Electronic Supplementary Information

Development of a handheld liquid extraction pen for on-site mass spectrometric analysis of daily goods

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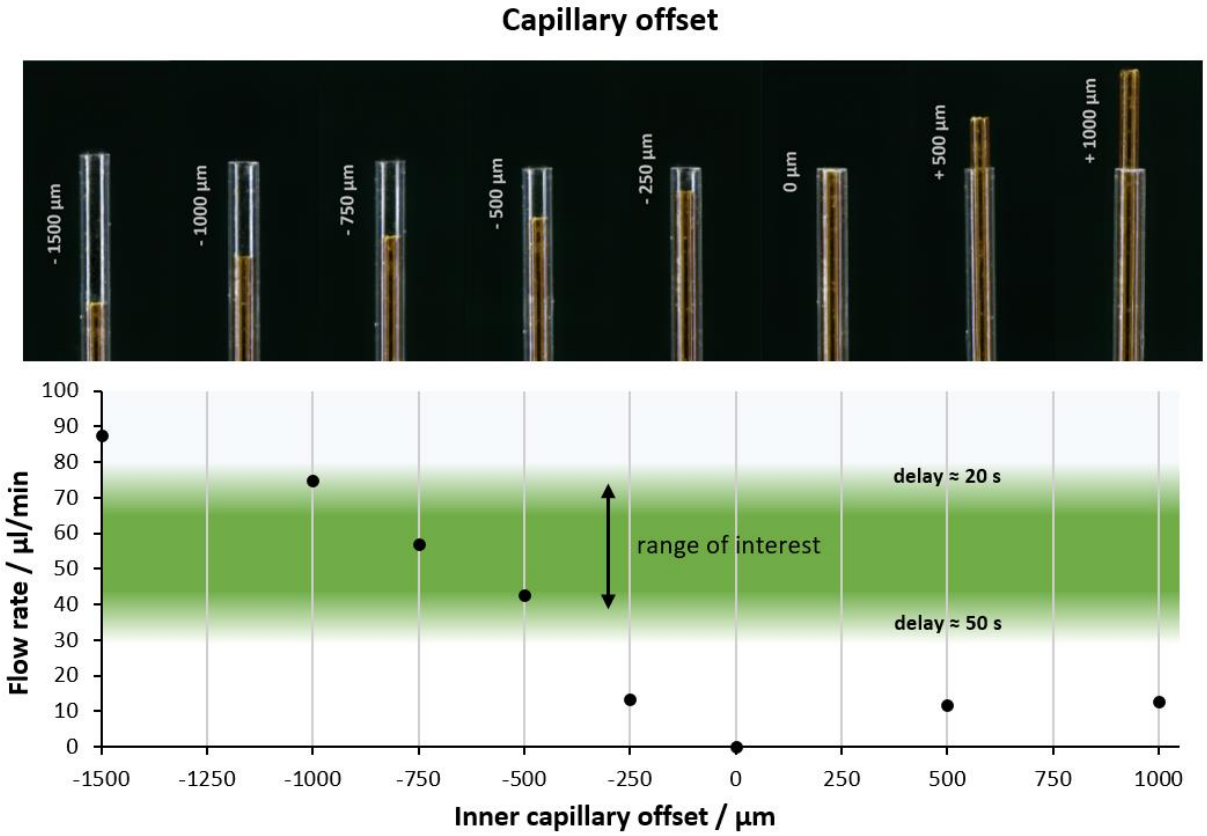
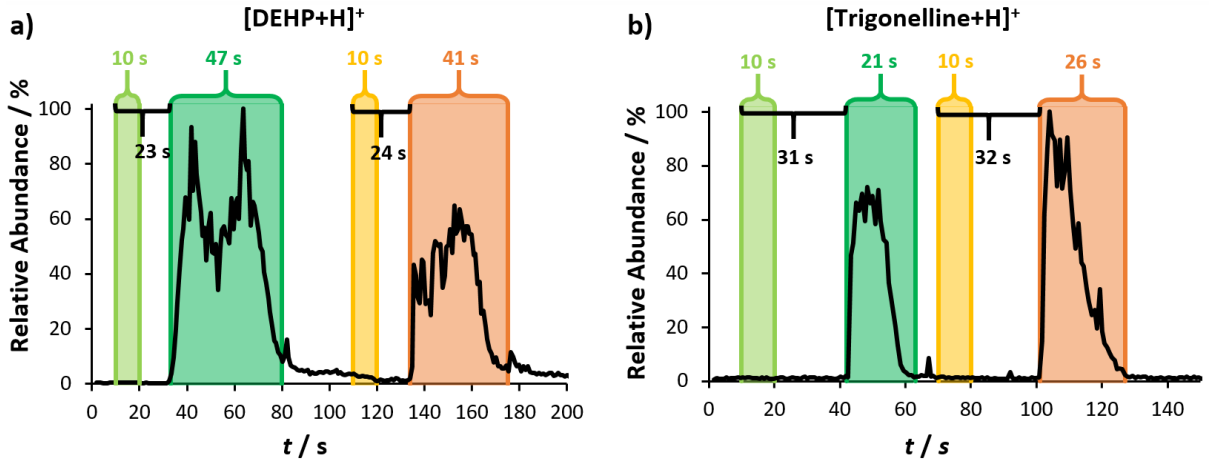
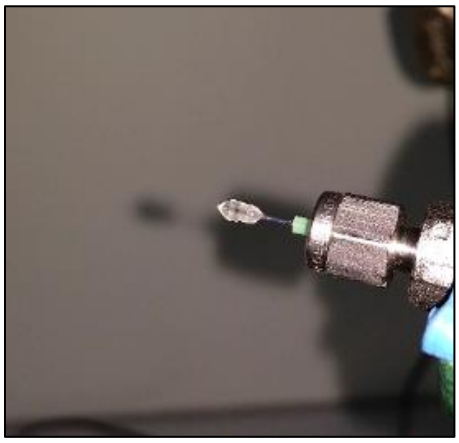


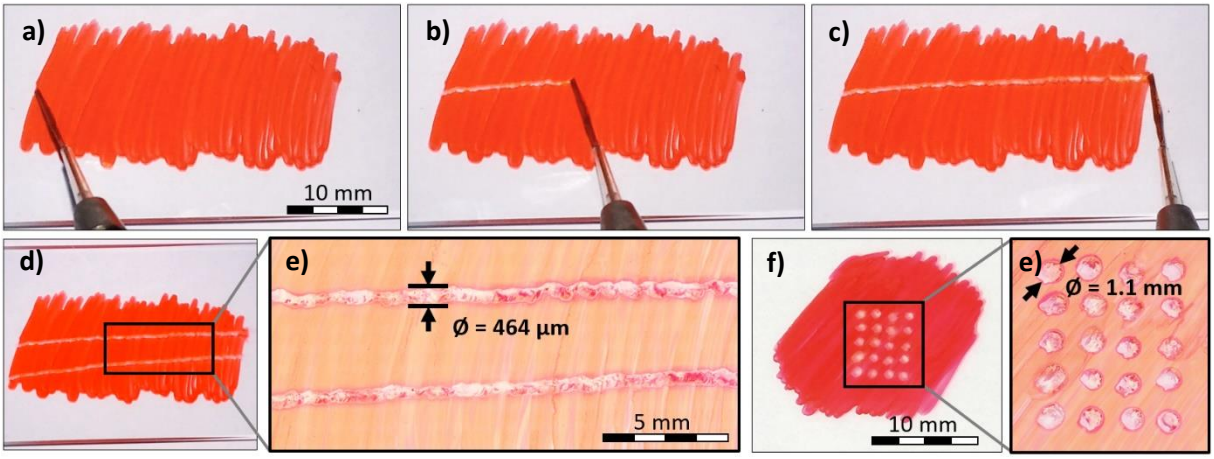
Supporting Figure 1. Influence of the spray capillary offset to the gas capillary within the ESI sprayer on the flow rate induced in the secondary capillary of the LEP, shown for a 9:1 acetonitrile:water mixture (for better visualization, an outer capillary without a droplet-preventing coating is shown).



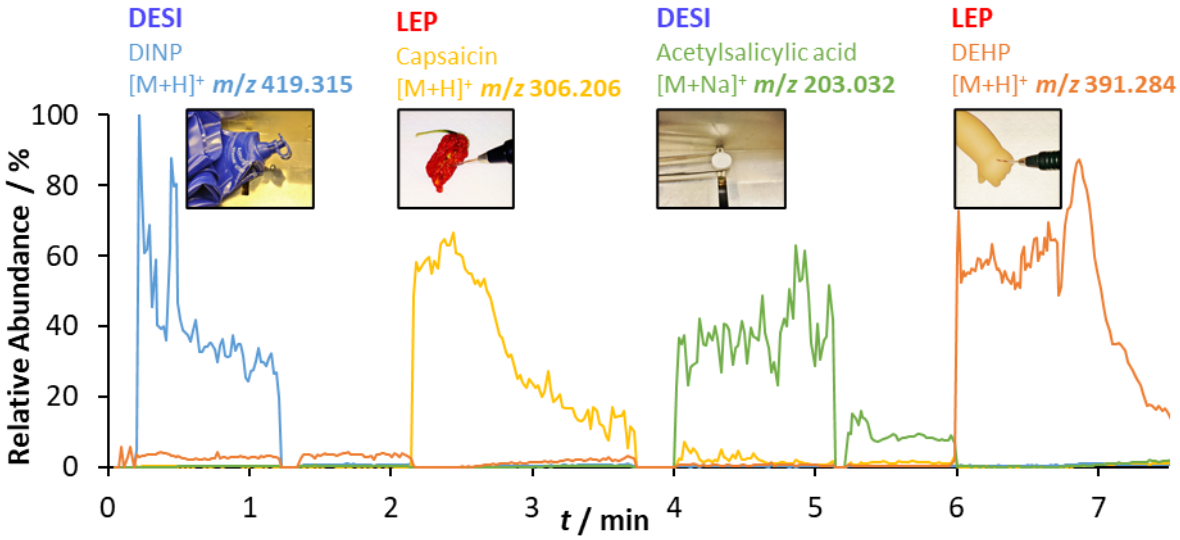
Supporting figure 2. a) Two consecutive measurements from a toy puppet (plasticizer: DEHP), using the optimized LEP setup described in the article. Methanol/water 9:1 was used as solvent with a flow rate of 40 µL/min. Shown is the signal intensity of the protonated DEHP ion after two 10 s measurement intervals. The DEHP signal appeared with a delay of 23 s and 24 s after the LEP contacted the sample and lasted for about 45 s. Therefore, it is recommended to flush the LEP for at least 30 seconds after each sample measurement. b) Two measurements from a roasted Arabica coffee bean (analyte: Trigonelline) with a reduced solvent flow rate of about 30 µL/min, resulting in an increased delay time. Compared to the plasticizer, the carry-over of Trigonelline was less pronounced.



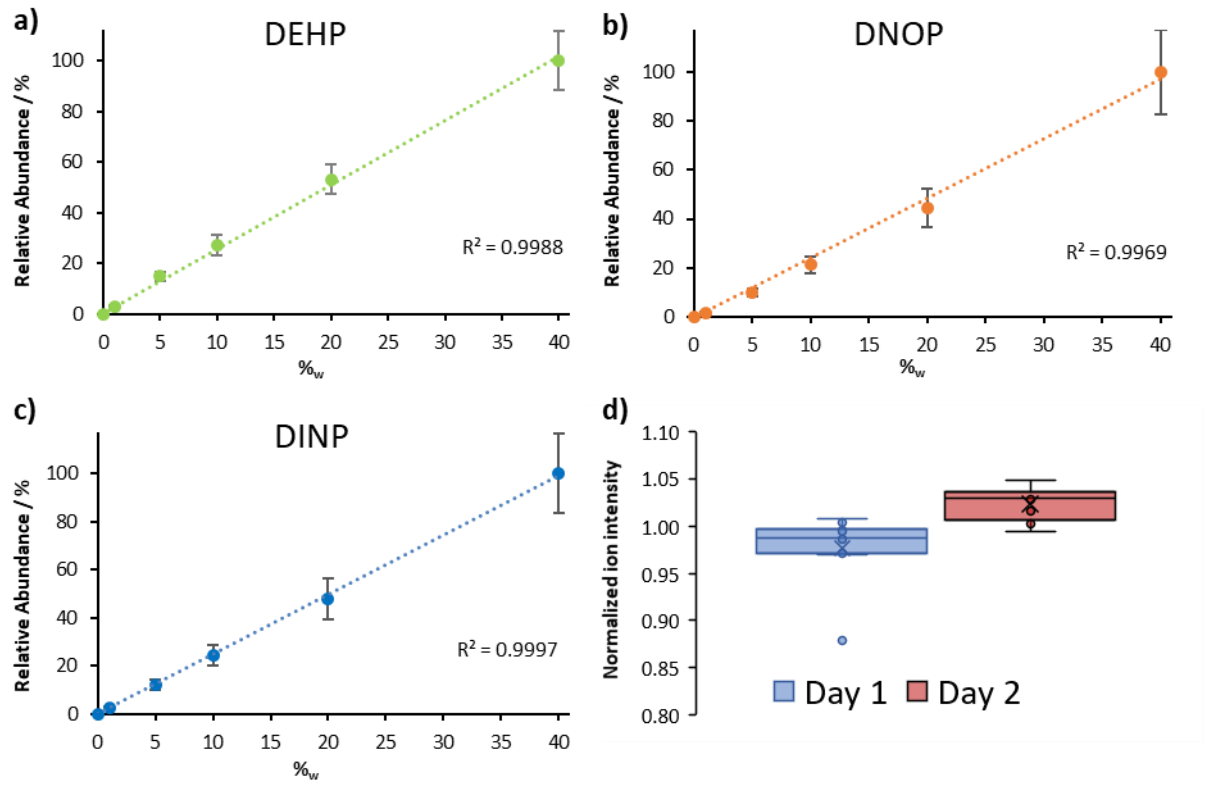
Supporting Figure 3. ESI sprayer tip: Gas capillary covered with thermoplastic polymer coating to prevent droplet formation.



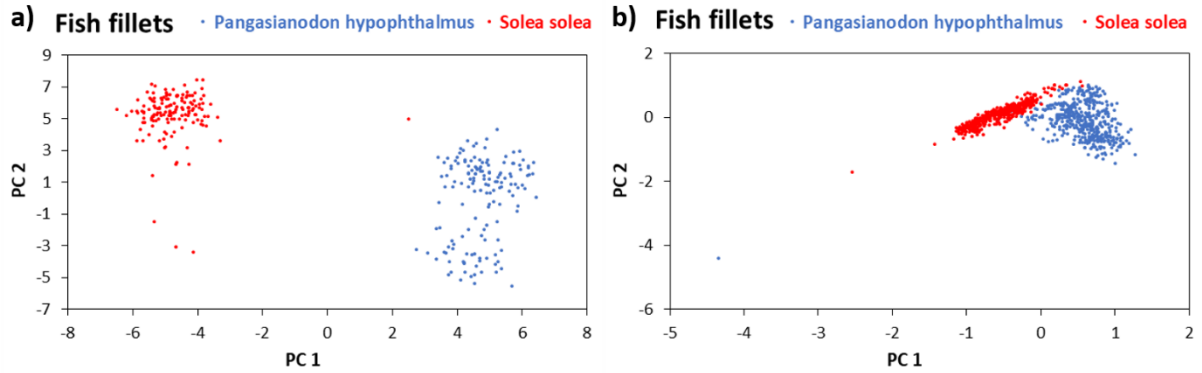
Supporting Figure 4. Visualized analyte consumption from a glass slide, covered with Rhodamine 6G. a)-c) Procedure of a manual LEP measurement. d) Sample after two line scans. e) Magnification of the line scans with averaged line width (n=40). f) Twenty spots measured from a glass slide. e) Magnification of the extraction spots with averaged spot diameter (n=40). MeOH/H_2O 9:1 was used as solvent with a flow rate in the range of 30-50 µl/min.



Supporting Figure 5. Fast switching between DESI and LEP demonstrates high-throughput capability, even in case of high sample diversity. The first sample was a beach ball, containing the plasticizer DINP, the second sample was a dried chili pepper *'Carolina Reaper',* containing Capsaicin, the third sample was a drug pill, containing acetylsalicylic acid and the fourth sample was a toy puppet, containing the plasticizer DEHP. MeOH/H_2O 9:1 was used as solvent with a flow rate in the range of 30-50 µl/min. For both modes, the same solvent flow and sprayer position were used. During DESI, the pen was placed on a clean glass slide, allowing the solvent to travel from the primary capillary to the secondary capillary without any contamination. The ESI sprayer was placed in a 60° angle and 1 cm distance relative to the mass spectrometer inlet capillary. Respective samples were placed on the sample table to allow analyte desorption. During LEP measurements the LEP was placed on the sample surface. A clean glass slide was placed on the sample table to direct the solvent/analyte plume towards the inlet capillary as it is done by the sample surface during DESI.

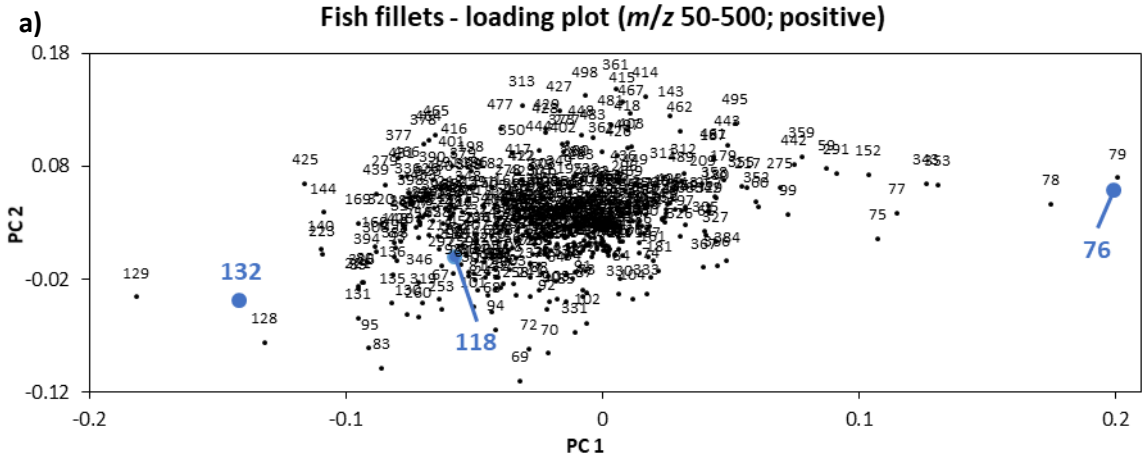


Supporting Figure 6. Quantitative analysis of phthalates from plastisol pills using the autarkic and portable LEP source, attached to an orbital-trapping mass spectrometer. Calibration curves were obtained for a) DEHP, b) DNOP and c) DINP. Data points represent averages of three replicates. Error bars indicate standard deviations. d) Intra-day (day 1 n=10, day 2 n=10) and inter-day reproducibility of signal intensities obtained from 20 $\%_w$ DNOP plastisol pill. Ion signals were normalized to the mean of both measurement days. In this case, a mixture of ACN/H_2O 9:1 with 0.1 % formic acid and additionally 7 mmol/L ammonium acetate was used. Ammonium acetate was added to suppress the formation of sodium and potassium adducts which were dominant for some real plasticizer samples in high-resolution measurements (shown in article figure 2 c)).

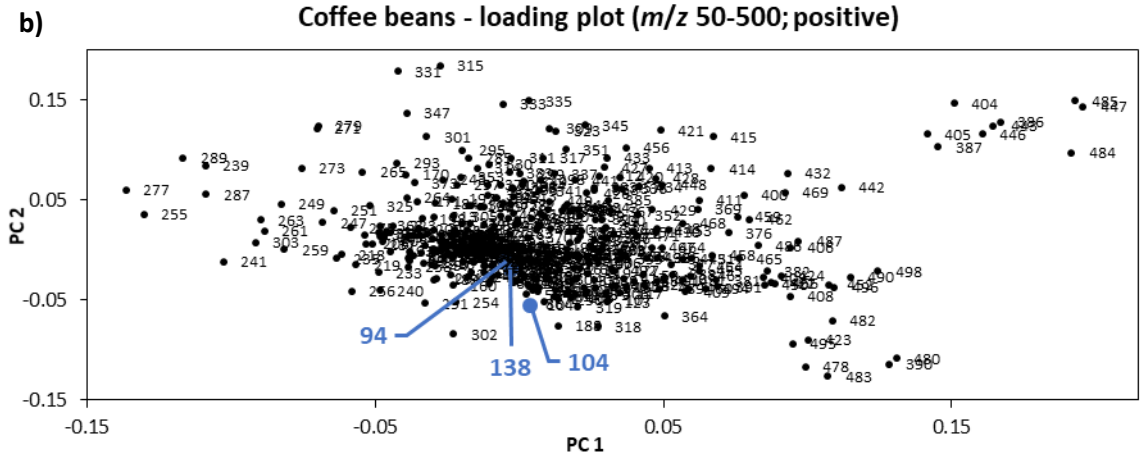


Supporting Figure 7. a) PCA score plots for the analyses of fish in negative-ion mode (*m/z* 50-500) and b) high mass range (*m/z* 700-900) in positive-ion mode. Cross validation of the PCA models via the leave-10 %-out method showed 100 % correct classification of the fish spectra to their species, using the LDA (linear discriminant analysis) coefficient as classifier.

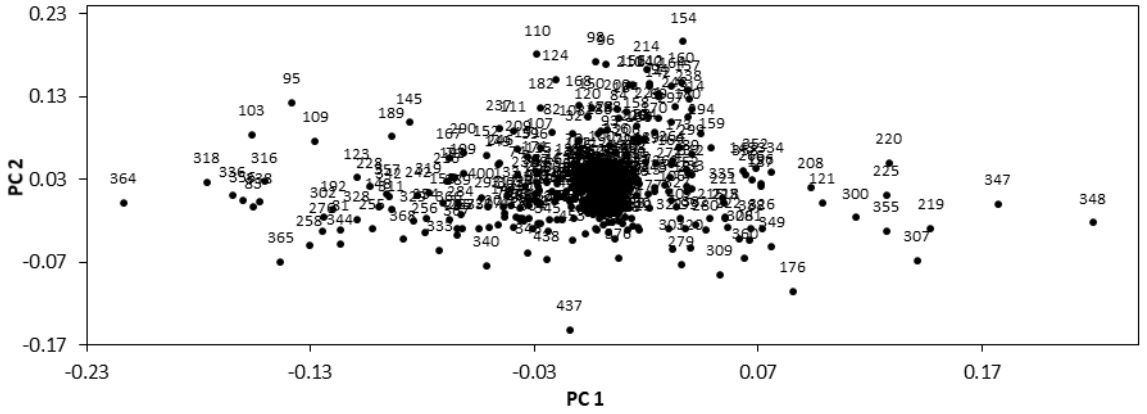
a)

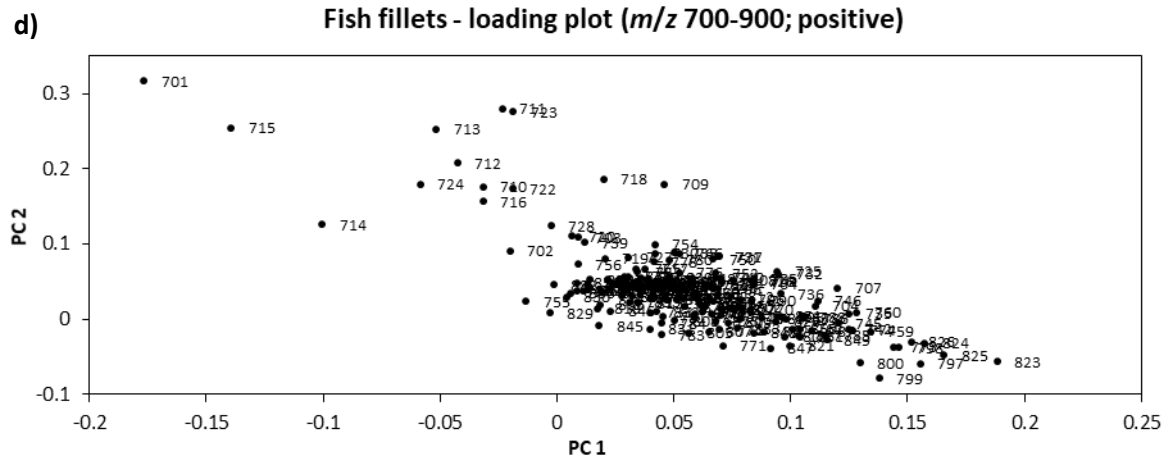

Fish fillets - loading plot (m/z 50-500; positive)
PC 2
PC 1
0.18
0.08
-0.02
-0.12
-0.2
-0.1
0
0.1
0.2
132
118
76

b)

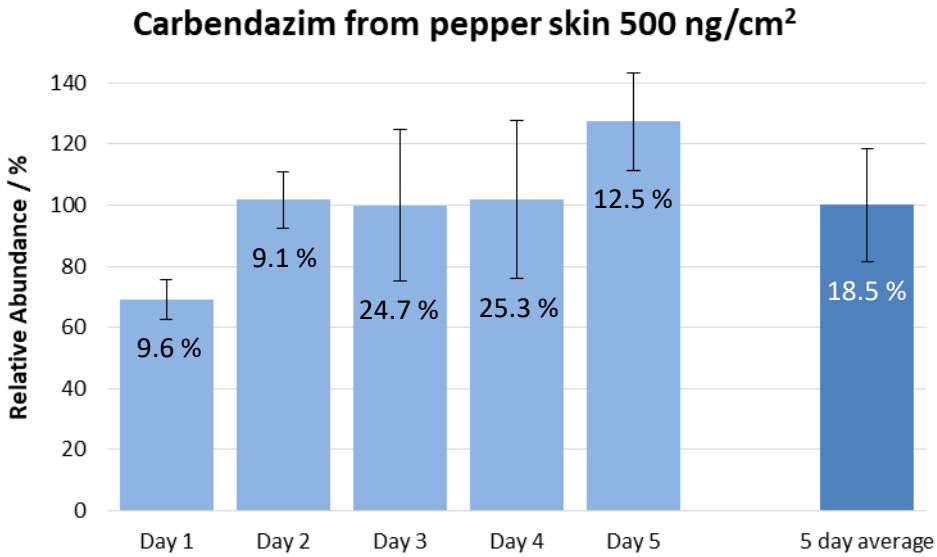

Coffee beans - loading plot (m/z 50-500; positive)
PC 2
PC 1
0.15
0.05
-0.05
-0.15
-0.15
-0.05
0.05
0.15
94
138
104

c)


Fish fillets - loading plot (m/z 50-500; negative)
PC 2
PC 1
0.23
0.13
0.03
-0.07
-0.17
-0.23
-0.13
-0.03
0.07
0.17



Supporting Figure 8. a) loading plot for the analyses of fish in positive-ion mode (*m/z* 50-500) with tentatively identified markers (see section `list of mass spectra´ for further details). b) loading plot for the analyses of coffee in positive-ion mode (*m/z* 50-500) and tentatively identified markers (see section `list of mass spectra´ for further details). c) loading plot for the analyses of fish in negative-ion mode (*m/z* 50-500 and d) loading plot for the analyses of fish in the high mass range (*m/z* 700-9000) in positive-ion mode. Numbers given in the loading plot correspond to the low end of the mass bin (e. g. 76 for the mass bin 76-77).



Supporting Figure 9. Carbendazim measured from pepper peel (c = 500 ng/cm²). Shown are deviations of five technical replicates measured per day on five consecutive days. Given numbers are the relative standard deviation for each day and the five-day average.

Supporting Table 1. Further information on the biological samples.

Sample	Cultivation area	Name	Retailer
Arabica (Coffee)	Kerala (India)	Indien Monsooned Malabar	Docklands Coffee
		Indien Monsooned Malabar	Mondo del Caffè
		Indien Monsooned Malabar	Schwarzwild
	Karnataka (India)	India Plantation	Fortezza
		Little Flower	19grams
		Bab Budan Giri	Roesttrommel
Robusta (Coffee)	Kerala (India)	Indien Cherry Robusta	Müller Kaffeerösterei
		Wayanad Espresso	Carles KaffeeRösterei
		Indien Monsooned Robusta	Docklands Coffee
	Karnataka (India)	Indien Perlbohne	Mondo del Caffè
		Indian Palthope Estate	Schwarzwild
		Höllentäler	Schwarzwild
Chili pepper	Central Germany (home grown)	Capsicum chinense *Carolina Reaper*	Chili Food (Seeds)
Sweet pepper	N/A	Capsicum annuum Yellow sweet pepper	Local supermarket Vegetable counter
Common sole (Fish)	North Atlantic Ocean (wild caught)	Solea Solea	World of Seafood Haak & Christ
Iridescent shark (Fish)	N/A	Pangasianodon hypophthalmus	Local wholesale Fish counter

Supporting Table 2. Comparison of quantitative data from LEP-MS and confirmatory methods.

SAMPLE	PLASTICIZER	CONFIRMED AMOUNT [%w]	FOUND WITH LEP-MS [%w]	REL. DEVIATION [%]
BAT (TOY)	DEHP	5.8[a]	8.6 ± 2.7	+ 47.9
CARNIVAL MASK	DEHP	2.7[b]	2.4 ± 1.2	- 10.7
TABLE MAT	DEHP	17.5[b]	16.8 ± 6.9	- 4.0
TOY PUPPET	DEHP	25.9[a]	26.1 ± 6.6	+ 0.8
STETHOSCOPE (TOY)	DEHP	31.0[b]	26.9 ± 1.2	- 13.4
CATERING GLOVE	DNOP	6.2[b]	5.8 ± 1.4	- 6.4
CARNIVAL MASK	DIBP	21.0[b]	21.3 ± 8.8	+ 1.4

Confirmed data obtained from the [a] Bavarian State Laboratory for Health and Food safety (Erlangen, Germany) (Quantification and Identification via HPLC-DAD) and the [b] State Laboratory of Rhineland-Palatinate (Koblenz, Germany) (Quantification via GC-FID, identification via GC-MS).

Capillary clogging and flushing

The sensitive equilibrium of solvent outflow and intake at the sampling tip of the LEP is a valuable indication for different types of possible malfunctions. The solvent delivery capillary (primary capillary) allows for constant solvent output onto the sample surface adjusted by the pressure above the solvent reservoir. The solvent intake through the secondary capillary can be controlled by the axial position of the spray capillary in the gas capillary of the ESI source. The pump capacity of each system is in a range, defined by the dimensions of the capillary system, supporting gas flow, pressure regulator sensitivity and solvent characteristics. A high pressure onto the solvent reservoir leads to a high flow rate whereas a low pressure gives a low flow rate.

If interruptions in the ESI spray or bubbles are observed in the secondary capillary, the solvent intake exceeds the solvent outflow. To recover the solvent flow equilibrium, a relocation of the spray capillary (see Supporting Figure 1) or a pressure increase on the reservoir is advised. If no improvement is obtained, the reservoir might be empty.

A visible droplet on the sample surface indicates, that the solvent outflow exceeds the solvent intake. In this case it is advised to reduce the pressure on the solvent reservoir, or the spray capillary must be moved to increase the solvent intake.

If insoluble particles enter the secondary capillary, they might reduce the solvent flow rate or completely cut it off. Such clogging was observed twice.

1. A slowly decreasing solvent intake by the secondary capillary over several minutes, inducing consecutive adjustments with the pressure regulator towards lower solvent outflow.
2. A sudden and complete clogging of the secondary capillary together with a quick development of a solvent droplet on the sample surface.

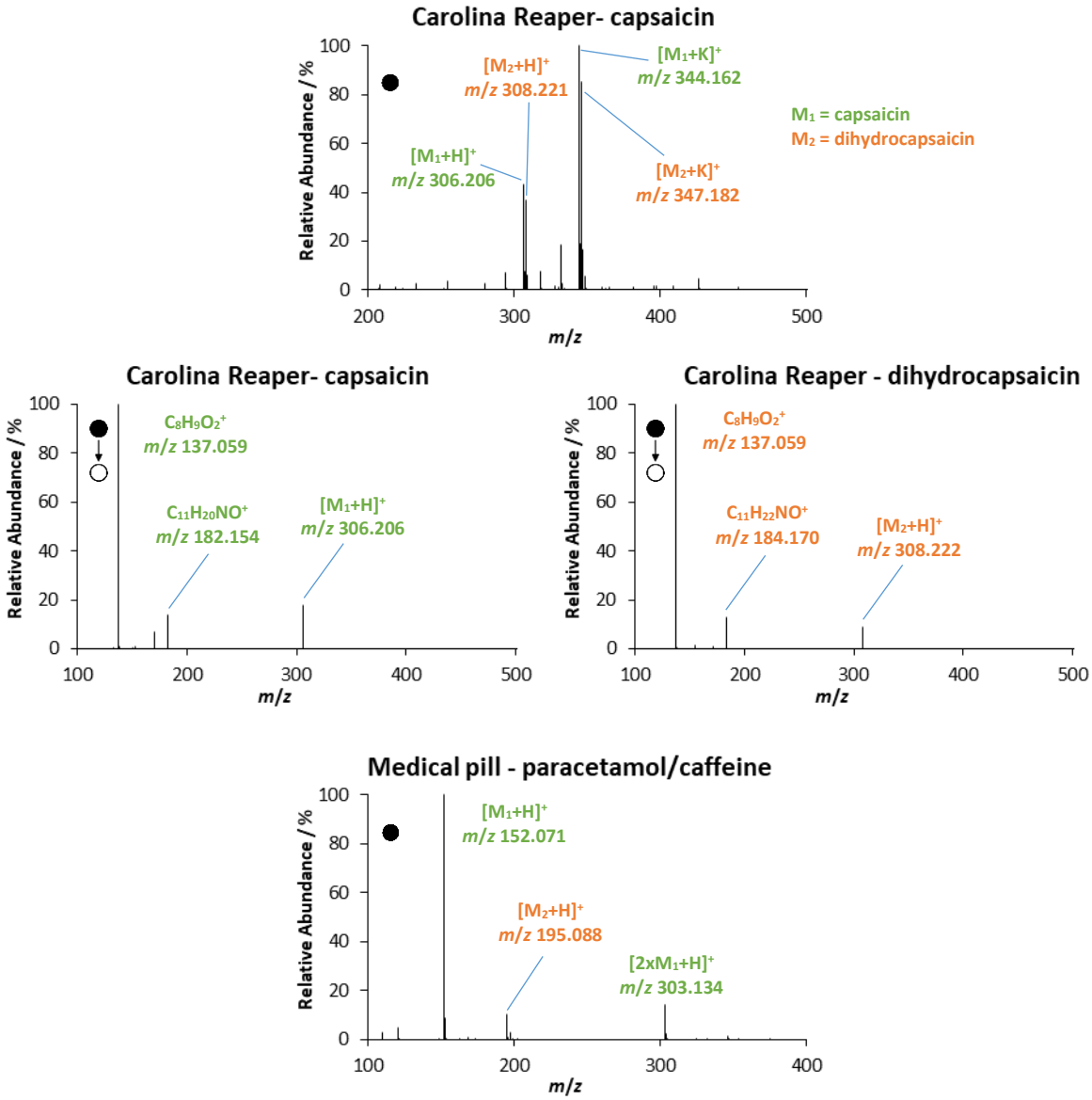
Both cases demand manual flushing of the secondary and spray capillary by the operator. Flushing procedure can be performed through the connection between those two capillaries, the high voltage connector. For that, the end of the connector which holds the secondary capillary in its sleeve must be unscrewed. An external fitting holding a sleeve that fits to a syringe cannula is then screwed into the high-voltage connector. Regular sub-milliliter syringes can be used to flush the high-voltage connector and the spray capillary. Then the connector end of the secondary capillary is placed back into the high-voltage connector. To flush the secondary capillary, the spray capillary end must be removed from the high-voltage connector. This way the high-voltage connector is flushed in both directions.

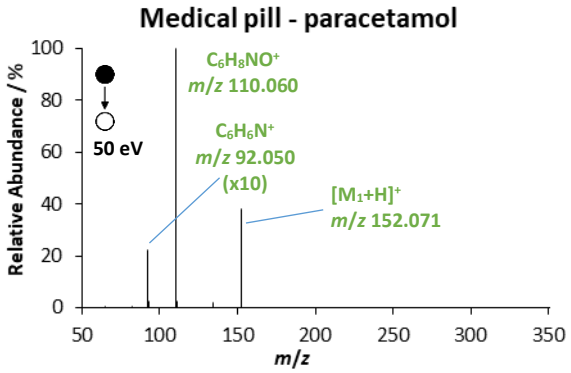
To reduce the risk of clogging, it is advised to perform measurements from particle-free samples. Furthermore, the operator should pull but not push the pen along a sample surface. This means, if the pen tip directs to the left, the movement should be forced to the right. This prevents digging into soft sample surfaces and reduces excessive stress on the sampling tip.

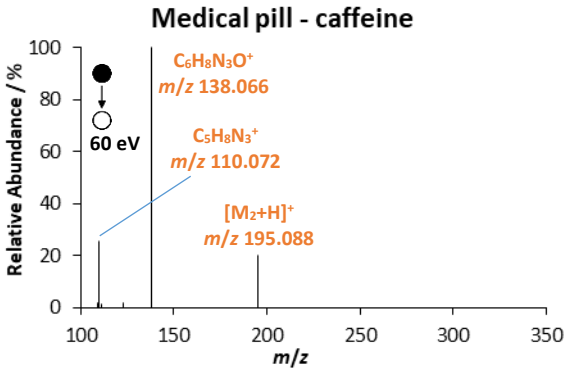
List of mass spectra

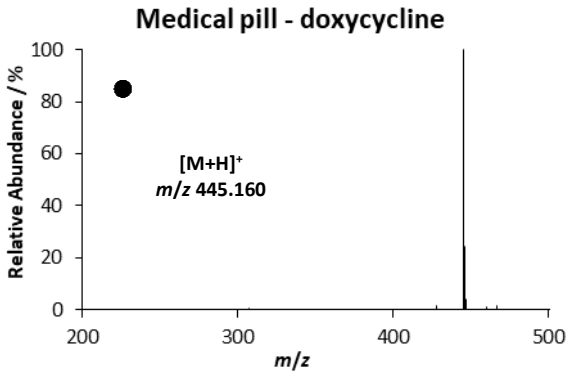
The following mass spectra were collected from real sample objects which were analyzed in a qualitative and/or semi-quantitative way. Shown are the mass spectra of the precursor ions of the found analytes and the corresponding fragment spectra observed via HCD. A HCD energy of 10 eV was used unless stated differently in the spectra. Sodium and potassium adducts are often present, but differ in relative intensity caused by different salt concentrations of the individual sample. For reasons of clarity the salt adducts were not tagged in all shown spectra. Some fragment signals with low relative

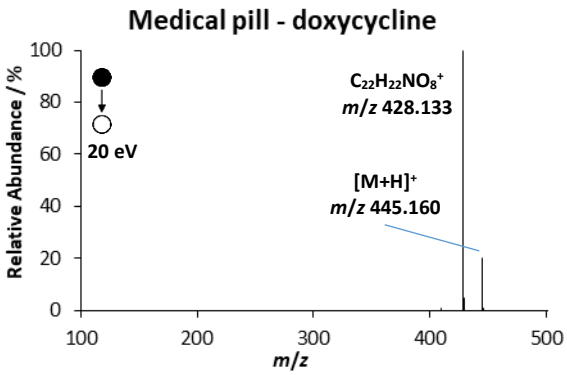
abundances were amplified as annotated. Precursor ion spectra were measured with an *Exactive* orbital trapping mass spectrometer (Thermo Fisher Scientific GmbH, Bremen, Germany). All fragmentation experiments were performed with a *Q Exactive HF-X* orbital trapping mass spectrometer (Thermo Fisher Scientific GmbH, Bremen, Germany). For both instruments, the inlet temperature was set to 250 °C and the injection time was limited to 500 ms. Mass resolutions of 100.000 (*Exactive*) and 240.000 (*Q Exactive HF-X*) were used. For all fragmentation experiments, the mass isolation window was set to Δ (*m/z*) ± 0.5 relative to the individual precursor ion. Structures of the indicated precursor and fragment ions can be found in the `list of fragments and expected structures´, following this section.

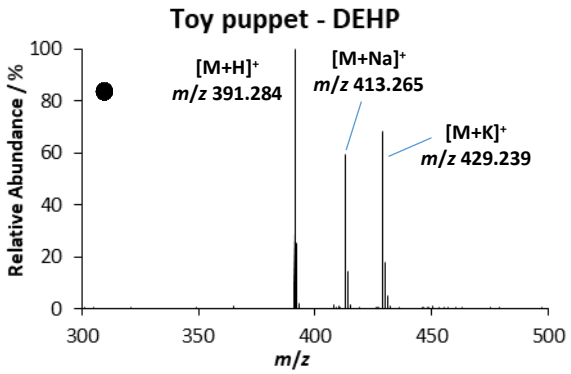


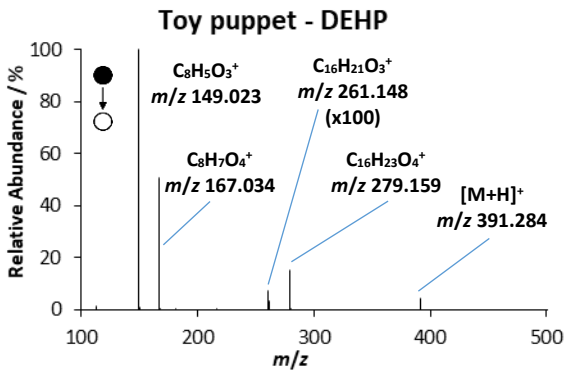

Medical pill - paracetamol
Relative Abundance / %
m/z
50 eV
C6H8NO+
m/z 110.060
C6H6N+
m/z 92.050
(x10)
[M1+H]+
m/z 152.071

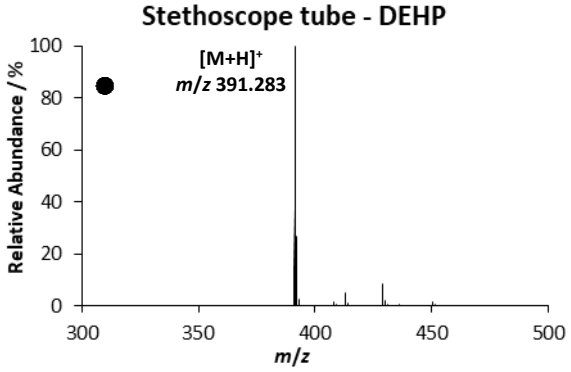

Medical pill - caffeine
Relative Abundance / %
m/z
60 eV
C6H8N3O+
m/z 138.066
C5H8N3+
m/z 110.072
[M2+H]+
m/z 195.088

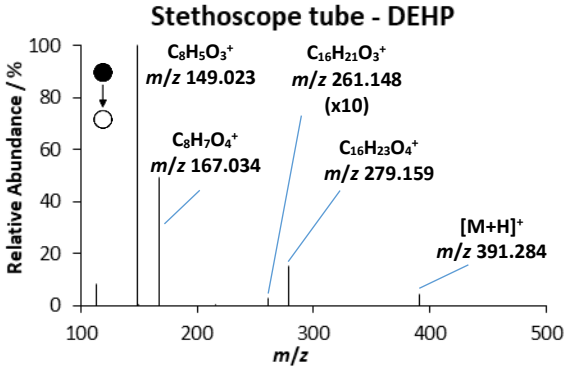

Medical pill - doxycycline
Relative Abundance / %
m/z
[M+H]+
m/z 445.160

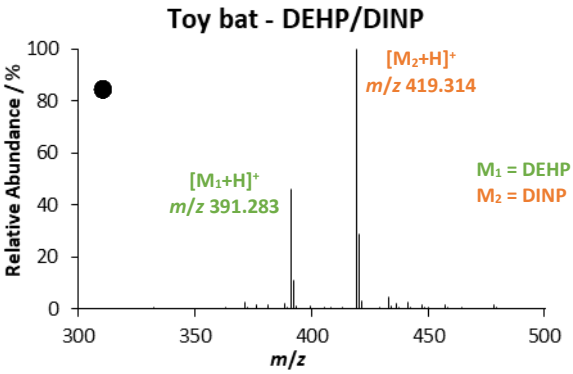

Medical pill - doxycycline
Relative Abundance / %
m/z
20 eV
C22H22NO8+
m/z 428.133
[M+H]+
m/z 445.160

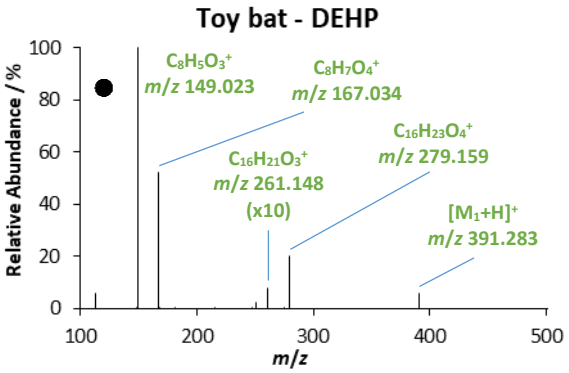

Toy puppet - DEHP
Relative Abundance / %
m/z
[M+H]+
m/z 391.284
[M+Na]+
m/z 413.265
[M+K]+
m/z 429.239

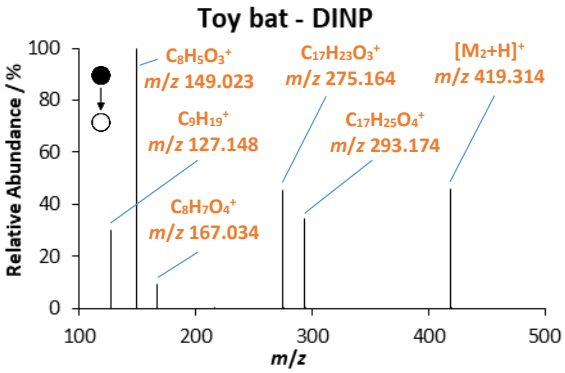

Toy puppet - DEHP
Relative Abundance / %
m/z
C8H5O3+
m/z 149.023
C16H21O3+
m/z 261.148
(x100)
C8H7O4+
m/z 167.034
C16H23O4+
m/z 279.159
[M+H]+
m/z 391.284


Stethoscope tube - DEHP
Relative Abundance / %
m/z
[M+H]+
m/z 391.283


Stethoscope tube - DEHP
Relative Abundance / %
m/z
C8H5O3+
m/z 149.023
C16H21O3+
m/z 261.148
(x10)
C8H7O4+
m/z 167.034
C16H23O4+
m/z 279.159
[M+H]+
m/z 391.284


Toy bat - DEHP/DINP
Relative Abundance / %
m/z
[M₂+H]⁺
m/z 419.314
[M₁+H]⁺
m/z 391.283
M₁ = DEHP
M₂ = DINP


Toy bat - DEHP
Relative Abundance / %
m/z
C8H5O3+ m/z 149.023
C8H7O4+ m/z 167.034
C16H21O3+ m/z 261.148 (x10)
C16H23O4+ m/z 279.159
[M1+H]+ m/z 391.283


Toy bat - DINP
Relative Abundance / %
m/z
C8H5O3+ m/z 149.023
C17H23O3+ m/z 275.164
[M2+H]+ m/z 419.314
C9H19+ m/z 127.148
C17H25O4+ m/z 293.174
C8H7O4+ m/z 167.034

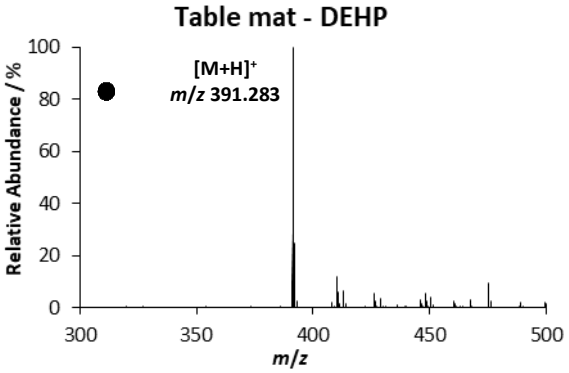


Table mat - DEHP
Relative Abundance / %
m/z
[M+H]+ m/z 391.283

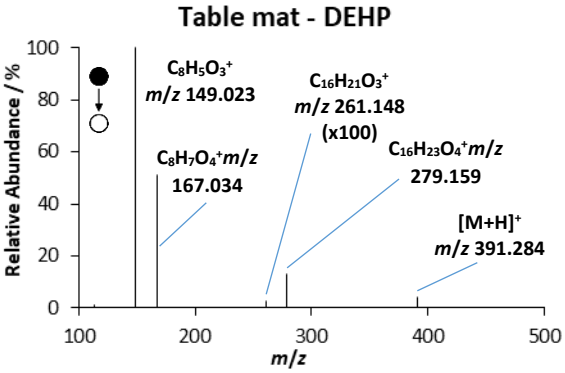
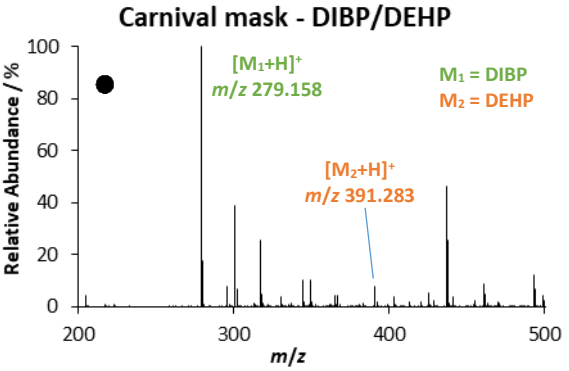
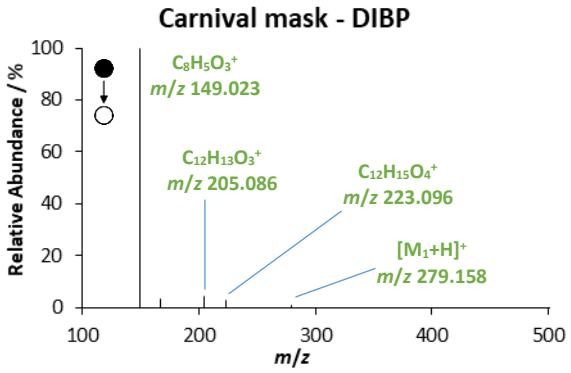
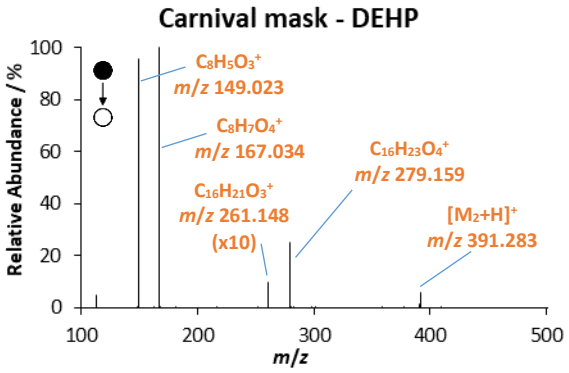
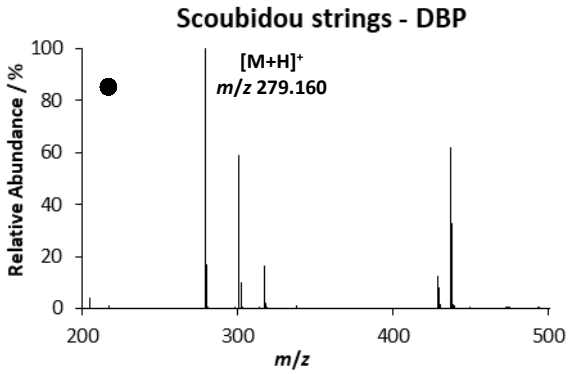


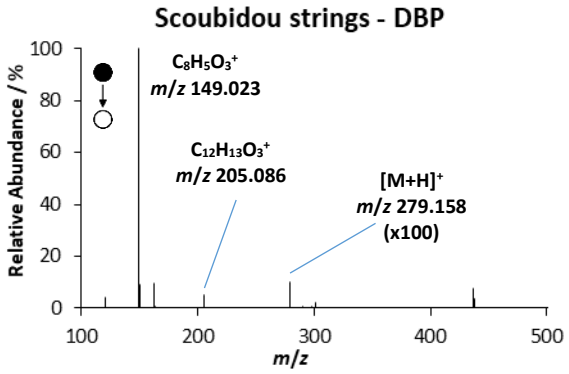
Table mat - DEHP
Relative Abundance / %
m/z
C8H5O3+ m/z 149.023
C16H21O3+ m/z 261.148 (x100)
C8H7O4+ m/z 167.034
C16H23O4+ m/z 279.159
[M+H]+ m/z 391.284

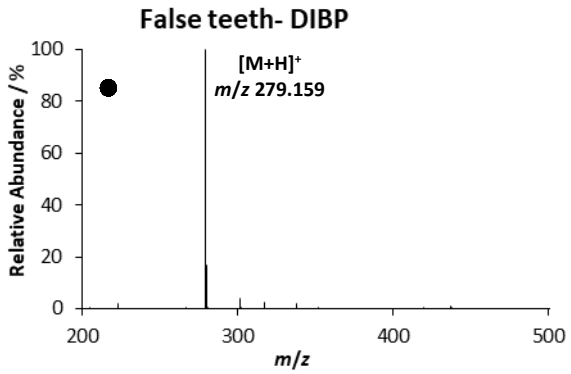

Carnival mask - DIBP/DEHP
Relative Abundance / %
m/z
[M1+H]+ m/z 279.158
M1 = DIBP
M2 = DEHP
[M2+H]+ m/z 391.283

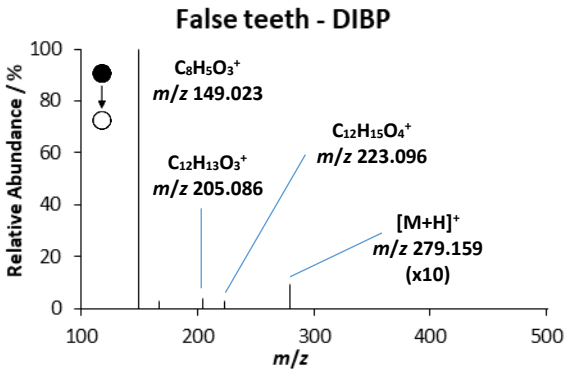

Carnival mask - DIBP
Relative Abundance / %
m/z
C8H5O3+ m/z 149.023
C12H13O3+ m/z 205.086
C12H15O4+ m/z 223.096
[M1+H]+ m/z 279.158

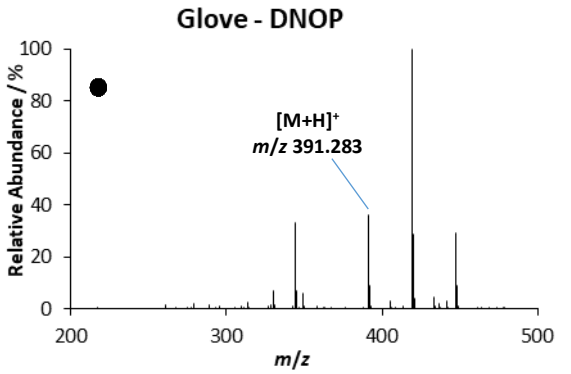

Carnival mask - DEHP
Relative Abundance / %
m/z
C8H5O3+ m/z 149.023
C8H7O4+ m/z 167.034
C16H23O4+ m/z 279.159
C16H21O3+ m/z 261.148 (x10)
[M2+H]+ m/z 391.283

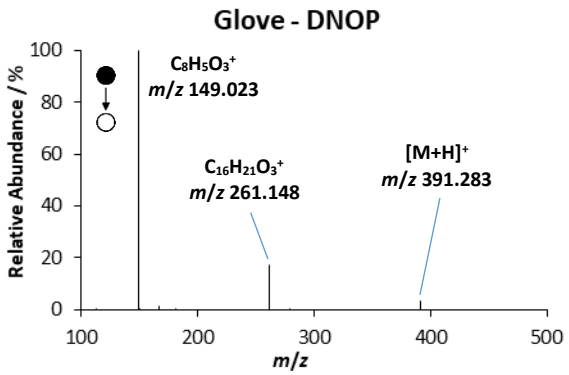

Scoubidou strings - DBP
Relative Abundance / %
m/z
[M+H]+ m/z 279.160

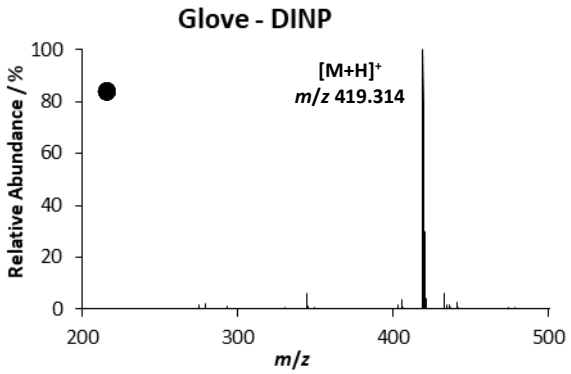

Scoubidou strings - DBP
Relative Abundance / %
m/z
C8H5O3+ m/z 149.023
C12H13O3+ m/z 205.086
[M+H]+ m/z 279.158 (x100)

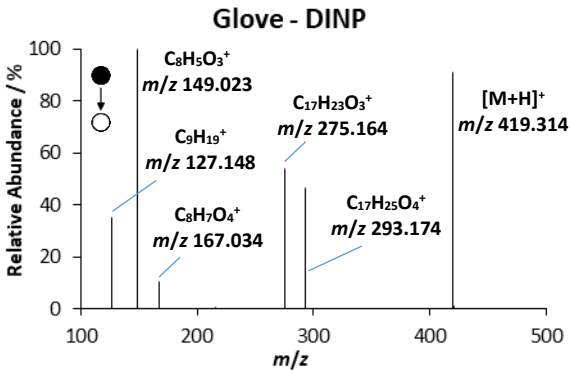

False teeth- DIBP
Relative Abundance / %
m/z
[M+H]+ m/z 279.159

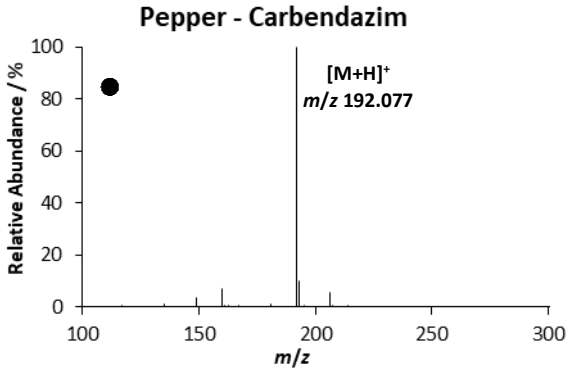

False teeth - DIBP
Relative Abundance / %
m/z
C8H5O3+ m/z 149.023
C12H13O3+ m/z 205.086
C12H15O4+ m/z 223.096
[M+H]+ m/z 279.159 (x10)

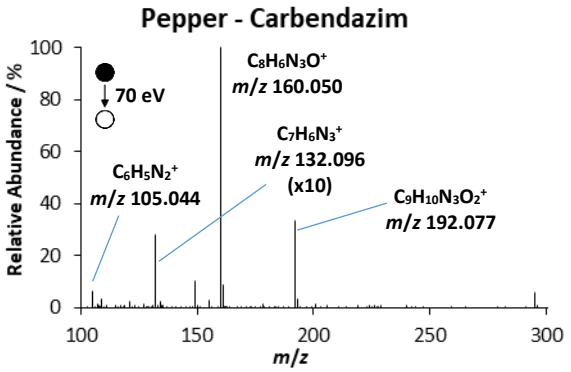

Glove - DNOP
Relative Abundance / %
m/z
[M+H]+ m/z 391.283

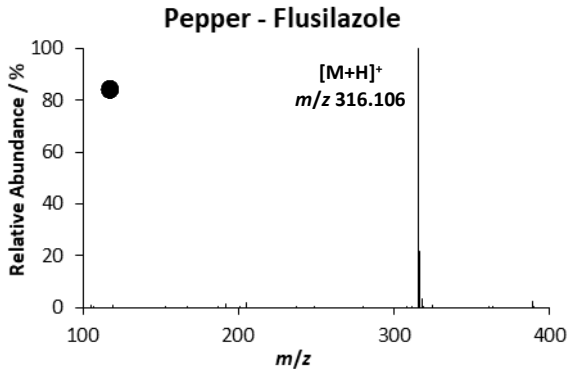

Glove - DNOP
Relative Abundance / %
m/z
C8H5O3+ m/z 149.023
C16H21O3+ m/z 261.148
[M+H]+ m/z 391.283

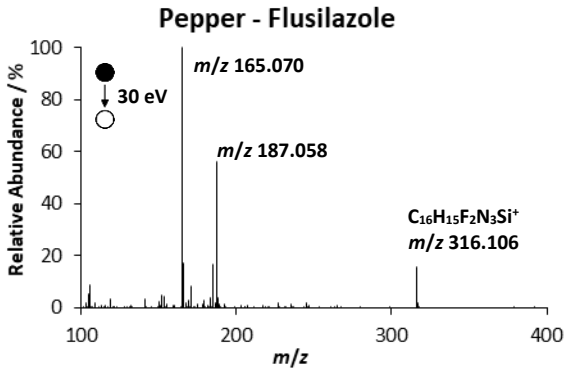




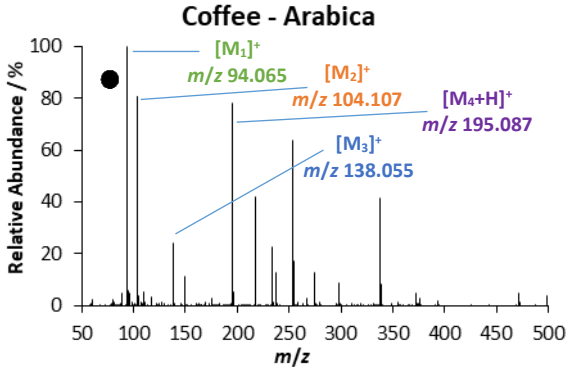


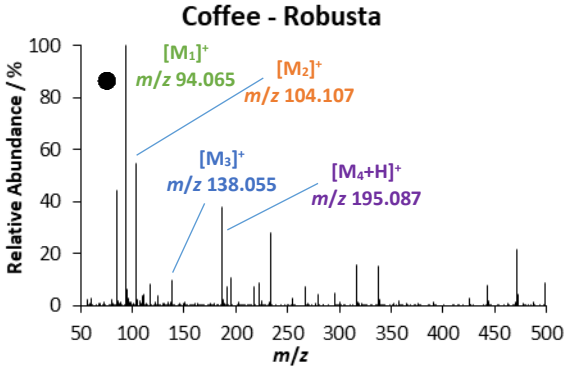


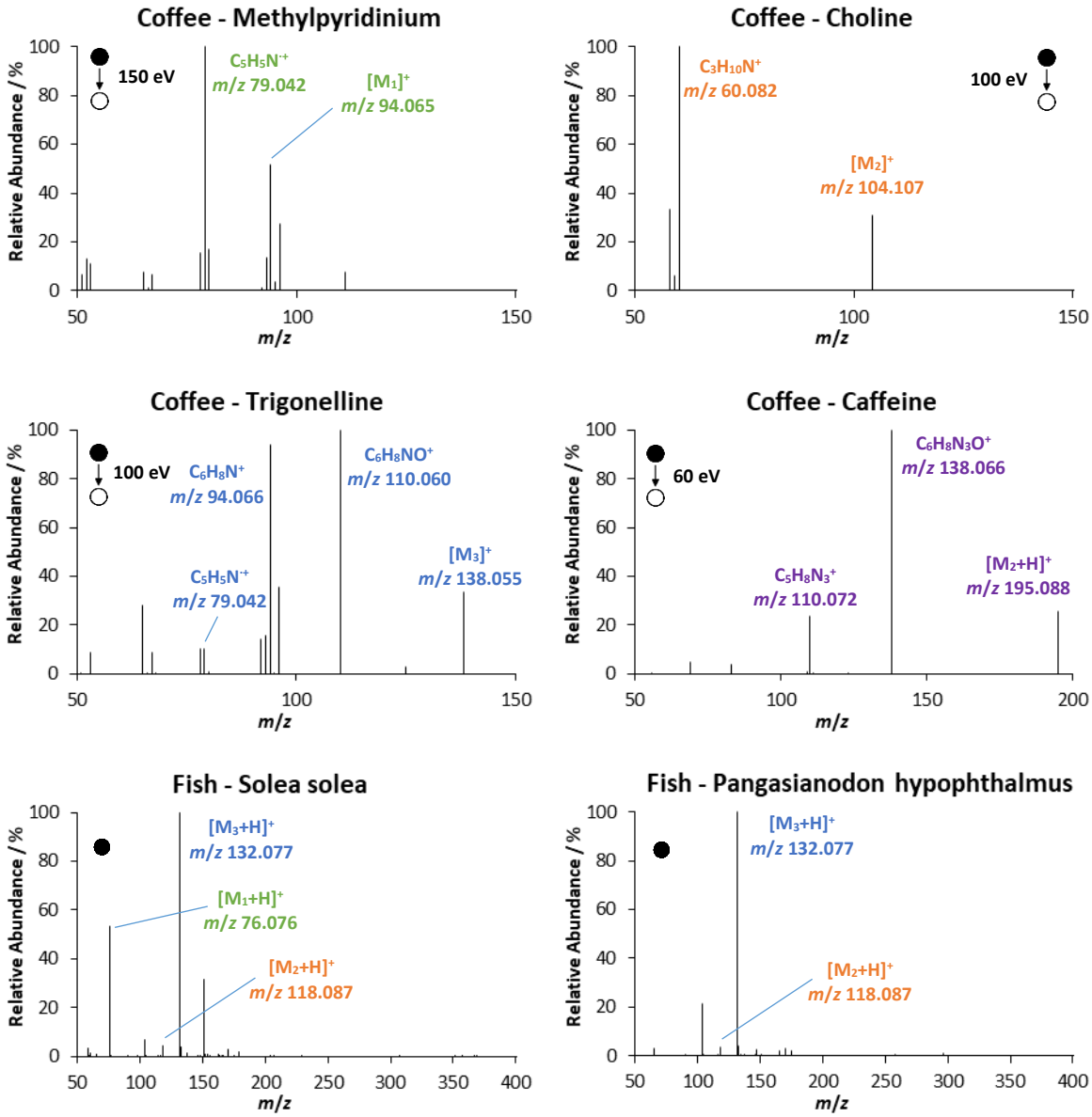


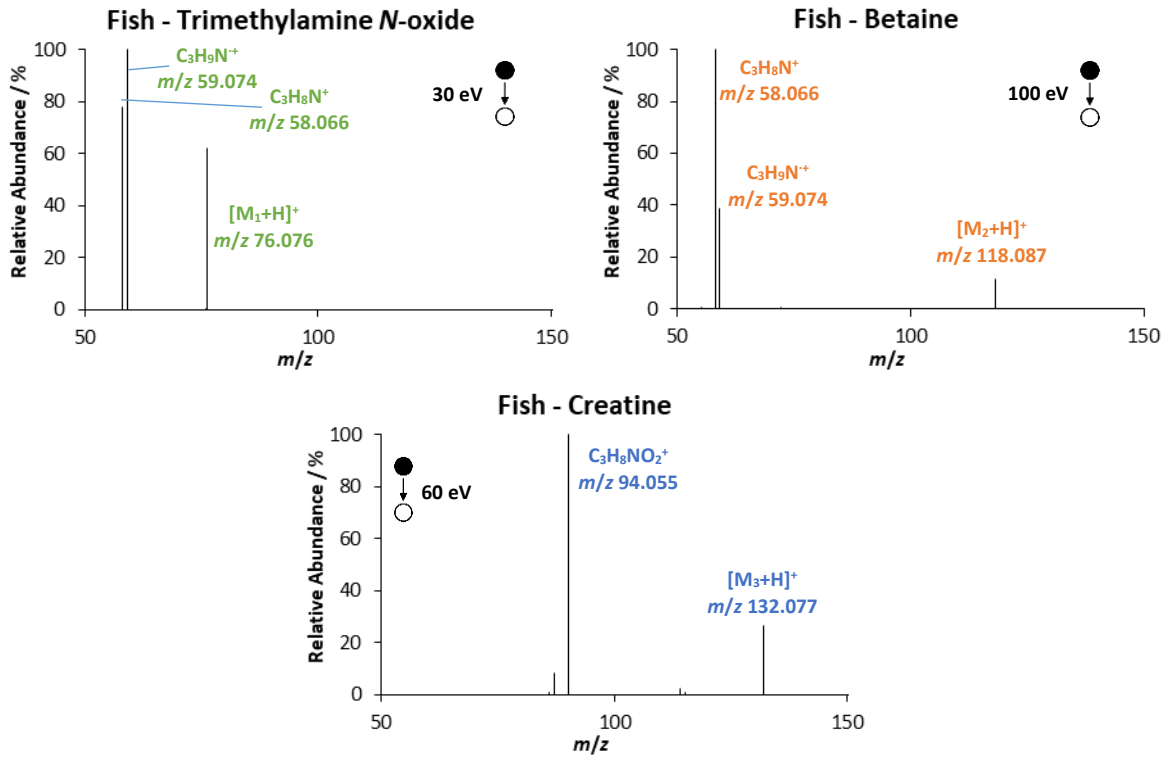


The fragmentation spectra of carbendazim and flusilazole measured from pepper skin show some background signals due to unselective fragmentation via an orbital trapping *Exactive* instrument.



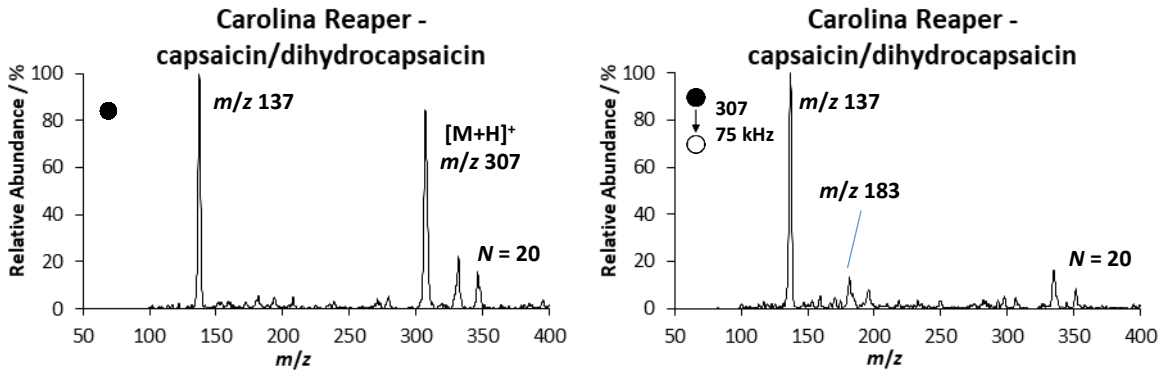



Coffee - Methylpyridinium
150 eV
$C_5H_5N^{+\cdot}$
m/z 79.042
$[M_1]^+$
m/z 94.065
Relative Abundance / %
m/z
Coffee - Choline
100 eV
$C_3H_{10}N^+$
m/z 60.082
$[M_2]^+$
m/z 104.107
Relative Abundance / %
m/z
Coffee - Trigonelline
100 eV
$C_6H_8N^+$
m/z 94.066
$C_6H_8NO^+$
m/z 110.060
$C_5H_5N^{+\cdot}$
m/z 79.042
$[M_3]^+$
m/z 138.055
Relative Abundance / %
m/z
Coffee - Caffeine
60 eV
$C_6H_8N_3O^+$
m/z 138.066
$C_5H_8N_3^+$
m/z 110.072
$[M_2+H]^+$
m/z 195.088
Relative Abundance / %
m/z
Fish - Solea solea
$[M_3+H]^+$
m/z 132.077
$[M_1+H]^+$
m/z 76.076
$[M_2+H]^+$
m/z 118.087
Relative Abundance / %
m/z
Fish - Pangasianodon hypophthalmus
$[M_3+H]^+$
m/z 132.077
$[M_2+H]^+$
m/z 118.087
Relative Abundance / %
m/z

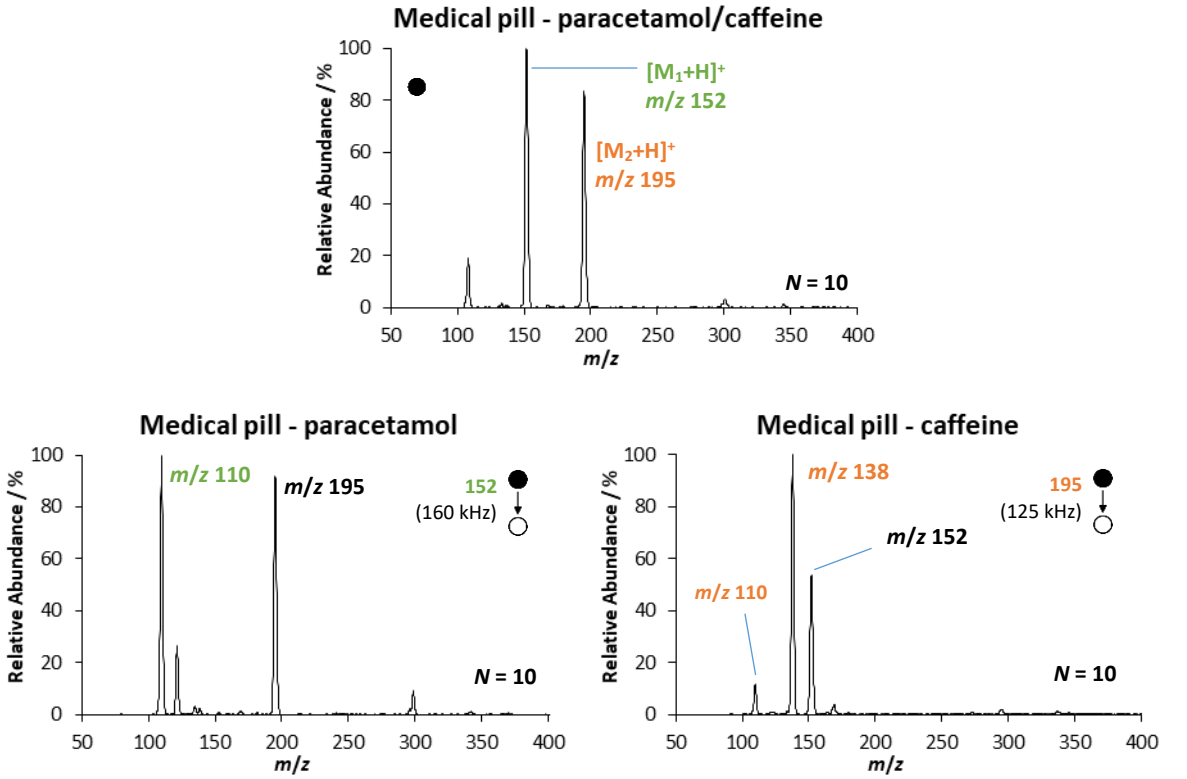


The shown fragment mass spectra from fish were detected from the species *Solea solea*.

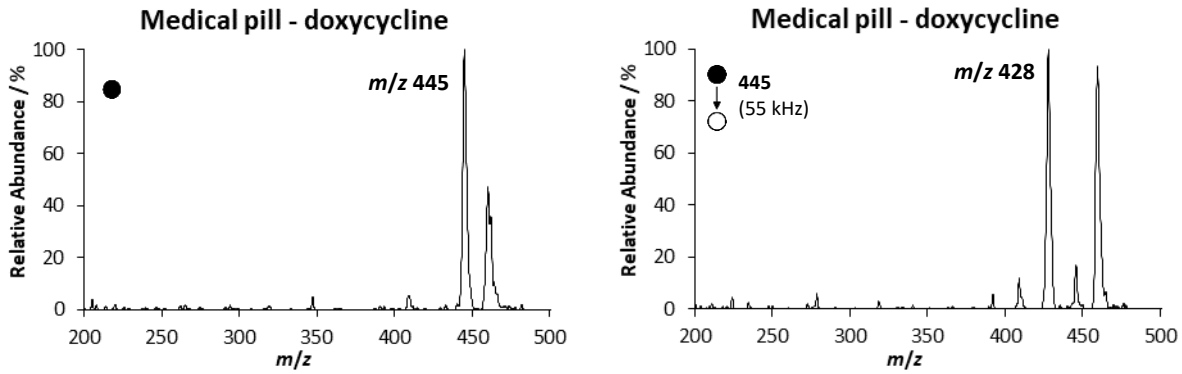
The following mass spectra show fragmentation experiments performed directly from the corresponding sample objects using the LEP source coupled to the prototype of the *Mini 11* mass spectrometer. Analytes of interest were drugs in medical pills, capsaicin in a chili pepper, and plasticizers in all of the presented real samples. Fragmentation was induced via CID by applying a specific AC resonance frequency (see annotation in spectra) of the individual precursor ion to the rectangular ion trap (no precursor ion isolation was performed). For all experiments, the AC voltage was set to 500 V. Some of the precurser spectra already showed signals of the fragments even if no AC frequency was applied.



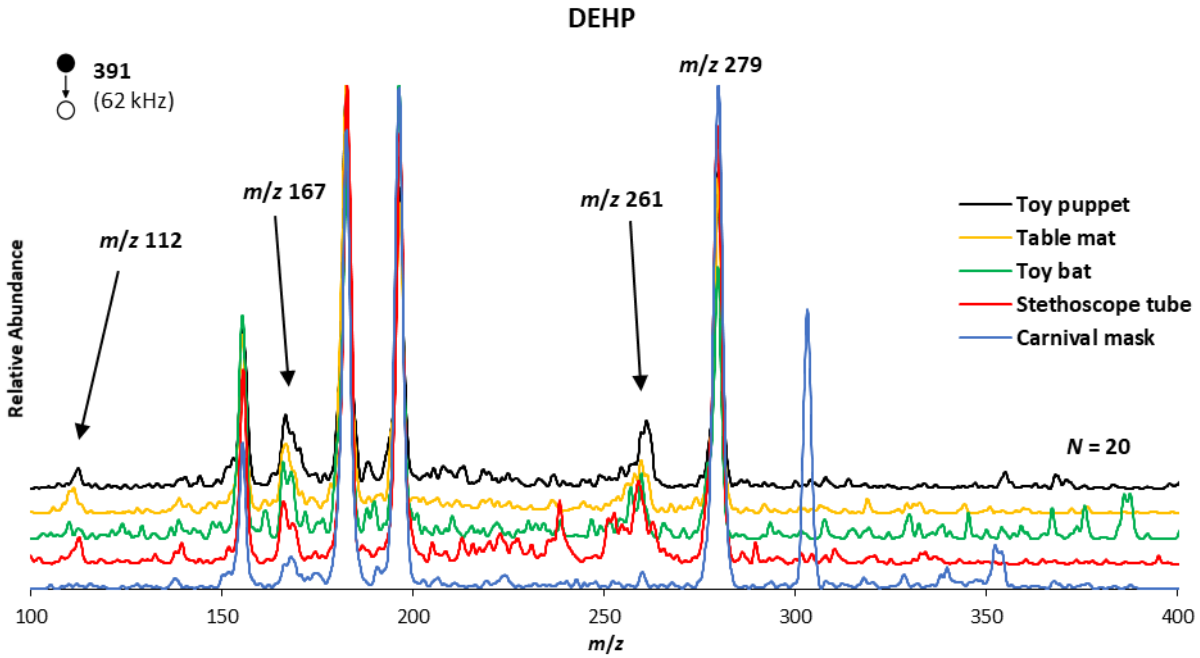
Due to the low resolving power of the Mini 11 prototype, capsaicin (*m/z* 206) and dihydrocapsaicin (*m/z* 208) were not separated. Also the two specific fragments of these compounds at *m/z* 182 and *m/z* 184 were not resolved.

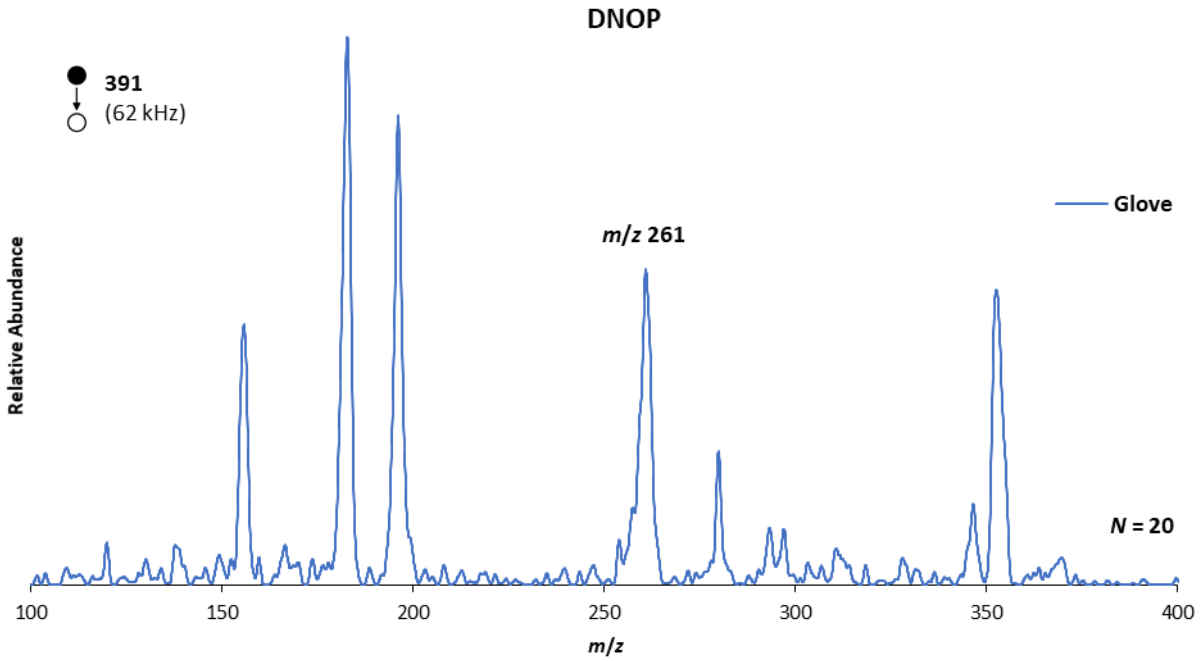


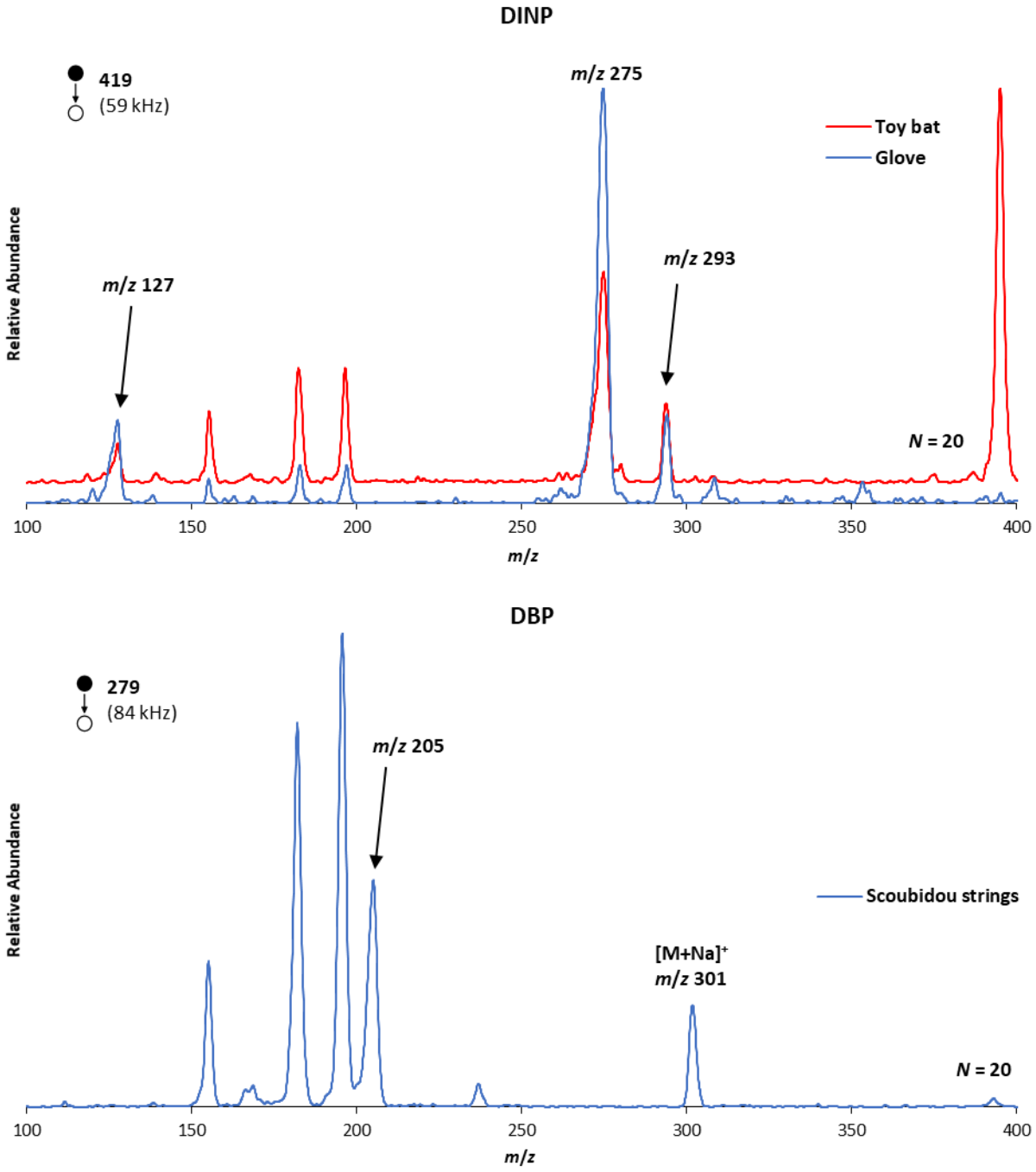
The low-abundant paracetamol fragment at *m/z* 92, detected with the orbital trapping mass spectrometer, was not found with the Mini 11 prototype.

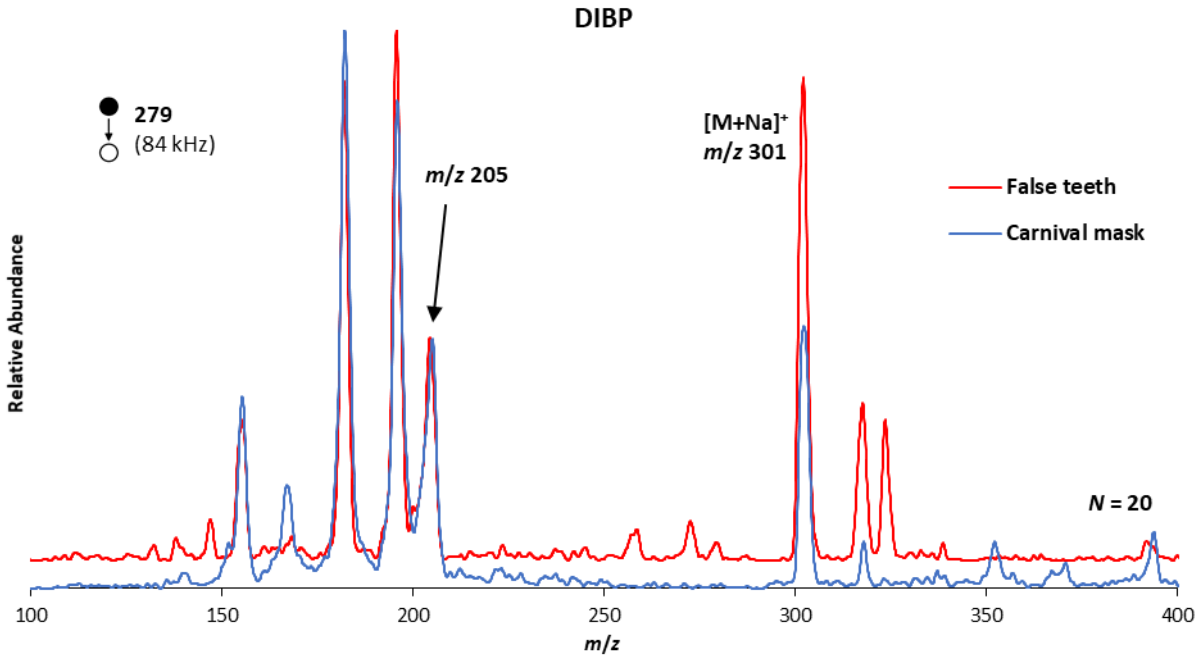


The plasticizers can be identified and differentiated by the mass-to-charge-number of the precursor ion and the specific fragments. In comparison to the HCD spectra collected with the laboratory-based orbital trapping instruments, not all fragments are visible. Especially the unspecific fragment at *m/z* 149 is missing in all Mini 11 spectra. A differentiation of the structural isomers DBP and DIBP was only possible via the Exactive instrument through the fragment at *m/z* 223 which is specific for DIBP. The unspecific signals at *m/z* 155, 182 and 196 which are visible in all plasticizer spectra were not further investigated.


DEHP
391
(62 kHz)
m/z 279
m/z 167
m/z 261
m/z 112
Toy puppet
Table mat
Toy bat
Stethoscope tube
Carnival mask
N = 20
Relative Abundance
100
150
200
250
300
350
400
m/z

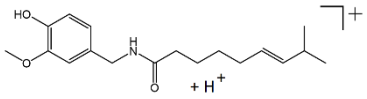
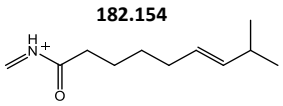
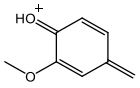
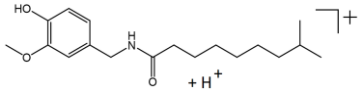
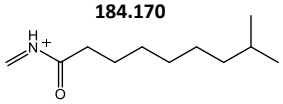
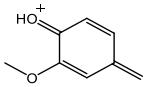
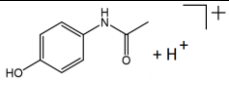
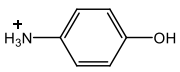
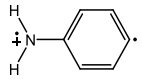
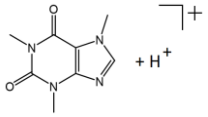
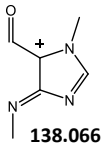
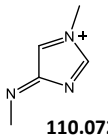
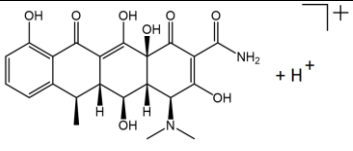
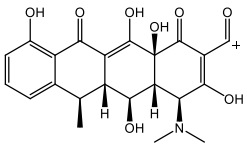

DNOP
391
(62 kHz)
Glove
m/z 261
N = 20
Relative Abundance
100
150
200
250
300
350
400
m/z

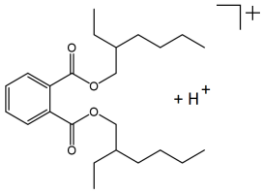
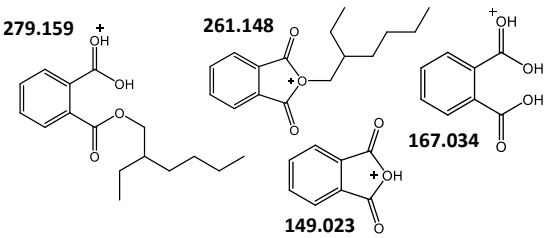
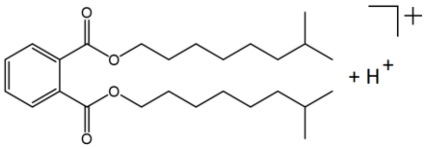
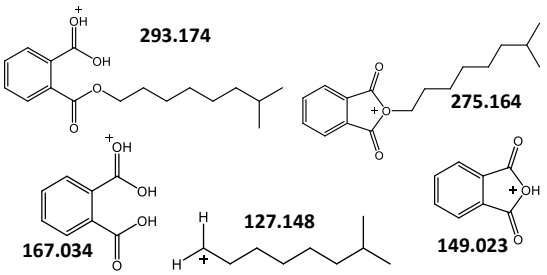
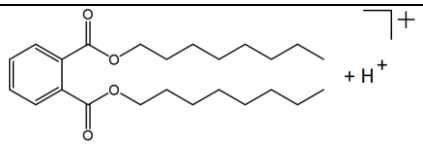
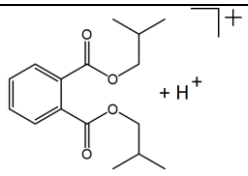
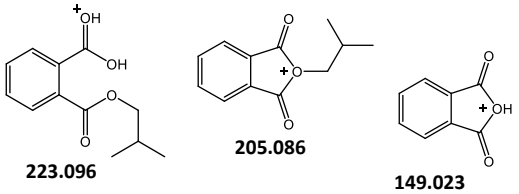
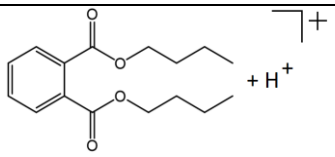
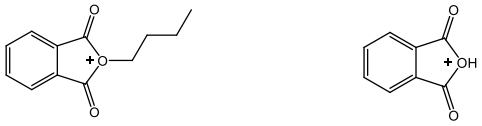
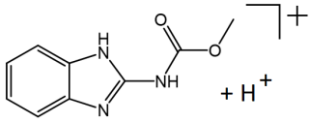
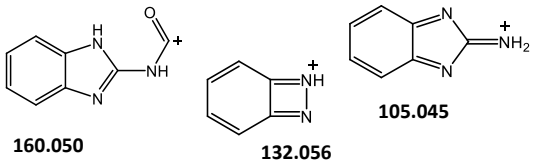
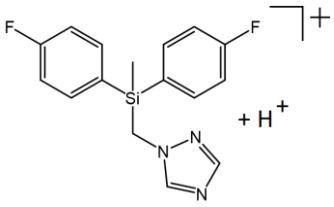
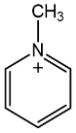
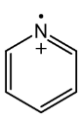

DINP
419
(59 kHz)
m/z 275
Toy bat
Glove
m/z 293
m/z 127
Relative Abundance
N = 20
100
150
200
250
300
350
400
m/z
DBP
279
(84 kHz)
m/z 205
Scoubidou strings
[M+Na]+
m/z 301
Relative Abundance
N = 20
100
150
200
250
300
350
400
m/z

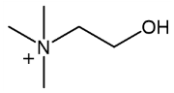
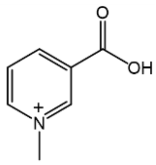
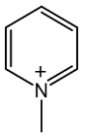
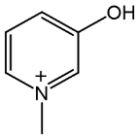
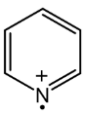
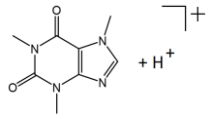
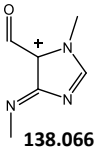
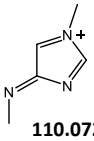
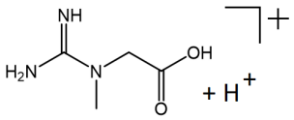
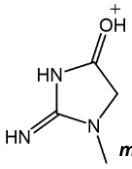
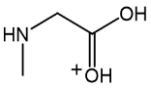
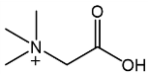


List of fragments and tentative structures

This list gives reliable *m/z*-values. Structures given are plausible, but not verified.

Sample	Molecule ion	Fragments
Chili pepper (Carolina Reaper)	 **[Capsaicin+H]⁺ *m/z* 306.206**	 **182.154**  **137.059**
	 **[Dihydrocapsaicin+H]⁺ *m/z* 308.221**	 **184.170**  **137.059**
Medical pill (Thomapyrin)	 **[Paracetamol+H]⁺ *m/z* 152.071**	 **110.060**  **92.050**
	 **[Caffeine+H]⁺ *m/z* 195.088**	 **138.066**  **110.072**
Medical pill (Doxycycline)	 **[Doxycycline+H]⁺ *m/z* 445.160**	 **428.133**

Toy puppet, Stethoscope tube, Toy bat, Table mat, Carnival mask,	 **[DEHP+H]⁺ *m/z* 391.284**	 **279.159** **261.148** **167.034** **149.023**
Toy bat, Glove	 **[DINP+H]⁺ *m/z* 419.314**	 **293.174** **275.164** **167.034** **127.148** **149.023**
Glove	 **[DNOP+H]⁺ *m/z* 391.284**	 **261.148** **149.023**
Carnival mask, False teeth	 **[DIBP+H]⁺ *m/z* 279.158**	 **223.096** **205.086** **149.023**
Scoubidou strings	 **[DBP+H]⁺ *m/z* 279.158**	 **205.086** **149.023**
Pesticide	 **[Carbendazim+H]⁺ *m/z* 192.077**	 **160.050** **132.056** **105.045**
Pesticide	 **[Flusilazole+H]⁺ *m/z* 316.106**	$C_8H_8FN_3^+$ **m/z 165.070** $C_9H_9N_3Si^+$ **m/z 187.058** Fragmentation pattern closely correlates to the MS/MS data found on the MoNA - MassBank of North America database: Spectrum AU256406 for Flusilazole.
Coffee	 **[Methylpyridinium]⁺ *m/z* 94.065**	 ***m/z* 79.042**

	 **[Choline]$^+$** ***m/z* 104.107**	 ***m/z* 60.082**
	 **[Trigonelline+H]$^+$** ***m/z* 138.055**	 ***m/z* 110.060**  ***m/z* 94.066**  ***m/z* 79.042**
	 **[Caffeine+H]$^+$ *m/z* 195.087**	 **138.066**  **110.072**
Fish	 **[Trimethylamine *N*-oxide+H]$^+$** ***m/z* 76.076**	 ***m/z* 58.066**  ***m/z* 59.074**
	 **[Creatine+H]$^+$ *m/z* 132.077**	 ***m/z* 114.066**  ***m/z* 90.055**
	 **[Betaine+H]$^+$** ***m/z* 118.087**	 ***m/z* 58.066**  ***m/z* 59.074**