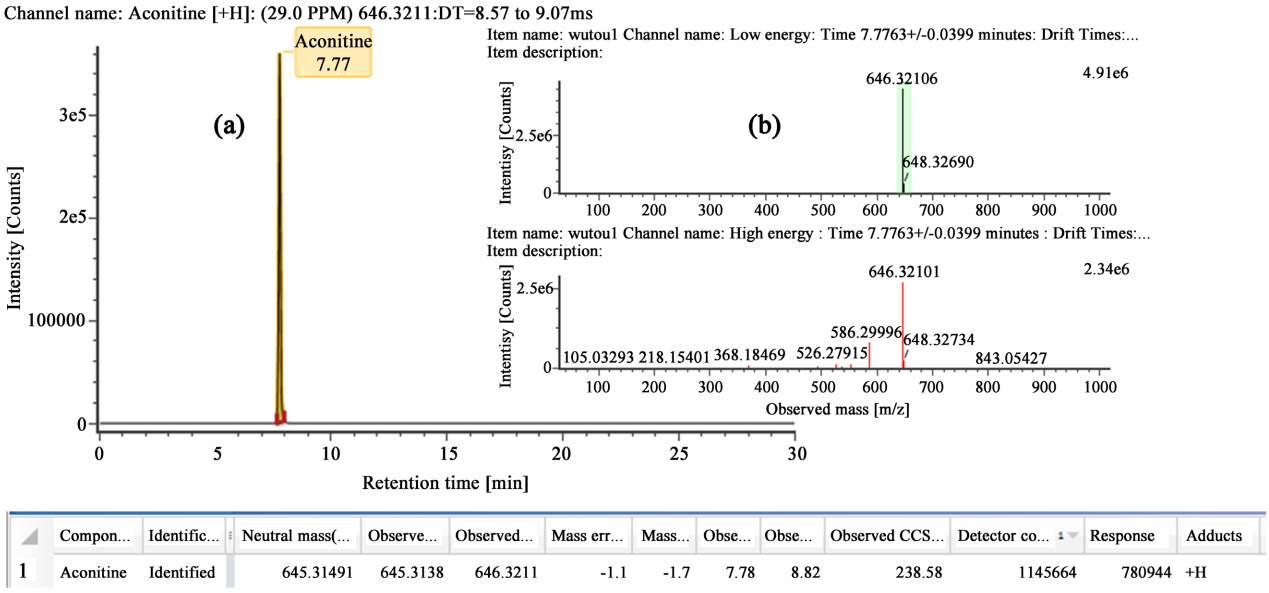


Figure 1. The relationship of CCS and mass of the compound.



	Compon...	Identific...	Neutral mass(...	Observe...	Observed...	Mass err...	Mass...	Obse...	Obse...	Observed CCS...	Detector co...	Response	Adducts
1	Aconitine	Identified	645.31491	645.3138	646.3211	-1.1	-1.7	7.78	8.82	238.58	1145664	780944	+H

Figure 2. The information of aconitine after processed by software.

log P of these compounds ranged from −1.88 to 7.1.

As an easy-to-use sample preparation, QuEChERS is used to purify the compounds in this study. The original QuEChERS method was designed for samples with water content between 25% and 80%. The honey sample contained little water which leading to disperse difficultly. The experimental parameters need to be optimized.

3.2.1. Amount of Water Added to the Honey

The different amounts of water (0.5, 1, 2 and 3 mL) were estimated from honey spiked with 100 μg/kg of analytes. The results demonstrated that the responses of solasodine were relatively low when the honey was dissolved in 0.5 mL water, may be the honey is not completely dispersed. On the contrary, the responses of mesaconine and seneciphylline decreased when the water volume was larger than 1 mL, may be because these compounds were water-soluble. So this study chose to dissolve 1 g honey in 1 mL water.

3.2.2. Amount of NaCl

Anhydrous magnesium sulfate ($MgSO_4$) and NaCl were used for salting out for determination of pyrrolizidine alkaloids in honey [27]. However, anhydrous $MgSO_4$ can promote the distribution of analytes in the organic phase mainly by absorbing water, thus the responses for some water-soluble compound would lower their responses in this process. Saturated NaCl aqueous solution would increases the solubility of compounds in organic phase. To separate the ACN and water layer, the amount of NaCl salt (0.5, 1, 2, 3 g) was optimized. The responses of the analytes increased when NaCl was from 0.5 g to 1 g, but decreased when 3 g of the NaCl was added. To ensure sufficient ion intensity of NaCl in different matrices, while not reduce the extraction efficiency, 1 g of NaCl was chosen to extraction.

3.2.3. Cleanup

The experiment compared SPE with QuEChERS sorbent (C18, PSA, EMR, Zsep, and Zsep+) to purify the herbal beverage (shown in **Figure 3(a)**). It was demonstrated that PSA sorbent could give the better result than other sorbents, which may due to PSA remove organic acids, pigments and metal ions in beverages. Meanwhile, the amounts of PSA were optimized (**Figure 3(b)**). The result found that 50 mg PSA can remove interference for 1.0 g of herbal beverage and honey effectively.

3.3. Method Validation

3.3.1. Matrix Effect

The matrix effect (ME, %) was calculated as the ratio between the area of post-extraction spike analytes and the area of standard solution under identical conditions and then multiplied by 100%. It is generally considered that the ME is

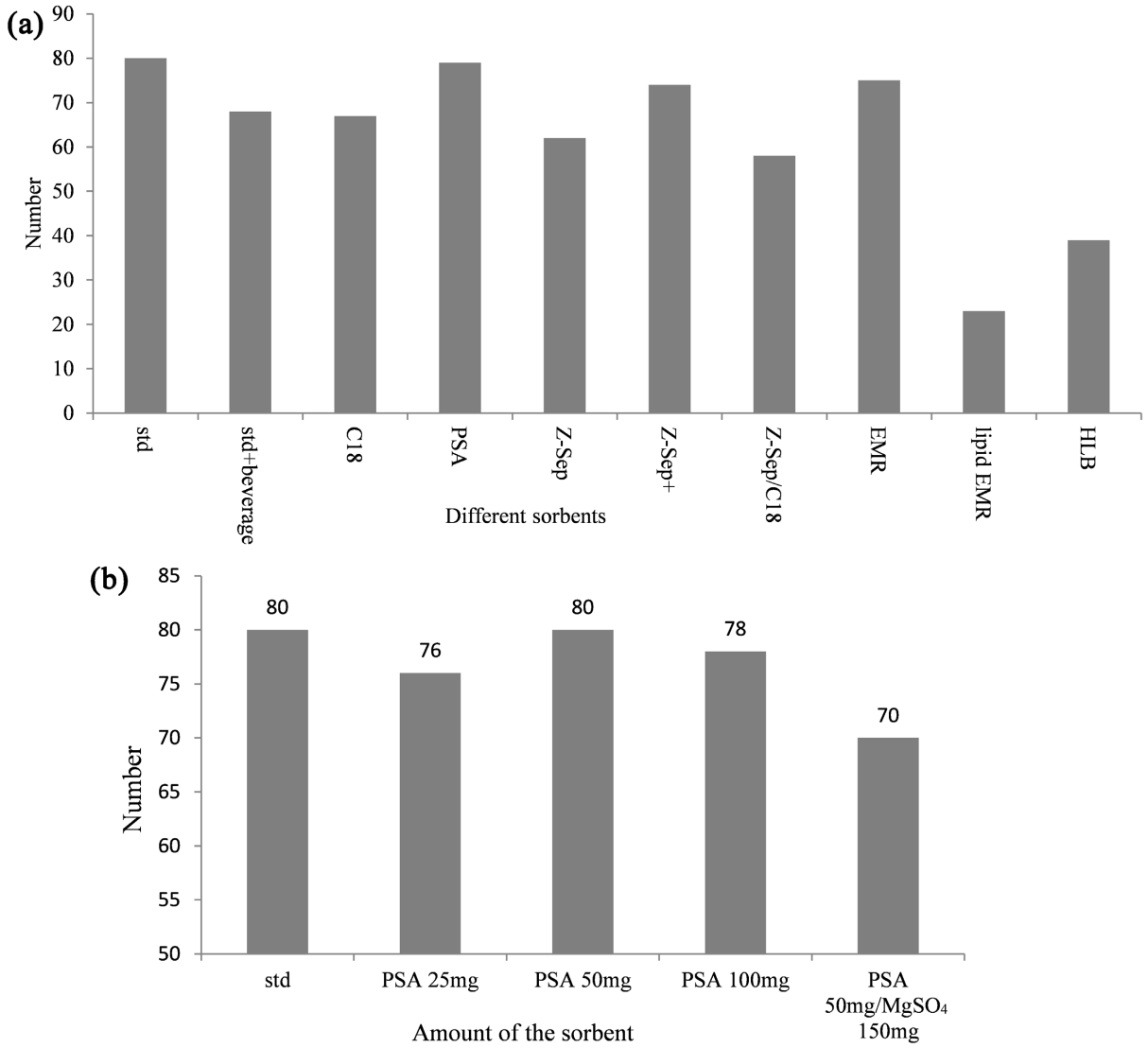


Figure 3. The statistics data of the plant toxins for different sorbents (a) and different amounts of PSA (b) in beverage.

ignored if the data is 80% - 120%. It is ME enhancement if the value is above 120% and inhibition if the value is lower than 80%. Compared the response of the standard in ACN/H_2O and in blank sample processed by PSA, we found that 10% of the compounds showed ME enhancement, and 25% of the compound showed inhibition (Figure 4). To reduce the interference of the ME, matrix-matched calibration curves were used for quantitative analysis.

3.3.2. Recovery and LOQs

Processed the sample that cannot contain the plant toxins according to the optimized sample preparation to form the matrix solution, and diluted the standard working solution with the matrix solution step by step to obtain a series of matrix-calibration curve with concentrations of 20, 50, 200, 500, 1000 μg/kg. The correlation coefficients were greater than 0.99. The sample spiked with 25 μg/kg and 100 μg/kg concentration was purified to evaluate recovery and accuracy. Six spiked samples were processed for each concentration level, and the average recovery and relative standard deviation (RSD) were calculated. The recovery results displayed that over 80% and 90% of the compounds in beverages for 25 μg/kg and 100 μg/kg were ranged from 80% - 120%, and over 80% and 90% of the compounds in honey for 25 μg/kg and 100 μg/kg were ranged from 70% - 120%. The average recoveries for two matrices at two levels ranged from 60.6% - 120.1%, with relative standard deviation (n = 6) less than 25% which can meet screening requirement. The minimum concentration of the standard curve was diluted with the matrix extract until the signal-to-noise ratio of each drug was equal to 10 (S/N = 10), which was determined as the limit of quantification (LOQ) of the compound. The data was shown in Table S2.

3.4. Detection of the Real Sample

The plant toxins database and the method were applied in detecting 20 honey and 20 herbal beverages and honey flavored tea beverage samples. This study

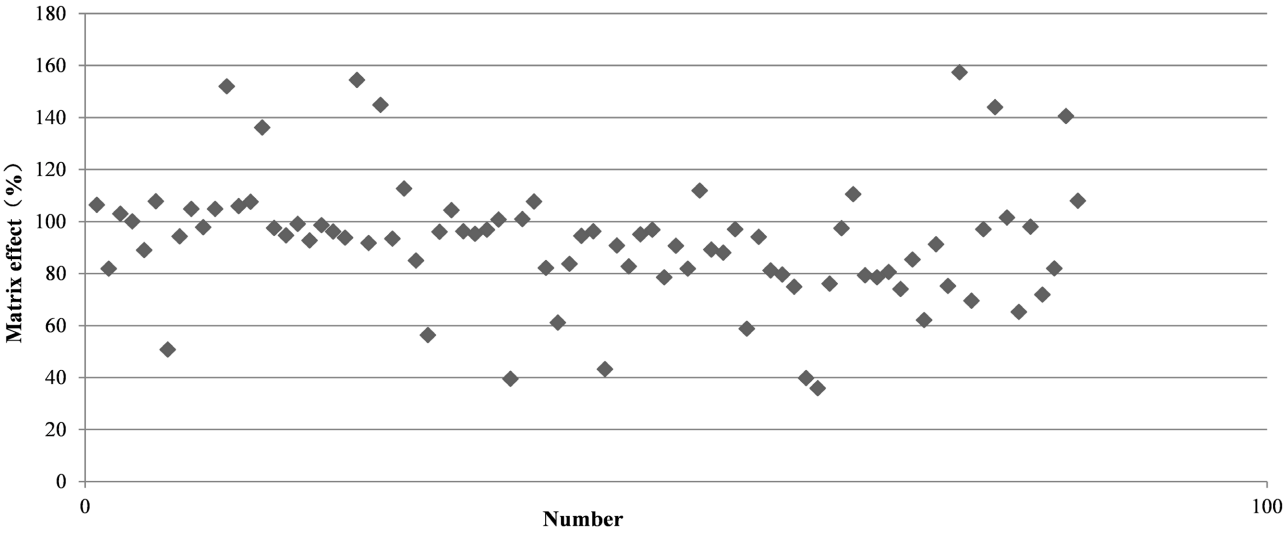


Figure 4. The matrix effect of the compounds in beverage.

adopts the methodological evaluation criteria for confirmation of identity of plant toxins referred to the office of foods and veterinary medicine (OFVM) of FDA in 2015 including RT, mass extraction window and so on. For confirmation, at least two accurate mass (generally one precursor and one production ion) and mass deviation for precursor ion should be less than or equal to 5 ppm and production ions should be less than or equal to 10 ppm. The set for RT is ±0.5 min and CCS is 5%. The deconvolution technique was used to automatically identify the candidate substances of each peak in the real sample by comparison with the standard spectra in the self-built library, which is easily and quickly identified. The result showed that berberine was detected in one honey sample with content was 1 μg/kg. Caffeine was present in tea beverages. The concentration of caffeine was between 200 and 5500 μg/kg. Studies have shown that women planning to be pregnant and women during pregnancy should not consume more than 300 mg of caffeine per day. The amount for children intaking caffeine does not exceed 2.5 mg/kg body weight/day [1], so there is a certain risk for pregnant women and children who often drink caffeine-containing beverages.

4. Conclusion

The study established a plant toxins database and a method for rapid screening plant toxins in honey and herbal beverages. The sample was extracted by ACN, purified by PSA sorbent and analyzed by UPLC-IM-QTOFMS. The recovery, precision and detection limit of this method met the screening requirements. This method is easy to operate and high practical in screening of plant toxins in honey and herbal beverages.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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Supplemental Information

Table S1. The information of toxic compounds in database.

CAS	Name	Molecular Formula	Monoisotopic mass	LogP	CCS	Retention Time (min)	Fragment ions
485-71-2	(−)-Cinchonidine	$C_{19}H_{22}N_2O$	294.1732	3.35	167.39	3.06	277.17024, 167.073, 168.08053, 235.12465, 130.06529
486-56-6	(−)-Cotinine	$C_{10}H_{12}N_2O$	176.0950	−0.23	141.79	0.55	146.06051, 80.04909, 118.06517, 117.05619, 149.07128
485-35-8	(−)-Cytisine	$C_{11}H_{14}N_2O$	190.1106	0.07	137.49	0.55	148.07555, 146.06033, 133.05311, 120.08138, 131.07201
490-46-0	(−)-Epicatechin	$C_{15}H_{14}O_6$	290.0790	0.49	162.49	3.01	139.03908, 147.04411, 123.04441, 163.03839
54-11-5	(−)-Nicotine	$C_{10}H_{14}N_2$	162.1157	0.72	147.12	0.56	133.07562, 147.09203, 121.07706, 135.09166, 122.09588
6106-81-6	(−)-Scopolamine N-oxide	$C_{17}H_{21}NO_5$	319.1420	−0.49	169.52	2.65	172.09697, 154.08654, 94.06543, 155.09351, 136.07622
485-49-4	(+)-Bicuculline	$C_{20}H_{17}NO_6$	367.1056	2.88	179.08	4.08	307.06043, 277.04977, 279.06483, 190.08645, 176.06796
13552-72-2	(+)-Isocorydine	$C_{20}H_{23}NO_4$	377.1394	–	180.93	4.15	279.10073, 308.12824, 264.07808, 265.08513, 311.12807
480-18-2	(+)-Taxifolin	$C_{15}H_{12}O_7$	304.0583	1.82	167.14	3.96	153.01885, 287.05523
7562-61-0	(+)-Usnic acid	$C_{18}H_{16}O_7$	344.0896	2.3	172.08	13.06	327.08637, 233.08098, 330.07354, 261.07594, 303.08658
53392-66-8	(±)-6'-Bromolaudanosine	$C_{21}H_{26}BrNO_4$	435.1045	4.78	192.38	5.63	206.11815, 311.1286, 314.15159, 228.98615, 405.07055
15251-47-5	(±)-Anabasine	$C_{10}H_{14}N_2$	162.1157	0.85	138.31	1.17	146.09542
500-64-1	(±)-Kavain	$C_{14}H_{14}O_3$	230.0943	1.69	149.63	8.24	129.06786
128-62-1	(±)-Noscapine	$C_{22}H_{23}NO_7$	413.1475	2.83	194.97	4.52	220.09683, 353.10218, 205.07304, 350.07839, 381.11988
564-20-5	(3aR)-(+)-Sclaerolide	$C_{16}H_{26}O_2$	250.1933	4.32	162.67	12.47	189.16413
41849-35-8	10-Hydroxyaconitine	$C_{34}H_{47}NO_{12}$	661.7370	0.32	240.57	8.89	602.29597, 542.27484, 570.26976, 552.25919, 612.28032
64439-81-2	10-Hydroxycamptothecin	$C_{20}H_{16}N_2O_5$	364.1059	1.32	188.35	4.98	321.12346, 265.09683, 184.06328, 264.08871, 247.08709
108664-98-8	16-Oxocafestol	$C_{19}H_{24}O_2$	284.1776	4.4	165.19	12.19	147.08108, 241.15973, 133.06724, 213.12742, 219.17459
471-53-4	18-β-Glycyrrhetinic acid	$C_{30}H_{46}O_4$	470.3396	6.57	215.33	12.96	453.33651, 317.21131, 425.34187, 407.33094, 189.16393
15345-89-8	5,6-Dehydrokawain	$C_{14}H_{12}O_3$	228.0786	1.8	151.78	8.81	201.09113, 152.06191, 186.06731, 168.05705, 183.08071
42079-78-7	5-Methoxyflavone	$C_{16}H_{12}O_3$	252.0786	3.47	150.56	8.3	238.06269, 237.05512, 210.06797, 108.02084, 136.01554
38183-04-9	6,7-Dihydroxyflavone	$C_{15}H_{10}O_4$	254.0579	3.62	152.6	6.55	237.05496, 129.03376, 153.01867, 107.01305, 77.03844

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5932-53-6	6-Hydroxytropinone	$C_8H_{13}NO_2$	155.0946	−1	134.91	0.49	138.09117, 98.05977
6665-86-7	7-Hydroxyflavone	$C_{15}H_{10}O_3$	238.0630	3.32	149.28	7.11	129.03364, 137.02345, 77.03838, 103.05418, 221.06074
18051-16-6	9,10-Dihydrolysergol	$C_{16}H_{20}N_2O$	256.1576	1.87	158.17	2.88	208.11224, 167.0735, 154.06539, 180.08141, 168.08015
480-44-4	Acacetine	$C_{16}H_{12}O_5$	284.0685	3.15	159.24	8.64	242.05737, 270.05244, 153.01848, 241.04957, 159.04516
509-20-6	Aconine	$C_{25}H_{41}NO_9$	499.5940	−1.63	204.03	2.93	450.24863, 468.25919, 418.22241, 482.27484, 436.23298
302-27-2	Aconitine	$C_{34}H_{47}NO_{11}$	645.3149	0.39	238.59	7.44	586.30083, 526.28009, 494.25337, 596.28516, 522.2498
4360-12-7	Ajmaline	$C_{20}H_{26}N_2O_2$	326.1994	0.78	172.63	4.37	182.09643, 144.08104, 220.11185, 239.15503, 167.07318
481-72-1	Aloe-emodine	$C_{15}H_{10}O_5$	270.0528	3.382	153.04	7.91	225.05459, 241.049, 253.04966, 224.04699, 235.03759
88321-09-9	Aloxistatin	$C_{17}H_{30}N_2O_5$	342.2155	2.36	187.56	8.97	228.12297, 172.09679, 182.0808, 325.21334, 140.03412
55869-99-3	Anisodamine	$C_{17}H_{23}NO_4$	305.1627	0.25	169.64	2.71	140.10724, 122.09678, 91.0545, 276.15754
642-15-9	Antimycin A1	$C_{28}H_{40}N_2O_9$	548.2734	4.68	229.14	15.03	243.07293, 265.01893, 287.06362, 186.01743, 307.18885
38966-21-1	Aphidicolin	$C_{20}H_{34}O_4$	338.2457	1.69	206.61	18.44	149.13299, 233.22664, 135.11702, 219.21051, 205.19398
520-36-5	Apigenin	$C_{15}H_{10}O_5$	270.0528	2.103	155.86	6.42	153.01809, 145.02877, 229.04894, 253.04886, 119.04931
313-67-7	Aristolochic acid A	$C_{17}H_{11}NO_7$	341.0536	3.41	168.53	9.22	267.06482, 239.06936, 308.05581
63968-64-9	Artemesinin	$C_{15}H_{22}O_5$	282.1467	2.27	167.4	9.74	205.12266
495-02-3	Auraptene	$C_{19}H_{22}O_3$	298.1569	5.69	169.37	13.64	189.05476, 175.03903, 215.07024, 203.0707, 227.07071
13395-02-3	Aristolactam I	$C_{17}H_{11}NO_4$	293.0688	2.97	161.99	9.19	279.05261, 251.05769
25274-27-5	Aristolone	$C_{15}H_{22}O$	218.1671	–	155.3	10.99	163.11174, 177.12739, 175.11174, 149.09609, 147.08044
55-48-1	Atropine	$C_{34}H_{46}N_2O_6$	289.1731	–	170.21	3.24	227.9906, 124.1118, 91.0541
19879-30-2	Bavachinin A	$C_{21}H_{22}O_4$	338.1518	4.93	188.49	11.59	219.10198, 271.09689, 283.09713, 147.04438, 269.08142
466-24-0	Benzoylaconine	$C_{32}H_{45}NO_{10}$	603.7000	0.9	236.01	6.02	554.27484, 572.28541, 522.24863, 586.30106, 540.25919
63238-66-4	Benzoylhypacoitine	$C_{31}H_{43}NO_9$	573.6740	–	229.39	6.27	542.27484, 480.23806, 510.24863, 460.21185, 384.21693
63238-67-5	Benzoylmesaconine	$C_{31}H_{43}NO_{10}$	589.6740	–	233.13	5.61	540.25919, 558.26976, 508.23298, 572.28541, 526.24354
2086-83-1	berberine	$C_{20}H_{18}NO_4+$	336.1240	−0.67	160.8	2.69	323.1745, 306.1693

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6078-17-7	Berbamine	$C_{37}H_{40}N_2O_6$	680.2420	–	241.68	0.54	381.18082, 578.25421, 593.26636, 367.16548, 174.09121
33570-04-6	Bilobalide	$C_{15}H_{18}O_8$	326.1002	−0.45	165.69	3.91	309.09666
491-80-5	Biochanin A	$C_{16}H_{12}O_5$	284.0685	3.139	160.93	8.87	269.04449, 253.04935, 158.03652, 152.01044, 153.01791
24939-16-0	Bis demethoxycurcumin	$C_{19}H_{16}O_4$	308.1049	3.39	180.56	9.06	147.04436, 119.04938, 131.04948, 189.05435, 107.04977
476-70-0	Boldine	$C_{19}H_{21}NO_4$	327.1471	2.32	178.22	3.27	265.08581, 297.1118, 282.08886, 239.07025, 267.06528
22260-51-1	Bromocriptine mesylate	$C_{33}H_{44}BrN_5O_8S$	749.2094	–	248.21	7.75	656.226, 303.0257
465-21-4	Bufalin	$C_{24}H_{34}O_4$	386.2457	3.42	197.47	8.45	351.23236, 369.24279, 255.21133, 333.22169, 305.22688
1354-84-3	Bullatine A	$C_{22}H_{33}NO_2$	343.2511	–	181.23	3.03	326.24784, 314.24784, 260.20089, 263.17943, 232.20598
107668-79-1	Bulleyaconotine A	$C_{35}H_{49}NO_{10}$	643.3356	1.67	247.35	8.19	584.32147, 552.29521, 520.26936, 524.26384, 612.31624
487-52-5	Butein	$C_{15}H_{12}O_5$	272.0685	2.66	162.66	6.28	255.06531, 163.03891, 137.02348, 145.02825, 135.04434
124753-97-5	C6 Ceramide	$C_{24}H_{47}NO_3$	397.3556	8.02	221.89	16.36	264.26884, 282.27979, 252.26905, 380.35284, 362.34236
469-83-0	Cafestol	$C_{20}H_{28}O_3$	316.2039	4.03	173.6	10.22	298.19282, 145.10157, 147.08106, 185.13092, 269.19033
81760-48-7	Cafestol acetate	$C_{22}H_{30}O_4$	358.2144	4.88	186.9	12.05	281.19027, 225.12802, 119.08588, 147.081, 131.08571
”58-08-2	Caffeine	$C_8H_{10}N_4O_2$	194.1900	–	137.79	2.75	195.08792, 138.06638, 110.07124, 139.06927
7689-03-4	Camptothecin	$C_{20}H_{16}N_2O_4$	348.1110	1.6	182.68	6.17	305.12872, 249.10211, 248.09503, 168.06882, 303.08853
404-86-4	Capsaicin	$C_{18}H_{27}NO_3$	305.1991	4.27	182.22	9.9	137.0599, 122.03643, 94.04105, 182.15386
19309-14-9	Cardamonin	$C_{16}H_{14}O_4$	270.0892	–	164.09	10.38	167.03389, 152.01041, 124.0155
1260-17-9	Carminic acid	$C_{22}H_{20}O_{13}$	492.0904	4.8	207.04	3.5	355.04621
2468-21-5	Catharanthine	$C_{21}H_{24}N_2O_2$	336.1838	4.05	179.25	5.76	144.08096, 143.07315, 219.10388, 218.0964, 248.14333
34157-83-0	Celastrol	$C_{29}H_{38}O_4$	450.2770	5.9	207.33	14.25	201.09101, 215.10666, 200.08318, 405.27881, 241.12231
483-17-0	Cephaeline	$C_{28}H_{38}N_2O_4$	466.2832	4.09	217.91	3.06	246.14901, 450.26393, 274.17962, 258.14914, 244.13291
481-49-2	Cepharanthine	$C_{37}H_{38}N_2O_6$	606.2730	5.229	241.48	5.07	365.14985, 174.09154, 576.23825, 380.17092, 591.24924
62-59-9	Cevadine	$C_{32}H_{49}NO_9$	591.3408	3.28	240.51	6.78	456.27477, 492.29586, 438.26465, 538.31728, 520.30681

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476-32-4	Chelidonine	$C_{20}H_{19}NO_5$	353.1263	–	180.45	5.14	323.0914, 305.08084, 336.12303, 295.09649
480-40-0	Chrysine	$C_{15}H_{10}O_4$	254.0579	2.88	151.85	8.5	153.01852, 213.05492, 129.0335, 237.05447, 77.03859
470-37-1	Cinobufagin	$C_{26}H_{34}O_6$	442.2355	2.43	209.76	9.18	365.21097, 401.23231, 347.20076, 383.22168, 337.216
25425-12-1	Citreoviridin	$C_{23}H_{30}O_6$	402.2043	3.04	223.94	9.11	297.14829, 285.14863, 315.1592, 191.06956, 259.13348
518-75-2	Citrinin	$C_{13}H_{14}O_5$	250.0841	1.2	150.23	7.42	233.08117, 205.08636, 203.03412, 215.07068, 191.07053
22373-78-0	Coban	$C_{36}H_{61}NaO_{11}$	692.4111	–	244.97	16.1	461.28701, 479.29749, 599.39235, 501.31807, 443.27643
64-86-8	Colchicine	$C_{22}H_{25}NO_6$	399.1682	0.92	194.22	5.69	358.16501, 310.11848, 295.09703, 341.13955, 267.10134
7633-69-4	Condelphine	$C_{25}H_{39}NO_6$	449.2777	−0.3	198.91	3.54	432.27446, 386.23281, 418.25908, 358.2375, 400.24811
546-06-5	Conessine	$C_{24}H_{40}N_2$	356.3192	5.71	197.16	3.7	312.26884, 269.22614, 310.25539, 270.223, 159.1167
518-69-4	Corydaline	$C_{22}H_{27}NO_4$	369.1940	4.19	191.48	5.66	192.10211, 354.16944, 176.07091, 165.09131, 177.07832
630-94-4	Corynoxeine	$C_{22}H_{26}N_2O_4$	382.1893	–	194.66	5.23	351.17032, 267.14919, 160.07569, 201.10224, 319.1441
479-13-0	Coumestrol	$C_{15}H_8O_5$	268.0372	2.94	153.02	6.43	225.05457, 224.04621, 252.04117
79592-91-9	Crassicauline A	$C_{35}H_{49}NO_{10}$	643.7640	1.67	248.5	8.25	584.32179, 552.29558, 520.26936, 612.31671, 488.24315
35825-57-1	Cryptotanshinone	$C_{19}H_{20}O_3$	296.1412	4.93	167.22	11.78	279.13839, 254.09379, 282.12537, 268.10925, 249.0912
66-81-9	Cycloheximide	$C_{15}H_{23}NO_4$	281.1627	0.56	167.54	5.69	264.15873, 177.12855, 219.13808
4449-51-8	Cyclopamine	$C_{27}H_{41}NO_2$	411.3137	5.44	217.34	6.87	394.31086, 321.22156, 377.28467, 213.1641, 157.10133
14930-96-2	Cytochalasin B	$C_{29}H_{37}NO_5$	479.2672	3.71	218.11	8.37	462.26429, 444.25384, 416.25918, 426.24238, 398.24927
486-66-8	Daidzein	$C_{15}H_{10}O_4$	254.0579	2.78	152.53	5.38	237.05475, 137.02338, 145.02874, 131.04986, 147.04455
552-66-9	Daidzin	$C_{21}H_{20}O_9$	416.1107	0.45	198.74	4.01	245.04522, 219.02909, 191.03453, 165.018, 195.02943
55486-00-5	Decylubiquinone	$C_{19}H_{30}O_4$	322.2144	5.5	187.58	16.17	197.08094, 151.07569, 182.05748, 136.05186, 139.0394
67909-49-3	Dehydroevodiamine	$C_{19}H_{15}N_3O$	301.1215	–	169.02	5.07	286.09749, 272.08184, 140.04948, 229.07602
522-17-8	Degeulin	$C_{23}H_{22}O_6$	394.1416	5.03	194.38	11.08	191.07049, 203.07062, 177.05479, 241.08614, 198.06778
52358-55-1	Delcorine	$C_{26}H_{41}NO_7$	479.2883	1.16	201.72	4.55	386.23279, 448.26925, 418.25915, 354.207, 358.23793

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509-18-2	Delsoline	$C_{25}H_{41}NO_7$	467.5950	−0.27	201.08	4.27	418.2588, 386.23258, 450.28501, 436.26936, 390.26389
6836-11-9	Deltaline	$C_{27}H_{41}NO_8$	507.6160	2.54	207.21	4.59	476.26428, 386.23258, 358.23767, 354.20637, 446.25371
474-08-8	Demissidine	$C_{27}H_{45}NO$	399.3501	7.46	204.52	8.06	98.09629, 161.13275, 255.21167, 382.3481, 159.1163
43043-74-9	Deoxyshikonin	$C_{16}H_{16}O_4$	272.1049	4.72	157.89	13.41	255.1016, 205.05031, 240.07801, 189.0561, 175.03928
10180-88-8	Desacetylmatricarin	$C_{15}H_{18}O_4$	262.1205	0.73	157.76	4.85	171.08071, 199.112, 172.08772, 184.08844, 217.1224
61939-05-7	Desoxypeganine	$C_{11}H_{12}N_2$	172.1001	0.16	134.79	2.29	144.06918, 130.06555, 117.05746, 143.0718, 118.06485
2270-40-8	Diacetoxyscirpenol	$C_{19}H_{26}O_7$	366.1678	1.33	180.29	6.57	175.11205, 159.08072, 173.09583, 91.05445, 105.07008
21851-07-0	Diacetylkorseveriline	$C_{31}H_{49}NO_5$	515.3611	5.65	238.5	6.94	456.34765, 396.3265, 378.31619, 454.33265, 394.31095
66-76-2	Dicoumarol	$C_{19}H_{12}O_6$	336.0634	3.548	168.32	11.61	163.03905, 121.02856, 175.03919, 77.0389, 95.04918
484-29-7	Dictamnine	$C_{12}H_9NO_2$	199.0633	–	136.25	7.86	185.04713
483-15-8	Dihydroberberine	$C_{20}H_{19}NO_4$	337.1314	–	180.6	5.01	322.10738, 292.09682, 294.11247, 280.09682
19408-84-5	Dihydrocapsaicin	$C_{18}H_{29}NO_3$	307.2147	–	189.47	11.06	137.05971, 122.03623, 94.04132, 172.16959
17479-19-5	Dihydroergocristine	$C_{35}H_{41}N_5O_5$	611.3108	–	238.06	7.56	270.16009, 350.1863, 594.30748, 253.13354, 225.13863
4382-33-6	Dihydrorobinetine	$C_{15}H_{12}O_7$	304.0583	0.8	166.96	2.64	137.02377, 287.05441, 179.03484
587-63-3	Dihydrokavain	$C_{14}H_{16}O_3$	232.1099	–	151.87	8.73	187.11174, 91.05423, 65.03858, 171.08044
6271-21-2	Dihydrolycorine	$C_{16}H_{19}NO_4$	289.1314	–	165.74	1.98	272.12812, 214.08626, 254.11756, 216.10191, 228.10191
20958-18-3	Dihydrotanshinone	$C_{18}H_{14}O_3$	278.0943	3.9	156.78	12.21	261.09135, 263.07057, 235.07642, 249.09111, 222.10371
520-34-3	Diosmetine	$C_{16}H_{12}O_6$	300.0634	3.1	164.49	6.76	258.05208, 286.04706, 257.04428, 153.01848, 161.06005
520-27-4	Diosmin	$C_{28}H_{32}O_{15}$	608.1741	2.05	247.07	4.85	301.07078, 463.12368, 286.04726, 258.05241, 407.07683
471-69-2	Dipterocarpol	$C_{30}H_{50}O_2$	442.3811	8.77	225.2	17.46	315.26748, 339.30589, 275.23989, 301.25331, 67.0541
14277-97-5	Domoic acid	$C_{15}H_{21}NO_6$	311.1369	0.61	168.73	2.98	266.13851, 248.12794, 220.13335, 202.12269, 193.12325
25316-40-9	Doxorubicin	$C_{27}H_{30}ClNO_{11}$	579.1508	–	229.29	5.78	321.076, 361.07113, 346.04709, 379.08129, 333.07679
22964-77-8	Dubinidine	$C_{15}H_{17}NO_4$	275.1158	1.35	159.27	3.95	216.10195, 188.07063, 186.05518, 258.11267, 170.06019

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118-08-1	D-β-Hydrastine	$C_{21}H_{21}NO_6$	383.1369	2.66	185.54	4.45	323.09159, 293.08043, 190.08623, 295.09693, 324.12064
76684-89-4	E-64-C	$C_{15}H_{26}N_2O_5$	314.1842	1.36	178.54	6.77	200.09168, 172.09814, 132.03069, 184.16859, 144.02831
520-68-3	Echimidine	$C_{20}H_{31}NO_7$	397.2100	−0.1	194.06	4.4	120.08078, 220.13321, 380.20676, 336.18055, 238.14377
476-66-4	Ellagic acid	$C_{14}H_6O_8$	302.0063	0.52	158.17	3.75	257.01021
519-23-3	Ellipticine	$C_{17}H_{14}N_2$	246.1157	4.8	153.26	5.1	231.0915
316-42-7	Emetine	$C_{29}H_{40}N_2O_4$	552.2521	–	222.16	3.89	272.16492, 246.14938, 464.28024, 274.17982, 230.11841
518-82-1	Emodin	$C_{15}H_{10}O_5$	270.0528	5.03	151.52	10.1	253.04946, 135.04455
989-51-5	Epigallocatechin	$C_{22}H_{18}O_{11}$	458.0849	2.08	209.51	3.02	139.03873
4049-38-1	Eriodictyol	$C_{15}H_{12}O_6$	288.0634	2.59	164.48	5.51	153.01858, 163.0393, 145.02855, 135.04456, 117.03352
28649-59-4	Euphorbiasteroid	$C_{32}H_{40}O_8$	552.2723	5.55	222.63	13.21	297.18556, 315.19541, 213.12818, 357.20795, 227.14307
518-17-2	Evodiamine	$C_{19}H_{17}N_3O$	303.1372	1.636	169.18	9.13	171.09165, 161.07092, 144.08072, 116.04992, 134.06038
4540-25-4	Fillalbin	$C_{16}H_{21}NO_4$	291.1471	2.55	173.02	3.16	124.11236, 278.1392, 151.03833, 93.06976, 277.13157
528-48-3	Fisetin	$C_{15}H_{10}O_6$	286.0477	2.52	160.45	4.8	269.04574, 137.02355, 231.0672, 149.02427, 179.03439
3420-72-2	Flavokawain A	$C_{18}H_{18}O_5$	314.1154	3.96	173.3	12	181.04973, 166.02613, 161.06008, 138.03143, 133.06509
1775-97-9	Flavokawain B	$C_{17}H_{16}O_4$	284.1049	4.01	164.93	12.21	181.04978, 166.0263, 138.03133, 103.05439, 267.10228
485-72-3	Formononetin	$C_{16}H_{12}O_4$	268.0735	2.961	156.75	7.55	253.04964, 237.05482, 118.04153, 137.02379, 136.01636
80665-72-1	Fuziline	$C_{24}H_{39}NO_7$	453.5690	−1.32	196.66	3.34	436.26936, 404.24315, 418.2588, 386.23258, 376.21185
548-83-4	Galangin	$C_{15}H_{10}O_5$	270.0528	2.83	154.63	8.77	153.01828, 215.07061, 213.05446, 77.0385, 253.04928
1954-04-4	Galanthamine	$C_{17}H_{21}NO_3$	368.1292	–	167.36	0.56	213.09087, 198.06738, 270.14868, 183.04394, 225.09105
2752-65-0	Gambogic acid	$C_{38}H_{44}O_8$	628.3036	10.3	241.56	16.94	601.31663, 447.18005, 255.10185, 561.24849, 501.26359
35306-33-3	Gelsemine	$C_{20}H_{22}N_2O_2$	358.1448	–	170.91	2.97	306.17035, 236.10723, 195.06811, 238.12261, 140.10726
15291-77-7	Ginkgolide B	$C_{20}H_{24}O_{10}$	424.1369	0.52	185.76	5.61	361.12789, 305.10161, 343.11746, 315.12282, 389.12168
67-99-2	Gliotoxin	$C_{13}H_{14}N_2O_4S_2$	326.0395	0.52	167.14	0.55	233.12937, 116.05654, 146.0611, 91.0545, 168.91735
485-61-0	Graveoline	$C_{17}H_{13}NO_3$	279.0895	3.5	159.46	6.4	265.07265, 252.1014, 250.08605, 236.07004, 264.06545

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304-21-2	Harmaline	$C_{13}H_{14}N_2O$	214.1106	0.66	146.57	4.24	200.0942, 174.09154, 159.06801, 131.07271, 157.07576
6028-00-8	Harmalol	$C_{12}H_{16}N_2O_3$	272.0928	–	142.47	2.7	160.07577, 184.07489, 159.06814, 158.06082, 142.06537
486-84-0	Harmane	$C_{12}H_{10}N_2$	182.0844	3.26	137.07	3.64	168.06825, 167.06187
442-51-3	Harmine	$C_{13}H_{12}N_2O$	212.0950	3.17	143.82	4.29	198.07929, 169.07605, 168.06853, 183.09267, 181.07521
40580-83-4	Harmol	$C_{12}H_{12}N_2O_2$	252.0666	–	140.42	2.85	184.06348, 169.07651, 181.07573, 183.05516
26833-85-2	Harringtonine	$C_{28}H_{37}NO_9$	531.2468	2.58	219.4	4.09	298.14408, 266.11788, 226.08673, 240.10217, 284.12823
303-33-3	Heliotrine	$C_{16}H_{27}NO_5$	313.1889	1.04	172.8	3.33	138.09147, 156.10176, 120.08099, 94.06509, 96.08074
6681-13-6	Hernandezine	$C_{39}H_{44}N_2O_7$	652.3149	2.75	254.17	5.46	411.19131, 622.28082, 606.24805, 174.09144, 426.21344
520-33-2	Hesperitine	$C_{16}H_{14}O_6$	302.0790	2.9	169.29	6.79	153.01853, 177.05485, 179.03405, 145.0288, 149.05979
3328-84-5	Heteratisine	$C_{22}H_{33}NO_5$	391.2359	0.07	183.11	2.74	342.20659, 360.21677, 374.23249, 181.08534, 297.14944
6879-74-9	Himbacine	$C_{22}H_{35}NO_2$	345.2668	4.64	184.88	6.61	302.28471, 185.13276, 328.26438, 269.22703, 145.10115
34000-39-0	Homobutein	$C_{16}H_{14}O_5$	286.0841	2.88	167.11	7.6	137.02366, 177.0548, 145.02856, 163.03902, 272.06805
446-71-9	Homoeriodictyol	$C_{16}H_{14}O_6$	302.0790	2.9	170.26	6.33	153.01841, 145.02841, 117.03356, 179.03354
4261-42-1	Homoorientin	$C_{21}H_{20}O_{11}$	448.1006	1.58	202.56	3.53	299.05509, 329.06537, 353.0653, 325.07057, 395.07593
102518-79-6	Huperzine A(-)	$C_{15}H_{18}N_2O$	242.1419	0.71	157.22	0.55	181.10216, 209.09469, 155.08821, 172.07557, 184.111
550-10-7	Hydrocotarnine	$C_{12}H_{15}NO_3$	221.1052	2.098	148.1	3.02	179.07062, 193.08638, 180.07823, 165.05398, 192.10173
63238-68-6	Hypaconine	$C_{24}H_{39}NO_8$	469.5680	−1.1	199.84	3.31	438.24863, 406.22241, 388.21185, 378.19111, 374.1962
6900-87-4	Hypaconitine	$C_{33}H_{45}NO_{10}$	615.7110	0.92	232.12	7.72	570.30614, 556.29049, 524.26428, 538.27993, 520.26936
77029-83-5	Hypocrellin A	$C_{30}H_{26}O_{10}$	546.1526	3.88	214.56	11.64	487.13891, 529.14961, 471.10784, 457.09213, 429.0968
123940-54-5	Hypocrellin B	$C_{30}H_{24}O_9$	528.1420	4.73	215.03	12.21	487.13854, 471.10726, 457.09153, 429.09657, 472.11241
18059-10-4	Imperialine	$C_{27}H_{43}NO_3$	429.3243	3.9	212.77	4.69	412.32106, 331.22692, 370.27501, 96.08087, 313.21771
4491-19-4	Indaconitine	$C_{34}H_{47}NO_{10}$	629.7380	0.54	241.41	7.71	570.30614, 538.27993, 520.26936, 506.25371, 552.29558

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479-41-4	Indirubin	$C_{16}H_{10}N_2O_2$	262.0742	2.48	152.19	9.48	132.04448, 77.03862
133-32-4	Indole-3-butyric acid	$C_{12}H_{13}NO_2$	203.0946	2.34	143.17	6.6	130.06536
59086-90-7	Ingenol 3,20-dibenzoate	$C_{34}H_{36}O_7$	556.2461	7.89	236.85	14.69	457.19823, 335.16185, 455.18273, 313.17972, 267.17463
418-19-3	Isorhamnetine	$C_{16}H_{12}O_7$	316.0583	1.76	167.39	6.82	302.04225, 285.03914, 245.04393, 153.01832, 257.04435
552-57-8	Isorhoifolin	$C_{27}H_{30}O_{14}$	578.1636	1.05	236.04	4.6	271.06009, 433.113, 153.01859, 381.09642
480-43-3	Isosakuranetin	$C_{16}H_{14}O_5$	286.0841	3.84	165.48	8.58	153.01842, 161.05994, 133.06502, 269.08032, 118.04134
776-86-3	Isoscopoletine	$C_{10}H_8O_4$	192.0423	0.83	134.41	3.66	178.02621, 150.03088, 122.03607, 149.02348, 121.02831
477-57-6	Isotetrandrine	$C_{38}H_{42}N_2O_6$	622.3043	3.55	247.9	0.55	381.18085, 592.26983, 174.09118, 384.1578, 400.19206
4759-48-2	Isotretinoin	$C_{20}H_{28}O_2$	300.2089	6.83	175.16	15.57	283.20693, 255.21161, 185.09581, 201.16533, 173.13239
469-59-0	Jervine	$C_{27}H_{39}NO_3$	425.2930	3.46	218.64	5.55	408.29, 313.21616, 295.20567, 391.26356, 311.20095
520-18-3	Kaempferol	$C_{15}H_{10}O_6$	286.0477	2.05	158.28	6.6	153.01834, 229.04933, 231.06525, 269.04468, 147.0439
17353-03-6	Kaempferol-7-neohesperidoside	$C_{27}H_{30}O_{15}$	594.1584	1.92	237.77	4.66	287.05492, 449.10734, 331.10017, 231.06407
81760-47-6	Kahweol Acetate	$C_{22}H_{28}O_4$	356.1988	4.23	205.03	10.54	267.13819
487-79-6	Kainic acid	$C_{10}H_{15}NO_4$	213.1001	0.5	143.87	0.56	174.09117, 168.10226, 122.09657, 150.09259, 179.07125
39089-30-0	Karacoline	$C_{22}H_{35}NO_4$	377.5180	−0.26	183.16	2.69	360.25332, 328.22711, 342.24276, 310.21654, 332.22202
142273-20-9	Kenpaullone	$C_{16}H_{11}N_2OBr$	326.0055	4.02	166.78	8.84	247.08645, 281.99244, 282.98819
82-02-0	Khellin	$C_{14}H_{12}O_5$	260.0685	1.77	148.87	6.55	231.02886, 163.00278, 246.05214, 203.03409, 230.05749
525-79-1	Kinetin	$C_{10}H_9N_5O$	215.0807	1.201	144.95	2.72	148.06192, 119.0356, 136.06201, 81.03331, 121.05116
32854-75-4	Lappaconitine	$C_{32}H_{44}N_2O_8$	584.7000	2.13	236.09	5.53	567.30648, 535.28026, 356.22202, 324.19581, 388.24824
25999-20-6	Lasalocid A	$C_{34}H_{53}NaO_8$	612.3638	–	242.49	15.97	377.26643, 393.24084, 359.2561, 481.25708, 237.18544
125697-92-9	Lavendustin A	$C_{21}H_{19}NO_6$	381.1212	3.61	184.63	4.22	136.03909, 256.06036, 148.03995, 258.07658, 154.0494
125697-91-8	Lavendustin B	$C_{21}H_{19}NO_5$	365.1263	4.44	180.72	5.55	240.06384, 242.08384, 148.03963, 241.07348, 77.03859
17946-87-1	Leucomisine	$C_{15}H_{18}O_3$	246.1256	1.92	155.17	7.18	173.09621, 158.07251, 159.07986, 201.12763, 191.14354

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1180-71-8	Limonin	$C_{26}H_{30}O_8$	470.1941	1.66	203.31	8.07	425.19641, 367.1913, 213.09182, 453.19222, 409.20116
154-21-2	Lincomycin	$C_{18}H_{34}N_2O_6S$	406.2137	0.91	199.63	0.56	359.21752, 126.12784, 389.21023, 393.20487, 317.2071
134-63-4	Lobeline	$C_{22}H_{22}NO_2$	373.1808	–	186.62	6.27	200.14373, 216.13847, 320.20126, 218.15442, 96.08094
491-70-3	Luteolin	$C_{15}H_{10}O_6$	286.0477	2.4	160.09	5.67	153.0183, 269.04469, 161.02357, 245.04468, 135.04352
52187-80-1	Luteolin-3',7-diglucoside	$C_{27}H_{30}O_{16}$	610.1534	−3.49	238.5	3.79	287.055, 449.10702
10285-07-1	Lycopsamine	$C_{15}H_{25}NO_5$	299.1730	–	169.99	2.4	156.10191, 138.09134, 94.06513, 120.08078, 256.15433
528-43-8	Magnolol	$C_{18}H_{18}O_2$	266.1307	3.938	161.13	11.59	197.06019, 211.07499, 225.09148, 239.10664, 181.06528
490-54-0	Maritimein	$C_{21}H_{20}O_{11}$	448.1006	−1.42	212.09	4.1	287.05458, 153.01804, 269.04466, 161.0236, 285.03922
519-02-8	Matrine	$C_{15}H_{24}N_2O$	248.1889	1.44	156.64	1.67	148.11269, 150.12739, 176.10689, 220.17153, 190.12255
73-31-4	Melatonin	$C_{13}H_{16}N_2O_2$	232.1212	0.96	154.87	4.72	174.0914, 158.06023, 144.07927, 117.05761
58-27-5	Menadion	$C_{11}H_8O_2$	172.0524	–	175.86	7.84	105.03394
6792-9-2	Mesaconine	$C_{24}H_{39}NO_9$	485.5680	−2.16	201.3	2.52	436.23298, 404.20676, 454.24354, 468.25919, 422.21733
2752-64-9	Mesaconitine	$C_{33}H_{45}NO_{11}$	631.7110	−0.14	235.9	7.18	572.28541, 540.25919, 512.26428, 522.24863, 582.26976
57432-61-8	Methylergonovine	$C_{24}H_{29}N_3O_6$	455.2056	–	184.53	3.46	223.12311, 208.076, 207.09138, 208.0989, 297.16008
13614-98-7	Minocycline	$C_{23}H_{22}N_3O_7$	493.1616	–	208.44	3.19	441.16568, 352.11786, 337.09503, 423.15595, 215.05784
315-22-0	Crotaline	$C_{16}H_{23}NO_6$	325.1525	−0.37	172.5	1.79	280.15411, 237.13624, 194.11796, 120.08096, 298.1635
529-44-2	Myricetin	$C_{15}H_{10}O_8$	318.0376	2.11	167.45	4.68	261.03926, 153.01827, 301.0345, 163.0391, 165.01806
35891-70-4	Myriocin	$C_{21}H_{39}NO_6$	401.2777	4.21	202.8	9.17	384.27543, 275.17572, 320.2584, 304.26466, 338.2686
607-91-0	Myristicin	$C_{11}H_{12}O_3$	192.0786	3.264	136.77	5	177.05746
480-41-1	Naringenin	$C_{15}H_{12}O_5$	272.0685	3.19	160.04	6.39	153.0184, 147.04449, 119.04937, 255.06401, 231.06458
466-26-2	Neoline	$C_{24}H_{39}NO_6$	437.5700	−1.69	195.59	3.51	420.27445, 388.24824, 356.22202, 370.23767, 362.23258
20069-05-0	Nitrarine	$C_{20}H_{25}N_3$	379.1582	–	174.02	2.76	223.123, 225.13798, 170.09664, 182.09548, 158.09669
6880-54-2	Norfluorocurarine	$C_{19}H_{20}N_2O$	292.1576	3.27	167.03	3.89	247.12397, 263.15466, 235.12337, 265.16972, 264.13635

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475-83-2	Nuciferine	$C_{19}H_{21}NO_2$	295.1570	–	171.63	5.8	265.12231, 235.07536, 250.09883, 219.08044, 207.08044
303-47-9	Ochratoxin A	$C_{20}H_{17}NO_6$	403.0823	4.31	187.73	9.49	239.0105, 221.00014, 193.0051, 358.08445, 165.01047
508-02-1	Oleanolic acid	$C_{30}H_{48}O_3$	456.3604	9.06	210.77	14.96	439.35762, 393.35232, 203.17996, 189.16416, 411.36268
579-13-5	Oligomycin A	$C_{45}H_{74}O_{11}$	790.5231	6.17	286.07	15.02	773.51968, 755.50894, 683.44917, 737.49852, 447.34702
484-12-8	Osthole	$C_{15}H_{16}O_3$	244.1099	3.87	155.58	10.56	189.05488, 161.05996, 159.04451, 203.07063, 187.03915
19666-76-3	Panaxadiol	$C_{30}H_{52}O_3$	460.3916	7.64	220.05	16.58	425.37836, 443.38893, 285.25843, 189.16415, 217.1957
32791-84-7	Panaxatriol	$C_{30}H_{52}O_4$	476.3866	5.94	222.26	11.85	459.38392, 441.37322, 187.14848, 189.16433, 367.30057
61-25-6	Papaverine	$C_{20}H_{21}NO_4$	375.1237	–	185.3	5.14	324.12315, 202.08628, 171.06788, 308.09194, 296.1282
36101-54-9	Peganole	$C_{11}H_{12}N_2O$	188.0950	−1.01	137.95	1.75	120.04451, 172.07565, 144.08095, 143.0731, 92.04976
1182-87-2	Peruvoside	$C_{30}H_{44}O_9$	548.2985	2.25	244.76	7.09	353.21152, 335.20165, 325.21709, 307.20661
57-47-6	Physostigmine	$C_{15}H_{21}N_3O_2$	275.1634	1.22	166.52	3.22	160.07593, 174.09142, 162.09156, 147.0676, 218.14151
554-62-1	Phytosphingosine	$C_{18}H_{39}NO_3$	317.2930	5.18	199.57	11.44	282.27907, 300.28967, 270.27904, 264.26856, 252.26862
10083-24-6	Piceatannol	$C_{14}H_{12}O_4$	244.0736	2.69	158.37	4.16	227.06915, 135.04347
17617-45-7	Picrotoxinin	$C_{15}H_{16}O_6$	292.0947	−0.13	156.52	5.04	247.09689, 275.0889, 219.10205, 193.05148
54-71-7	Pilocarpine	$C_{11}H_{16}N_2O_2$	208.1212	−0.09	146.33	1.74	163.12327, 95.0602, 147.09241, 191.11742, 135.09176
94-62-2	Piperine	$C_{17}H_{19}NO_3$	285.1365	2.66	173.37	9.44	201.05459, 171.04433, 173.05957, 135.04425, 159.04435
5947-49-9	Podocarpic acid	$C_{17}H_{22}O_3$	274.1569	4.27	160.15	0.55	210.06592, 131.05055, 105.03266, 109.06562, 157.06617
487-24-1	Pratol	$C_{16}H_{12}O_4$	268.0735	3.59	157.25	7.21	226.06266, 254.05757, 225.0551, 255.06254, 137.02365
14152-28-4	Prostaglandin A_1	$C_{20}H_{32}O_4$	336.2301	3.61	192.26	8.18	289.21701, 117.06994, 105.06963, 191.14253, 275.2016
124-97-0	Protoveratrine B	$C_{41}H_{63}NO_{15}$	809.4198	0.75	299.48	6.52	792.41709, 774.40698, 732.395, 658.3587, 714.38581
6164-62-1	Pseudopelletierine	$C_9H_{15}NO$	189.0920	–	135.83	0.56	112.11292, 96.0813, 113.11846, 94.06372
76-78-8	Quassin	$C_{22}H_{28}O_6$	388.1886	2.22	184.35	6.7	223.09706, 208.07339, 163.07566, 177.09097, 203.1066

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6151-25-3	Quercetin	$C_{15}H_{14}O_9$	338.0638	–	162.63	5.72	245.04436, 285.03932, 153.01859, 287.05367, 247.05897
56-54-2	Quinidine	$C_{20}H_{24}N_2O_2$	324.1837	–	174.69	3.54	307.18068, 264.13803, 253.13418, 160.07588, 172.07562
130-95-0	Quinine	$C_{20}H_{24}N_2O_2$	324.1837	–	176.88	3.65	307.18088, 253.13436, 172.07573, 184.07573, 160.07578
61281-38-7	R(+)-Schisandrin A	$C_{24}H_{32}O_6$	416.2199	5.87	196.91	13.12	402.20411, 347.14914, 386.20901, 355.15432, 317.102
12772-57-5	Radicicol	$C_{18}H_{17}ClO_6$	364.0714	1.53	174.29	7.02	197.00021, 224.99493, 192.0419, 227.01056, 347.06928
50-55-5	Reserpine	$C_{33}H_{40}N_2O_9$	608.2734	4.046	252.45	8.06	397.21181, 195.06549, 448.19682, 365.18613, 174.09158
501-36-0	Resveratrol	$C_{14}H_{12}O_3$	228.0786	3.139	154.29	5.92	211.07427, 210.06858
480-54-6	Retrorsine	$C_{18}H_{25}NO_6$	351.1682	−0.14	180.73	3.11	324.18139, 276.15996, 322.16577, 120.08111, 138.09181
90-19-7	Rhamnetine	$C_{16}H_{12}O_7$	316.0583	2.58	167.65	7.77	271.05991, 302.04185, 167.03416, 299.05505, 257.04404
17306-46-6	Rhoifolin	$C_{27}H_{30}O_{14}$	578.1636	1.72	235.37	4.7	271.05961, 433.11307, 153.01811, 313.06905, 270.05276
13292-46-1	Rifampicin	$C_{43}H_{58}N_4O_{12}$	822.4052	1.09	289.5	10.14	791.38636, 399.16586, 469.17304, 163.11205, 299.06632
82-08-6	Rottlerin	$C_{30}H_{28}O_8$	516.1784	8.66	221.6	14.58	323.12803, 219.0654, 335.12804, 231.06563, 177.05487
84-26-4	Rutaecarpine	$C_{18}H_{13}N_3O$	287.1059	2.031	162.28	9.37	271.08699, 243.09071, 242.08391, 169.07613, 262.09893
61281-37-6	S(-)-Schisandrin A	$C_{23}H_{28}O_6$	400.1886	6.46	190.69	13.71	386.17331, 331.11835, 370.1782, 371.18442, 355.15425
101467-40-7	Salsoline	$C_{11}H_{15}NO_2$	193.1103	0.87	145.61	1.66	162.09158, 146.06105
493-48-1	Salsolodine	$C_{12}H_{17}NO_2$	207.1259	1.63	151.25	2.52	191.10616, 176.08289, 161.05916
481-06-1	Santonin	$C_{15}H_{18}O_3$	246.1256	1.6	155.54	6.79	173.09627, 158.07256, 201.12769, 157.06482, 172.08785
20310-89-8	Saponarin	$C_{27}H_{30}O_{15}$	594.1584	−1.21	239.7	3.49	283.06018, 313.07072, 337.07094, 379.08135, 397.09203
126-19-2	Sarsasapogenin	$C_{27}H_{44}O_3$	416.3290	6.21	212.39	17.13	255.2108, 273.22125, 173.13258, 159.11727, 147.11713
549-23-5	Sclerotiorin	$C_{21}H_{22}IO_5$	390.1234	3.12	202.46	13.66	303.11524, 349.12074, 331.11028, 181.00535, 259.05244
92-61-5	Scopoletin	$C_{10}H_8O_4$	192.0423	1.28	133.8	3.88	178.02615, 150.03079, 122.03617, 149.02396, 121.0292
5610-40-2	Securinine	$C_{13}H_{15}NO_2$	217.1103	0.596	146.99	1.24	84.08004, 172.11183
130-01-8	Senecionine	$C_{12}H_{15}NO_3$	221.1052	2.098	177.92	3.97	308.18611, 120.08133, 138.09147, 290.17594, 220.13402

Continued

480-81-9	Seneciphylline	$C_{18}H_{23}NO_5$	333.1580	−1.88	176.54	3.46	306.16998, 120.08078, 288.15942, 138.09134, 94.06513
2318-18-5	Senkirkine	$C_{19}H_{27}NO_6$	365.1840	−0.27	180.74	4.35	168.10191, 150.09134, 348.18055, 122.06004, 140.07061
-	Sevedindione	$C_{27}H_{41}NO_3$	427.3087	3.21	210.82	5.09	410.30527, 398.30538, 380.25921, 126.12682, 162.12728
22888-70-6	Silybine	$C_{25}H_{22}O_{10}$	482.1213	2.59	212.03	6.46	435.10847, 419.11263, 465.11919, 153.01884, 311.05591
2306-27-6	Sinensetine	$C_{20}H_{20}O_7$	372.1209	3.08	186.64	8.14	343.0812, 357.0969, 329.10206, 315.08634, 313.0707
115-53-7	Sinomenine	$C_{19}H_{23}NO_4$	329.1627	1.25	173.96	2.78	207.04413, 223.07513, 239.07017, 241.08629, 209.05944
32685-93-1	SipeiMine-3β-D-glucoside	$C_{33}H_{53}NO_8$	591.3771	–	271.68	4.32	574.3738, 412.32, 430.3315
83-95-4	Skimmianine	$C_{14}H_{13}NO_4$	259.0845	2.86	149.84	6.89	227.05758, 244.06036, 216.06555, 202.04948, 201.04212
80-78-4	Solasodine	$C_{27}H_{43}NO$	397.3345	7.1	203.64	6.28	380.33192, 382.31164, 327.28993, 98.0958, 253.1961
509-24-0	Songorine	$C_{22}H_{31}NO_3$	357.2304	0.71	178.46	2.82	340.22711, 322.21674, 296.14101, 294.18479, 306.18719
6160-12-9	Spartein	$C_{15}H_{38}N_2O_9S$	422.2298	–	154.11	2.09	98.0962, 190.15894
10048-13-2	Sterigmatocystin	$C_{18}H_{12}O_6$	324.0634	1.62	164.88	9.59	281.04424, 310.04699, 253.04943, 254.05582, 309.03933
3930-19-6	Streptonigrin	$C_{25}H_{22}N_4O_8$	506.1438	−0.43	224.12	8.69	461.14659, 489.1415, 446.12283, 431.09967, 429.11665
120-05-8	Sulfuretine	$C_{15}H_{10}O_5$	270.0528	1.98	159.62	5.36	253.04965, 161.02423, 147.04417, 149.02369, 163.03933
20501-56-8	Talatisamine	$C_{24}H_{39}NO_5$	421.5700	−0.5	194.88	3.91	390.26389, 358.23767, 372.25332, 340.22711, 326.21146
568-73-0	Tanshinone IIA	$C_{18}H_{12}O_3$	276.0786	4.443	153.8	11.64	221.09506, 206.07203
33069-62-4	Taxol	$C_{47}H_{51}NO_{14}$	853.3309	7.38	293.81	10.5	531.19937, 308.08969, 591.22003, 324.06401, 469.18367
6474-90-4	Teterahydroalstonine	$C_{21}H_{24}N_2O_3$	352.1787	2.88	182.95	5.49	144.08082, 222.11306, 143.07312, 321.15958, 178.08621
518-34-3	Tetrandrine	$C_{38}H_{42}N_2O_6$	622.3043	3.55	249.29	5.22	381.18117, 580.26809, 174.09124
77-59-8	Tomatidine	$C_{27}H_{45}NO_2$	415.3450	6.15	209.56	8.39	398.34217, 255.21097, 273.22177, 161.13267, 159.1175
33224-01-0	Trans-4-Cotininecarboxylic acid	$C_{11}H_{12}N_2O_3$	220.0848	−0.6	150.74	1.13	185.13289, 143.08513, 129.06869, 145.10081, 131.08528
302-79-4	tretinoin	$C_{20}H_{28}O_2$	300.2089	6.83	175.97	15.31	283.20691, 159.11708, 213.12697
38748-32-2	Triptolide	$C_{20}H_{24}O_6$	360.1570	0.2	185.87	6.17	255.10157, 229.08592
38647-11-9	Triptonide	$C_{20}H_{22}O_6$	358.1420	–	186.15	8.08	313.14344, 344.12544, 271.09649

Continued

74285-86-2	Triptophenolide	$C_{20}H_{24}O_3$	312.1730	4	181.67	10.32	225.12739, 253.12231, 267.17434, 271.13287, 185.09609
13220-57-0	Tryptanthrin	$C_{15}H_8N_2O_2$	248.0586	2.163	146.29	7.68	130.02892, 75.02269, 194.06005, 90.03379, 171.01851
69-33-0	Tubericidin	$C_{11}H_{14}N_4O_4$	266.1015	−0.12	158.03	0.55	135.06666, 118.04036, 117.05746, 177.07549, 119.06819
77-52-1	Ursolic acid	$C_{30}H_{48}O_3$	456.3604	9.01	212.77	15.03	439.35737, 203.18036, 189.16454, 191.18, 119.08614
50591-64-5	Vasicine	$C_{11}H_{12}N_2O$	188.0950	−0.997	138.72	1.94	171.09189, 154.06564, 118.06532, 144.0807, 143.07338
60-70-8	Veratramine	$C_{27}H_{39}NO_2$	409.2981	4.9	214.61	5.74	295.20596, 392.29529, 171.11721, 277.19536, 157.10148
71-62-5	Veratridine	$C_{36}H_{51}NO_{11}$	673.3462	3.48	271.28	6.43	492.29528, 456.2743, 603.31543, 162.1268, 354.18914
143-67-9	Vinblastine	$C_{46}H_{58}N_4O_9$	810.4203	4.18	290.32	6.86	751.40589, 542.30137, 793.41458, 749.38941, 524.28823
1617-90-9	Vincamine	$C_{21}H_{26}N_2O_3$	354.1943	3.1	181.02	4.99	337.19101, 294.14884, 280.13308, 308.1625, 264.10185
2068-78-2	Vincristine	$C_{46}H_{58}N_4O_{14}S$	922.3670	–	291.11	6.37	809.41158, 807.39511, 765.38615, 763.36812, 705.3636
2182-14-1	Vindoline	$C_{25}H_{32}N_2O_6$	456.2260	2.2	198.24	6.62	188.10739, 397.2129, 173.08371, 439.2234, 379.20264
71486-22-1	Vinorelbine	$C_{45}H_{54}N_4O_8$	778.3942	4.69	283.56	7.87	510.27632, 617.34985, 719.38262, 619.36171, 615.33479
42971-09-5	Vinpocetin	$C_{22}H_{26}N_2O_2$	350.1994	5.14	185.27	7.07	280.13307, 266.11736, 322.17775, 294.14866, 308.16447
82-57-5	Visnagin	$C_{13}H_{10}O_4$	230.0579	2.26	140.91	6.6	216.04211, 187.03947, 176.01077, 148.01579, 147.00811
3681-93-4	Vitexin	$C_{21}H_{20}O_{10}$	432.1057	1.28	196.35	3.97	313.07099, 283.06033, 415.10255, 397.092, 337.07125
524-12-9	Wedelolactone	$C_{16}H_{10}O_7$	314.0427	2.75	163.37	5.93	297.03944, 269.0449, 259.06024, 161.02375, 299.02005
37239-51-3	Wilfordine	$C_{43}H_{49}NO_{19}$	883.2900	1.2	284.97	10.06	856.30224, 866.28659, 838.29168, 674.24433, 176.07061
37239-47-7	Wilforgine	$C_{41}H_{47}NO_{19}$	857.2740	1.2	276.95	10.34	840.27094, 686.24433, 178.08626, 798.26038, 746.26546
11088-09-8	Wilforine	$C_{43}H_{49}NO_8$	867.2950	2.2	282.15	11.1	850.29168, 686.24433, 746.26546, 178.08626, 808.28111
84104-71-2	Wilforlide A	$C_{30}H_{46}O_3$	454.3450	6.9	209.31	14.97	437.3409, 201.1644
37239-48-8	Wilfortrine	$C_{41}H_{47}NO_{20}$	873.2690	0.3	281.6	9.28	846.2815, 856.26585, 828.27094, 674.24433, 176.07061
632-85-9	Wogonin	$C_{16}H_{12}O_5$	284.0685	2.14	158.16	8.44	270.0521, 241.04929, 252.04142, 269.0441, 168.00566

Continued

19545-26-7	Wortmannin	$C_{23}H_{24}O_8$	428.1471	0.81	193.08	7.44	266.14835, 143.07223, 283.09857, 268.07454, 247.09901
500-62-9	Yangonin	$C_{15}H_{14}O_4$	258.0892	1.75	159.63	8.82	231.10205, 216.07856, 171.08104, 199.07548, 161.06023
65-19-0	Yohimbine	$C_{21}H_{26}N_2O_3$	390.1710	–	186.8	4.62	144.08077, 212.12806, 143.07301, 224.12944, 321.15984
70578-24-4	Yunaconitine	$C_{35}H_{49}NO_{11}$	659.7640	0.61	250.81	7.77	600.31671, 568.29049, 550.27993, 536.26428, 582.30614
17924-92-4	Zearalenone	$C_{18}H_{22}O_5$	318.1467	3.83	172.87	9.27	301.14391, 185.05954, 189.05474, 187.07561, 203.07092
471-05-6	Zerumbone	$C_{15}H_{22}O$	218.1671	5.34	151.84	11.87	163.11234, 149.09644, 135.08088, 161.09631, 121.06486
18695-01-7	*α*-Apo-Oxytetracycline	$C_{22}H_{22}N_2O_8$	442.1376	−0.85	195.27	3.86	426.11856, 408.10867, 229.05008, 390.09912, 337.07011
20562-02-1	*α*-Solanine	$C_{45}H_{73}NO_{15}$	867.4980	5.67	345.59	6.28	398.34176, 380.33183, 473.35207
5289-74-7	*β*-Ecdysone	$C_{27}H_{44}O_7$	480.3087	−0.53	222.6	5.81	409.27407, 445.2965, 299.16476, 463.30461, 311.20223
4707-32-8	*β*-Lapachone	$C_{15}H_{14}O_3$	242.0943	2.82	149.95	8.9	159.04412, 187.03897, 183.04415, 225.09093, 105.03367

Table S2. The recoveries, LODs and LOQs for some plant toxins in honey and beverage.

Name	Beverage		Honey		LOQ μg/kg	LOD μg/kg
	25 μg/kg	100 μg/kg	25 μg/kg	100 μg/kg		
(−)-Cotinine	82.3	91.2	79.7	94.4	8	3
(−)-Nicotine	106.9	87.5	102.7	75.8	20	10
13-Dehydroxyindaconintine	91.0	93.8	88.1	99.8	1	0.2
9,10-Dihydrolysergol	79.9	85.4	79.6	87.0	8	3
Aconine	80.6	90.4	73.4	100.9	3	1
Aconitine	60.9	88.5	69.8	84.8	5	2
Anisodamine	101.9	96.2	86.4	97.3	15	6
Aristolactam I	85.6	84.1	78.8	89.3	10	5
Aristolone	93.1	93.3	94.4	87.9	2	0.5
Atropine	83.9	89.0	88.1	89.7	8	3
Benzoylaconine	87.4	92.0	101.6	93.4	1	0.2
Berbamine	95.4	101.3	76.8	88.6	20	10
Berberine	89.2	95.3	71.9	85.6	0.5	0.2
Bromocriptine	76.1	86.8	61.5	81.5	15	6
Bufalin	84.0	70.6	75.7	86.9	2	0.5
Bullatine A	77.8	88.7	73.5	91.2	10	5

Continued

Capsaicin	99.0	93.4	90.1	99.4	5	2
Cardamonin	86.7	85.1	83.5	80.2	5	2
Catharanthine	111.4	110.1	60.6	96.4	1	0.2
Celastrol	99.6	94.3	96.9	101.5	2	0.5
Chelidonine	83.6	92.9	87.7	99.4	2	0.5
Cinobufagin	73.4	90.7	85.7	92.7	3	1
Colchicine	82.1	85.9	66.6	88.5	5	2
Corydaline	103.9	94.5	84.4	97.2	2	0.5
Corynoxeine	86.9	81.6	84.0	86.2	2	0.5
Crassicauline A	87.9	100.1	68.4	83.5	0.5	0.1
Crotaline	83.5	87.8	85.7	95.4	15	6
Dehydroevodiamine	101.6	80.0	103.9	82.6	1	0.2
Delsoline	78.1	98.8	63.7	94.2	3	1
Deltaline	89.1	98.4	114.4	97.3	1	0.2
Dictamnine	88.0	92.5	93.8	79.3	1	0.2
Dihydroberberine	119.7	76.9	87.4	96.6	1	0.2
Dihydrocapsaicin	100.6	95.2	101.4	98.8	5	2
Dihydroergocristine	79.4	84.5	74.6	95.1	5	2
Dihydrokavain	97.1	93.1	90.8	91.7	5	2
Dihydrolycorine	90.8	90.6	72.2	105.7	15	6
Echimidine	83.5	97.5	80.1	110.3	8	3
Fuziline	73.0	95.5	74.5	92.8	5	2
Gelsemine	77.4	85.7	76.0	87.3	8	3
Hypaconine	76.7	92.9	80.7	99.3	3	1
Hypaconitine	81.7	92.8	79.6	98.5	2	0.5
Indaconitine	120.0	110.4	118.6	92.7	1	0.2
Isoscopoletin	86.9	89.6	77.8	96.8	15	6
Karacoline	82.3	93.0	80.0	90.3	8	3
Lappaconitine	77.8	93.8	67.0	89.4	3	1
Lycopsamine	85.4	87.4	71.9	87.9	15	6
Lysergol	80.6	92.0	78.6	96.3	10	5
Mesaconine	83.1	90.3	73.0	99.1	5	2
Mesaconitine	103.4	93.8	76.9	104.5	2	0.5
Methylergonovine	92.7	87.3	84.9	79.6	8	3
Neoline	75.8	84.5	74.2	95.1	5	2

Continued

Nuciferine	83.7	93.9	93.6	99.5	3	1
Papaverine	82.5	79.1	104.7	89.9	1	0.2
Pilocarpine	112.3	83.9	90.3	95.3	20	10
Retrosine	90.3	86.7	80.3	87.6	10	5
Senecionine	82.8	90.8	70.9	96.5	8	3
Seneciphylline	88.6	91.5	82.3	99.9	8	3
Senkirkine	90.1	72.3	80.6	87.4	5	2
Sinomenine	81.9	87.0	69.3	79.8	15	6
SipeiMine-3β-D-glucoside	88.4	72.5	89.2	80.1	8	3
Skimmianine	83.1	92.9	83.1	89.9	0.5	0.1
Solasodine	92.0	89.4	85.2	109.4	3	1
Songorine	78.4	92.1	74.2	90.0	8	3
Talatisamine	88.5	91.8	79.9	89.7	10	5
Tetrandrine	91.8	89.4	65.4	85.9	0.5	0.1
Tomatidine	86.2	98.0	120.1	114.6	10	5
Triptolide	77.2	90.1	72.0	97.5	10	5
Triptonide	87.9	90.0	74.2	89.3	8	3
Triptophenolide	89.2	92.7	83.9	98.6	20	10
Veratridine	101.4	98.0	73.0	99.5	5	2
Vincamine	82.9	94.4	83.0	89.6	2	0.5
Vindoline	86.3	94.7	84.0	108.5	1	0.2
Vinorelbine	87.4	92.7	70.8	93.9	20	10
Vinpocetine	82.1	94.8	98.1	89.5	3	1
Wilfordine	83.1	92.1	74.7	90.1	5	2
Wilforgine	84.9	93.2	97.4	113.2	2	0.5
Wilforine	86.4	98.5	85.2	100.7	1	0.2
Wilfortrine	85.7	93.3	77.8	89.7	3	1
Yunaconitine	87.6	69.2	88.0	89.8	1	0.2
α-Solanine	85.2	93.3	92.0	97.8	3	1