

SUPPORTING INFORMATION

Identification of 24 unknown substances (NIAS/IAS) from food contact polycarbonate by LC-Orbitrap Tribrid HRMS-DDMS³. Safety assessment

Vicent Yusà^{a,b*}, Antonio López^a, Pablo Dualde^a, Olga Pardo^a, Igor Fochi^c, Clara Coscolla^a

a Foundation for the Promotion of Health and Biomedical Research in the Valencian Region, FISABIO-Public Health, Av. Catalunya, 21, 46020 Valencia, Spain

b Public Health Laboratory of Valencia, 21, Avenida Cataluña, 46020 Valencia, Spain

c Thermo Fisher, Rodano (MI), Italy

*Corresponding author.

E-mail address: yusa_vic@gva.es (V. Yusà).

Figures	Page
Figure SI-1. Workflow for the ddMS ³ used in AcquireX Deep Scan Mode	2
Figure SI-2: Workflow for the ddMS ³ used in AcquireX IPE Mode	5
Figure SI-3: Compound Discover Workflow	8
Figure SI-4. Log P and Retention Time (Rt) of the quality control compounds	9
Tables	
Table SI-1. Description of the different nodes of the CD workflow	12
Table SI-2. Calculation of the average response factor	23
Table SI-3. Experimental MS3 transitions	24

Figure SI-1: Workflow for the ddMS³ used in AcquireX Deep Scan Mode

The figure illustrates the workflow and configuration for ddMS³ in AcquireX Deep Scan Mode. It is divided into three horizontal sections, each showing a workflow diagram on the left and a configuration panel on the right.

Workflow Diagrams: Each diagram shows a vertical sequence of steps: MS OT (0.6 sec), Dynamic Exclusion, Targeted Mass Exclusion, Targeted Mass, ddMS² OT HCD (2 scans), Precursor Selection Range, Intensity, Precursor Ion Exclusion, and ddMS³ IT CID. The top diagram has 'MS OT' highlighted with a blue border and a close button. The middle diagram has 'Dynamic Exclusion' highlighted. The bottom diagram has 'Targeted Mass Exclusion' highlighted.

MS Scan Properties:

- Orbitrap Resolution: 120000
- Scan Range (m/z): 100-900
- RF Lens (%): 45
- Maximum Injection Time (ms): 50
- Polarity: Positive
- Use EASY-IC™:

Dynamic Exclusion Properties:

- Use Common Settings:
- Exclude after n times: 1
- Exclusion duration (s): 2.5
- Mass Tolerance: ppm
- Low: 5
- High: 5
- Exclude Isotopes:

Targeted Mass Exclusion Properties:

MASS LIST

- Include Start/End Times:
- Include Intensity Threshold:
- Add Mass List Targets Determined by Xcalibur AcquireX:
- Mass List Type: m/z

Compound	m/z	t start (min)	t stop (min)	Inten
1	524.265	0	15	1.0e20

Exclusion mass width: ppm

- Low: 5
- High: 5

Data-Dependent MSⁿ Scan Properties [Show All](#)

Isolation Window (m/z)	1.5
Isolation Offset	Off
Activation Type	HCD
Collision Energy Mode	Stepped
HCD Collision Energies (%)	20,40,90
Detector Type	Orbitrap
Orbitrap Resolution	15000
Maximum Injection Time (ms)	22
Use EASY-IC™	<input checked="" type="checkbox"/>

Precursor Selection Range Properties

Selection Range Mode	Mass Range
Mass Range (m/z)	125-2000

Intensity Properties

Filter Type	Intensity Threshold
Intensity Threshold	5.0e3

```

graph TD
    A[MS OT] --> B[Dynamic Exclusion]
    B --> C[Targeted Mass Exclusion]
    C --> D[Targeted Mass]
    D --> E[ddMS² OT HCD]
    E --> F[Precursor Selection Range]
    F --> G[Intensity]
    G --> H[Precursor Ion Exclusion]
    H --> I[ddMS³ IT CID]
    
```

Precursor Ion Exclusion Properties

Exclusion mass width	m/z
Low	0.5
High	3

```

graph TD
    A[MS OT] --> B[Dynamic Exclusion]
    B --> C[Targeted Mass Exclusion]
    C --> D[Targeted Mass]
    D --> E[ddMS² OT HCD]
    E --> F[Precursor Selection Range]
    F --> G[Intensity]
    G --> H[Precursor Ion Exclusion]
    H --> I[ddMS³ IT CID]
    
```

Data-Dependent MSⁿ Scan Properties Show All

MS ⁿ Level	3
MS Isolation Window (m/z)	1.8
MS2 Isolation Window (m/z)	2
Isolation Offset	Off
Activation Type	CID
CID Collision Energy (%)	30
Detector Type	Ion Trap
Ion Trap Scan Rate	Rapid
Maximum Injection Time (ms)	35

Figure SI-2: Workflow for the ddMS³ used in AcquireX IPE Mode

The figure illustrates the ddMS³ workflow in AcquireX IPE Mode, divided into three panels. Each panel shows a sequence of steps in a flowchart and a corresponding configuration window.

Panel 1: Intensity Properties

The flowchart shows the following steps: MS OT, Intensity (0.6 sec), Dynamic Exclusion, Targeted Mass Exclusion, ddMS² OT HCD, Precursor Selection Range, Intensity (2 scans), Precursor Ion Exclusion, and ddMS³ IT CID.

The Intensity Properties window shows:

- Filter Type: Intensity Threshold
- Intensity Threshold: 4.0e4

Panel 2: Dynamic Exclusion Properties

The flowchart shows the following steps: MS OT, Intensity (0.6 sec), Dynamic Exclusion, Targeted Mass Exclusion, ddMS² OT HCD, Precursor Selection Range, Intensity (2 scans), Precursor Ion Exclusion, and ddMS³ IT CID.

The Dynamic Exclusion Properties window shows:

- Use Common Settings:
- Exclude after n times: 1
- Exclusion duration (s): 2.5
- Mass Tolerance: ppm
- Low: 5
- High: 5
- Exclude Isotopes:

Panel 3: Targeted Mass Exclusion Properties

The flowchart shows the following steps: MS OT, Intensity (0.6 sec), Dynamic Exclusion, Targeted Mass Exclusion, ddMS² OT HCD, Precursor Selection Range, Intensity (2 scans), Precursor Ion Exclusion, and ddMS³ IT CID.

The Targeted Mass Exclusion Properties window shows:

- Include Start/End Times:
- Include Intensity Threshold:
- Add Mass List Targets Determined by Xcalibur AcquireX:
- Mass List Type: m/z

MASS LIST

Compound	m/z	t start (min)	t stop (min)	Inten
1	524.265	0	15	1.0e20

Exclusion mass width: ppm

- Low: 5
- High: 5

Data-Dependent MSⁿ Scan Properties [Show All](#)

Isolation Window (m/z)	1.5
Isolation Offset	Off
Activation Type	HCD
Collision Energy Mode	Stepped
HCD Collision Energies (%)	20,40,90
Detector Type	Orbitrap
Orbitrap Resolution	15000
Maximum Injection Time (ms)	22
Use EASY-IC™	<input checked="" type="checkbox"/>

Precursor Selection Range Properties

Selection Range Mode	Mass Range
Mass Range (m/z)	125-2000

Intensity Properties

Filter Type	Intensity Threshold
Intensity Threshold	5.0e3

```

graph TD
    A[MS OT] --> B[Intensity]
    B --> C[Dynamic Exclusion]
    C --> D[Targeted Mass Exclusion]
    D --> E[ddMS² OT HCD]
    E --> F[Precursor Selection Range]
    F --> G[Intensity]
    G --> H[Precursor Ion Exclusion]
    H --> I[ddMS³ IT CID]
    
```

0.6 sec

2 scans

Precursor Ion Exclusion Properties

Exclusion mass width	m/z
Low	0.5
High	3

```

graph TD
    A[MS OT] --> B[Intensity]
    B --> C[Dynamic Exclusion]
    C --> D[Targeted Mass Exclusion]
    D --> E[ddMS² OT HCD]
    E --> F[Precursor Selection Range]
    F --> G[Intensity]
    G --> H[Precursor Ion Exclusion]
    H --> I[ddMS³ IT CID]
    
```

0.6 sec

2 scans

Data-Dependent MSⁿ Scan Properties Show All

MS ⁿ Level	3
MS Isolation Window (m/z)	1.8
MS2 Isolation Window (m/z)	2
Isolation Offset	Off
Activation Type	CID
CID Collision Energy (%)	30
Detector Type	Ion Trap
Ion Trap Scan Rate	Rapid
Maximum Injection Time (ms)	35

Figure SI-3. Compound Discover Workflow

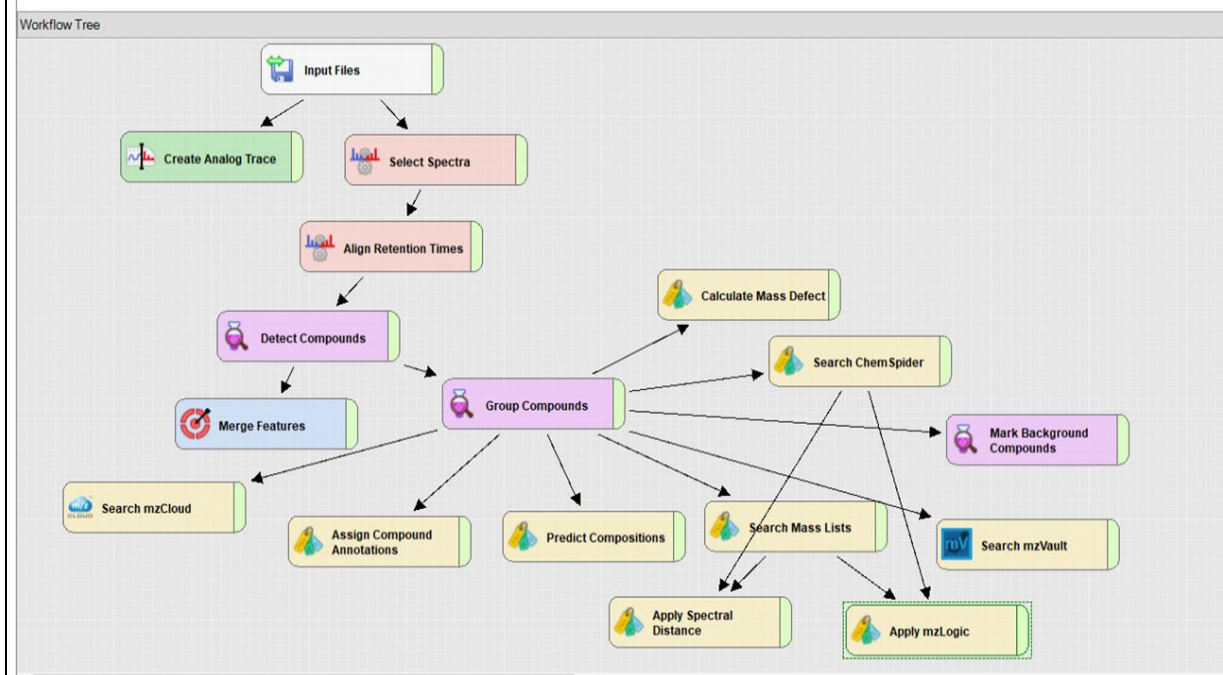
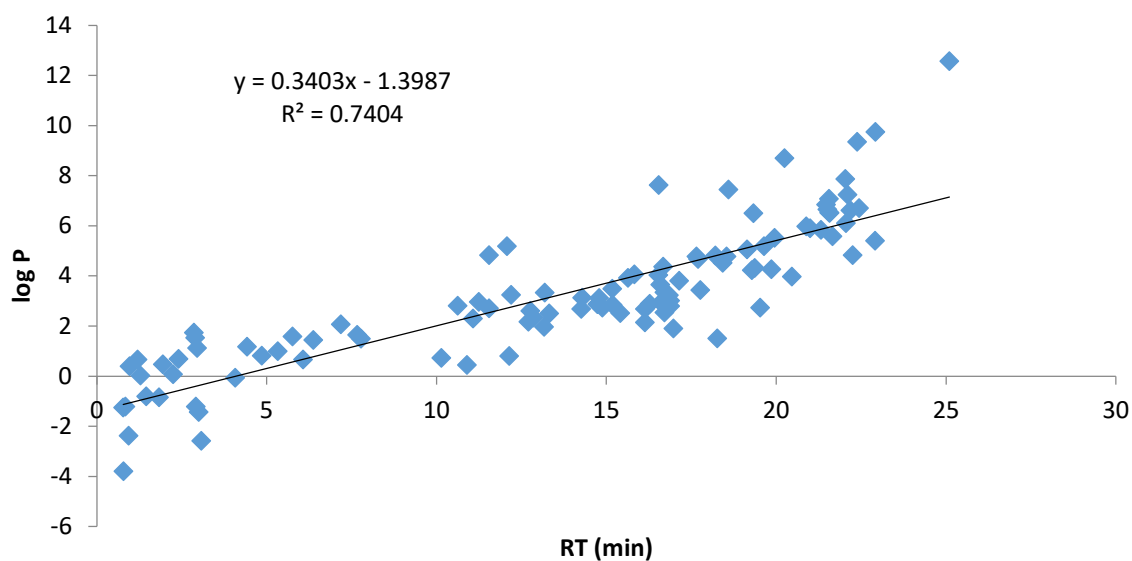


Figure SI-4. Log P and Retention Time (Rt) of the quality control compounds

Analyte	Rt	log P
Sulfaguanidine	0,85	-1,22
Val-Tyr-Val	4,86	0,8
Reserpine	13,19	3,32
Caffeine	4,08	-0,07
Acetaminophen	1,95	0,46
Sulfadimethoxine	7,67	1,63
Terfenadine	16,55	7,62
2,4-D	12,77	2,59
2-diethylamino-6-methyl pyrimidin-4-ol/one	2,96	1,11
3,5,6-Trichloro-2-pyridinol	12,71	2,16
3-phenoxybenzoic acid	15,64	3,91
4-Fluoro-3-phenoxybenzoic acid	15,83	4,05
4-nitrophenol	5,77	1,57
5-hydroxy-thiabendazole	2,86	1,73
6-Chloronicotinic acid	5,33	0,98
Acetochlor	16,61	2,92
Acetochlor mercapturate	14,75	2,86
Alachlor mercapturate	14,75	2,86
Bentazone	10,63	2,8
Benzophenone-3 (Oxybenzone)	16,59	3,64
Carbendazim	2,9	1,52
Chlorfenvinphos	18,43	4,51
Chlormequat	0,79	-3,8
Desisopropylatrazine	4,43	1,16
Diethylthiophosphate	2,41	0,68
Dimethyldithiophosphate	1,2	0,65
Fenhexamid	16,54	4,02
Fenvalerate free acid	16,72	3,33

Fipronil	17,66	4,76
Fipronil sulfone	18,6	7,44
Fluopyram	16,68	4,36
Hydroxy-tebuconazole	15,42	2,5
Isoproturon	12,86	2,32
Malathion dicarboxylic acid	7,78	1,48
Mecoprop	15,19	2,84
Metolachlor	16,89	3
N,N-diethyl-m-toluamide ou DEET	13,17	1,96
Omethoate	2,25	0,06
Prochloraz	17,15	3,8
p-Toluenesulfonamide	12,15	0,79
Triclosan glucuronide	16,72	2,53
Triclosan sulfate	17,71	4,66
acetamiprid-N-desmethyl	6,08	0,65
Acephate	1,84	-0,85
Avermectin B1a (Abamectin)	21,57	6,51
Benodanil	12,2	3,23
benzoic acid	16,98	1,89
Bromoxynil	11,25	2,95
Butocarboxim	18,27	1,49
Cefoperazone	6,38	1,43
Dichlorvos	10,15	0,71
Dinoterb	17,77	3,42
Flamprop	15,18	3,47
Inabenfide	14,27	2,67
Ivermectin B1a	22,19	6,61
MCPA	13,32	2,49
Methamidophos	1,46	-0,82
Nigericin	22,26	4,82
Phenytoin	11,08	2,29
Rifaximin	16,85	3,22
Salicylic acid	7,19	2,06
salinomycin	22,06	6,1
Simazine 2-Hydroxy	2,92	-1,22
Spinosad A (Spinosyn A)	18,21	4,8
TCMTB	14,29	3,12
Tepraloxydim	16,28	2,88
Trichlorfon (Dylox)	10,9	0,43
triclosan	19,65	5,17
Valproic acid	14,89	2,72
Vancomycin	3	-1,44
1-Stearyl glycerol	22,11	7,23
4-tert-Butylcyclohexyl acetate	20,47	3,96
Bis(2-ethylhexyl)adipate	22,04	7,85

Citroflex A-4	19,34	6,49
Dibutyl phthalate	11,55	4,82
Dibutyl sebacate	20,89	5,97
Diethyl phthalate	11,55	2,7
Dimethyl sebacate	16,89	2,79
Dipentyl phthalate	21	5,89
Erucamide	22,93	9,74
Ethyl Oleate	20,25	8,69
Galaxolidone	19,96	5,5
Hexadecanamide	21,48	6,84
Hexadecanedioic acid	19,15	5,05
L-Histidine	0,78	-1,26
Monobutyl phthalate	19,53	2,72
N,N'-Dicyclohexylurea	14,79	3,1
Octyl decyl phthalate	22,39	9,336
Oleamide	21,56	7,07
Palmitoleic acid	21,51	6,64
Palmitoyl ethanolamide	21,32	5,82
PEG n5	3,08	-2,59
Pyrene	12,08	5,17
L-Pyroglutamic acid	0,94	-2,39
Tributyl phosphate	19,86	4,26
Triethyleneglycol bis(2-ethylhexanoate)	21,66	5,57
L-Tyrosine	0,97	0,38
Urocanic acid	1,29	0,01
Dibutyl hexanodioate	19,291	4,22
Benzyl octyl adipate	21,58	6,5
D,L-Camphor	16,139	2,13
Irgafos 168	25,103	12,56
Benazol P	19,378	4,3
3,5-ditert-butyl-4-hydroxybenzaldehyde	18,544	4,77
Methyl dihydrojasmonate	16,142	2,67
Stearamide	22,447	6,7
Dodecyl sulfate	22,916	5,39

Table SI-1. Description of the different nodes of the CD workflow

NODE		
<p>CREATE AMONG TRACE</p>	<p>Parameters of 'Create Analog Trace'</p> <p>Show Advanced Parameters</p> <ul style="list-style-type: none"> 1. General Settings <ul style="list-style-type: none"> Trace Type UV RT Offset [min] 0 Custom Label UV trace 2. PDA Settings <ul style="list-style-type: none"> Total Scan False Spectrum Maxir False Wavelength Rar True Min. Wavelengt 190 Max. Wavelengt 800 	
<p>SELECT SPECTRA</p>	<p>Parameters of 'Select Spectra'</p> <p>Show Advanced Parameters</p> <ul style="list-style-type: none"> 1. General Settings <ul style="list-style-type: none"> Precursor Selection Use MS(n - 1) Precursor Provide Profile Spectra Automatic 2. Spectrum Properties Filter <ul style="list-style-type: none"> Lower RT Limit 0 Upper RT Limit 0 First Scan 0 Last Scan 0 Ignore Specified Scans Lowest Charge State 0 Highest Charge State 0 Min. Precursor Mass 100 Da Max. Precursor Mass 5000 Da Total Intensity Threshold 0 Minimum Peak Count 1 3. Scan Event Filters <ul style="list-style-type: none"> Mass Analyzer (Not specified) MS Order Any Activation Type (Not specified) Min. Collision Energy 0 Max. Collision Energy 1000 Scan Type Any Polarity Mode (Not specified) 4. Peak Filters <ul style="list-style-type: none"> S/N Threshold (FT-only) 1.5 5. Replacements for Unrecognized Properties <ul style="list-style-type: none"> Unrecognized Charge Replace 1 Unrecognized Mass Analyzer ITMS <p>Precursor Selection Specifies which precursor to use for higher order MSn spectra: - 'Use MS1 Precursor': Uses the precursor of the associated MS1 scan, - 'Use MS(n - 1) Precursor': Uses the precursor of the direct parent scan of the spectrum, - 'Use MS(n - 1) with Parent Precursors': Uses the precursor of the direct parent scan and all preceding precursors up to the MS1 scan.</p>	

ALIGN RETENTION TIME

Parameters of 'Align Retention Times'	
Show Advanced Parameters	
▼ 1. General Settings	
Alignment Model	Adaptive curve
Maximum Shift [min]	2
Mass Tolerance	5 ppm

Alignment Model

This defines the Model, which is used for the alignment. The adaptive curve calculates a flexible curve for retention time shift for each retention time point. The linear model uses one linear function through the complete retention time range.

GROUP COMPOUNDS

Parameters of 'Group Compounds'	
Show Advanced Parameters	
▼ 1. Compound Consolidation	
Mass Tolerance	5 ppm
RT Tolerance [min]	0.1
▼ 2. Fragment Data Selection	
Preferred Ions	[M+H] ⁺ +1; [M+NH ₄] ⁺ +1; [M-H] ⁻ -1

Mass Tolerance

This parameter specifies the mass tolerance to be used for grouping.

Minimum value = 0.1 ppm

Maximum value = 20 ppm

DETECT COMPOUND

Parameters of 'Detect Compounds'

Show Advanced Parameters

1. General Settings

Mass Tolerance (ppm)	5 ppm
Intensity Tolerance (%)	30
S/N Threshold	3
Min. Peak Intensity	100000
Ions	-Na)+2; [M+H-NH4)+2; [M+H-H2O)+1; [M+H-NH3)+1; [M+K)+1; [M+Na)+1; [M+NH4)+1; [M-2H]-2; [M-2H+K)-1; [M-H
Min. Element Counts	C H
Max. Element Counts	C90 H190 Br3 Cl4 K2 N10 Na2 O18 P3 S5

Ions
This parameter allows selection of multiple ion definitions to be considered.

CALCULATE MASS DEFECT

Parameters of 'Calculate Mass Defect'

Show Advanced Parameters

1. Mass Defect

Fractional Mass	False
Standard Mass Defect	False
Relative Mass Defect	False
Kendrick Mass Defect	True

2. Kendrick Formula

Formula 1	C2 H4 O
Formula 2	C2 H3 Cl
Formula 3	C2 H2 F2
Formula 4	C3 H6
Formula 5	C8 H8

Fractional Mass
This parameter specifies whether fractional mass should be calculated.

MERGE FEATURES

Parameters of 'Merge Features'

Show Advanced Parameters

1. Peak Consolidation

Mass Tolerance	5 ppm
RT Tolerance [min]	0.2

Mass Tolerance

This parameter specifies the mass tolerance to be used for peak merging.

Minimum value = 0.1 ppm
Maximum value = 20 ppm

SEARCH CHEMSPIDER

Parameters of 'Search ChemSpider'

Show Advanced Parameters

▼ 1. Search Settings

Database(s)	Alfa Chemistry; EPA DSSTox; EPA Toxcast; NIST; PurePEG; Sigma-Aldrich; TCI
Search Mode	By Formula or Mass
Mass Tolerance	5 ppm
Max. # of results per compound	10
Max. # of Predicted Compositions to be searched per	3

Database(s)
The selected databases are searched.

MARK BACKGROUND COMPOUNDS

Parameters of 'Mark Background Compounds'

Show Advanced Parameters

1. General Settings

Max. Sample/Blank	5
Max. Blank/Sample	0
Hide Background	True

Max. Sample/Blank

This parameter specifies the maximum allowed ratio of the sample vs. blank to be considered as background. Set to 0 to skip this rule.

Minimum value = 0.0

Maximum value = (unchecked)

SEARCH mzCLOUD

Parameters of 'Search mzCloud'

Show Advanced Parameters

- 1. General Settings**

Compound Classes	All
Library	Autoprocessed; Reference
- 2. DDA Search**

Identity Search	HighChem HighRes
Match Activation Type	True
Match Activation Energy	Match with Tolerance
Activation Energy Toleranc	20
Apply Intensity Threshold	True
Similarity Search	Similarity Forward
Match Factor Threshold	60
- 3. DIA Search**

Use DIA Scans for Search	True
Max. Isolation Width [Da]	500
Match Activation Type	True
Match Activation Energy	Any
Activation Energy Toleranc	100
Apply Intensity Threshold	True
Match Factor Threshold	20

Compound Classes
The Compound Classes used for the search.

ASSIGN COMPOUND ANNOTATIONS

Parameters of 'Assign Compound Annotations'

Show Advanced Parameters

- 1. General Settings**

Mass Tolerance	5 ppm
----------------	-------
- 2. Data Sources**

Data Source #1	mzCloud Search
Data Source #2	mzVault Search
Data Source #3	MassList Search
Data Source #4	Predicted Compositions
Data Source #5	ChemSpider Search
Data Source #6	
Data Source #7	
- 3. Scoring Rules**

Use mzLogic	True
Use Spectral Distance	True
SFit Threshold	20
SFit Range	20

Mass Tolerance
This parameter specifies the mass tolerance to be used to validate annotations.
Minimum value = 0.1 ppm
Maximum value = 20 ppm

PREDICT COMPOSITION

Parameters of 'Predict Compositions'

Show Advanced Parameters

1. Prediction Settings

Mass Tolerance	5 ppm
Min. Element Counts	C H
Max. Element Counts	C200 H800 Br5 Cl4 F5 N5 O80 Si15
Min. RDBE	0
Max. RDBE	40
Min. H/C	0.1
Max. H/C	3.5
Max. # Candidates	10

2. Pattern Matching

Intensity Tolerance [%]	30
Intensity Threshold [%]	0.1
S/N Threshold	3
Use Dynamic Recalibration	True

3. Fragments Matching

Use Fragments Matching	True
Mass Tolerance	5 ppm
S/N Threshold	3

Mass Tolerance

This parameter specifies the mass tolerance to be used for prediction.

Minimum value = 0.1 ppm

Maximum value = 20 ppm

SEARCH MASS LIST

Parameters of 'Search Mass Lists'

Show Advanced Parameters

▼ 1. Search Settings

Mass Lists	\\Extractables and Leachables HRAM Compound Database.massList
Use Retention Time	True
RT Tolerance [min]	0.1
Mass Tolerance	5 ppm

Mass Lists
This parameter allows the selection of several registered mass list files:
The .masslist files can be edited using the file manager.

SEARCH mz VAULT

Parameters of 'Search mzVault'

Show Advanced Parameters

▼ 1. Search Settings

mzVault Library	\\mzVault Reference May 2019.db\mzVault Autoprocessed May 2019.db
Compound Classes	All
Match Ion Activation Type	True
Match Ion Activation Energy	Match with Tolerance
Ion Activation Energy Tolerance	20
Match Ionization Method	True
Apply Intensity Threshold	True
Precursor Mass Tolerance	10 ppm
Match Analyzer Type	True
Search Algorithm	HighChem HighRes
Match Factor Threshold	50
RT Tolerance [min]	2
Use Retention Time	False

mzVault Library

This parameter allows the selection of registered mzVault database files.

**APPLY
SPECTRAL
DISTANCE**

Parameters of 'Apply Spectral Distance'

Show Advanced Parameters

▼ **1. Pattern Matching**

Mass Tolerance	5 ppm
Intensity Tolerance [%]	30
Intensity Threshold [%]	0.1
S/N Threshold	3
Use Dynamic Recalibration	True

Mass Tolerance
This parameter specifies the mass tolerance to be used for isotope search.
Minimum value = 0.1 ppm
Maximum value = 20 ppm

**APPLY
mzLOGIC**

Parameters of 'Apply mzLogic'

Show Advanced Parameters

▼ **1. Search Settings**

Max. # Compounds	0
Max. # mzCloud Similarity Results to consider per	10
Match Factor Threshold	30

Max. # Compounds
The maximum number of compounds for which candidates should be scored.
0 means all candidates of all compounds are scored.
Minimum value = 0
Maximum value = (unchecked)

Table SI-2. Calculation of the average response factor			
Analytes	Area	Concentration (ng·mL⁻¹)	Response factor
Sulfaguanidine	826910	10	82691
Val-Try-Val	3709775	10	370978
Reserpine	3548764	10	354876
Caffeine	2631124	10	263112
Acetaminophen	4351886	10	435189
Sulfadimethoxine	5639812	10	563981
Terfenadine	19167123	10	1916712
AVERAGE			569648

Table SI-3. Experimental MS³ transitions	
Substance	¹ Acquired MS ³ (m/z MS ² precursor > m/zMS ³ fragment)
3,5-ditert-butyl-4-hydroxybenzaldehyde	179.1063 > 123.05
4-tert-butylcyclohexyl acetate	135.1166 > 107.08
Benazol P	183.0679 > 155.06
Benzyl octyl adipate	129.0544 > 100.93
Bis(2-ethylhexyl)adipate	129.0545 > 111.06
Citroflex A-4	129.0180 > 111.00
D,L-Camphor	-
DEET	173.449 > 131.02
Dibutyl hexanodioate	129.0536 > 111.08
Dibutyl phthalate	149.0231 > 121.04
Dibutyl sebacate	185.1172 > 139.03
Diethyl phthalate	177.0546 > 149.05
Dipentyl phthalate	149.0229 > 121.08
Dodecyl sulfate	247.0226 > 219.03
Erucamide	321.3157 > 163.23
Galaxolidone	255.17455 > 227.24
Hexadecanamide	130.1224 > 88.02
Irgafos 168	147.1167 > 132.09
Methyl dihydrojasmonate	153.1271 > 97.06
N,N'-Dicyclohexylurea	143.1181 > 60.92
Octyl decyl phthalate	149.0231 > 121.04
Oleamide	135.1166 > 107.08
Palmitoyl ethanolamide	283.2638 > 109.12
Stearamide	130.1222 > 88.02
¹ The fragmentation of the MS ² precursor in the Linear Ion Trap was performed at 40 eV	