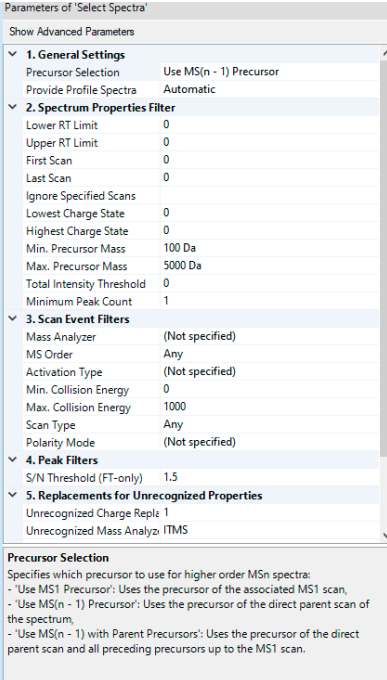
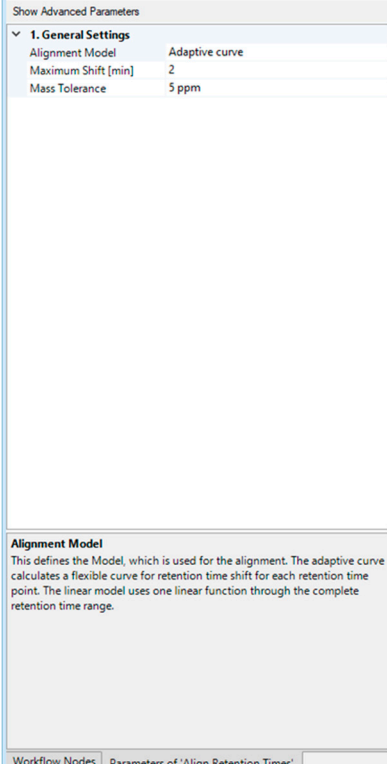


Supplementary Materials: Identification of Unknown Substances in Ambient Air (PM₁₀), Profiles and Differences between Rural, Urban and Industrial Areas

Antonio López, Esther Fuentes, Vicent Yusà, María Ibáñez and Clara Coscollà

Table S1. Description of the different nodes of the CD workflow.

NODE	
<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 Repl: 1 Unrecognized Mass Analyz: TMS <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>
<p>ALIGN RETENTION TIME</p>	 <p>Show Advanced Parameters</p> <ul style="list-style-type: none"> 1. General Settings <ul style="list-style-type: none"> Alignment Model: Adaptive curve Maximum Shift [min]: 2 Mass Tolerance: 5 ppm <p>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.</p> <p>Workflow Nodes Parameters of 'Align Retention Times'</p>

CREATE TRACE PATTERN

Show Advanced Parameters

1. General Settings

Isotope Ratios	CI
Mass Tolerance	5 ppm
Intensity Tolerance [%]	30
MS Order	MS1
Polarity	+
Custom Label	1CI Trace

Isotope Ratios

This parameter specifies the isotope ratios to be searched.

DETECTED COMPOUNDS

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	1000000
Ions	[2M+ACN+H] ⁺ 1; [2M+ACN+Na] ⁺ 1; [2M+FA-
Min. Element Counts	C H
Max. Element Counts	C90 H190 Br3 Cl4 F6 K2 N10 Na2 O18 P3 S5

Mass Tolerance [ppm]

This parameter specifies the mass tolerance to be used for extracted ion chromatogram creation.

Minimum value = 1 ppm
Maximum value = 20 ppm

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]⁺; [M-H]⁻

Mass Tolerance

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

Minimum value = 0.1 ppm
Maximum value = 20 ppm

MERGE FEATURES

Show Advanced Parameters

1. Peak Consolidation

Mass Tolerance 5 ppm
RT Tolerance [min] 0.1

Mass Tolerance

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

Minimum value = 0.1 ppm
Maximum value = 20 ppm

FILL GAPS

Parameters of 'Fill Gaps'

Show Advanced Parameters

1. General Settings

Mass Tolerance	5 ppm
S/N Threshold	1.5

Mass Tolerance

This parameter specifies the mass tolerance to be used for similar features search and XIC creation.

Minimum value = 0.1 ppm
Maximum value = 20 ppm

NORMALIZED AREAS

Show Advanced Parameters

1. QC-based Area Correction

Min. QC Coverage [%]	50
Max. QC Area RSD [%]	30

2. Area Normalization

Normalization Type	[None]
Exclude Blanks	False

3. Scaling Factor

Study Factor Name

Min. QC Coverage [%]

This parameter specifies the minimum percentage of the QC samples where particular compound must be detected, otherwise the compound will not be used for quantification.

Minimum value = 25
Maximum value = 100

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)

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 F4
Formula 2	C2 F3 O
Formula 3	C2 H4
Formula 4	C3 H6
Formula 5	C8 H8

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

SEARCH MzVault

Show Advanced Parameters

▼ 1. Search Settings

mzVault Library	\\mzVault Autoprocessed May 2019.db
Compound Classes	All
Match Ion Activation Type	True
Match Ion Activation Energ	Match with Tolerance
Ion Activation Energy Toler	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.

PATTERN SCORING

Parameters of 'Pattern Scoring'

Show Advanced Parameters

▼ 1. General Settings

Isotope Patterns	CI
Mass Tolerance	5 ppm
Intensity Tolerance [%]	30
SN Threshold	3
Min. Spectral Fit [%]	0

Isotope Patterns
This parameter specifies the isotope patterns to be searched.

SEARCH MzCloud

Parameters of 'Search MzCloud'

Show Advanced Parameters

1. General Settings	
Compound Classes	All
Library	Autoprocessed; Reference
2. DDA Search	
Identity Search	Cosine
Match Activation Type	True
Match Activation Energy	Match with Tolerance
Activation Energy Tolerance	20
Apply Intensity Threshold	True
Similarity Search	Confidence Forward
Match Factor Threshold	60
3. DIA Search	
Use DIA Scans for Search	True
Max. Isolation Width [Da]	500
Match Activation Type	False
Match Activation Energy	Any
Activation Energy Tolerance	100
Apply Intensity Threshold	True
Match Factor Threshold	20

Compound Classes

The Compound Classes used for the search.

PREDICT COMPOSITIONS

Parameters of 'Predict Compositions'

Show Advanced Parameters

1. Prediction Settings	
Mass Tolerance	5 ppm
Min. Element Counts	C H
Max. Element Counts	C90 H190 Br3 Cl8 F18 N10 O18 P3 S5
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

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

SEARCH MASS LIST

Parameters of 'Search Mass Lists'

Show Advanced Parameters

1. Search Settings

Mass Lists \EFS HRAM Compound Database.masslist(...)

Use Retention Time	True
RT Tolerance [min]	0.5
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.

APPLY MzLogic

Parameters of 'Apply mzLogic'

Show Advanced Parameters

1. Search Settings

Max. # Compounds	0
Max. # mzCloud Similarity	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)

SEARCH ChemSpider

Parameters of 'Search ChemSpider'

Show Advanced Parameters

1. Search Settings

Database(s)	ACToR: Aggregated Computational Toxicology Resource
Search Mode	By Formula or Mass
Mass Tolerance	5 ppm
Max. # of results per compound	20
Max. # of Predicted Compositions	3

Database(s)
The selected databases are searched.

<p>APPLY SPECTRAL DISTANCE</p>	<p>Parameters of 'Apply Spectral Distance'</p> <p>Show Advanced Parameters</p> <p>1. Pattern Matching</p> <table border="1"> <tr><td>Mass Tolerance</td><td>5 ppm</td></tr> <tr><td>Intensity Tolerance [%]</td><td>30</td></tr> <tr><td>Intensity Threshold [%]</td><td>0.1</td></tr> <tr><td>S/N Threshold</td><td>3</td></tr> <tr><td>Use Dynamic Recalibration</td><td>True</td></tr> </table> <p>Mass Tolerance This parameter specifies the mass tolerance to be used for isotope search. Minimum value = 0.1 ppm Maximum value = 20 ppm</p>	Mass Tolerance	5 ppm	Intensity Tolerance [%]	30	Intensity Threshold [%]	0.1	S/N Threshold	3	Use Dynamic Recalibration	True
Mass Tolerance	5 ppm										
Intensity Tolerance [%]	30										
Intensity Threshold [%]	0.1										
S/N Threshold	3										
Use Dynamic Recalibration	True										
<p>DIFFERENTIAL ANALYSIS</p>	<p>Parameters of 'Differential Analysis'</p> <p>Show Advanced Parameters</p> <p>1. General Settings</p> <table border="1"> <tr><td>Log10 Transform Values</td><td>True</td></tr> </table> <p>Log10 Transform Values This parameter specifies whether area values should be log10 transformed prior to analysis.</p>	Log10 Transform Values	True								
Log10 Transform Values	True										

Table S2. Average response factor of internal standards.

Internal standard	Response factor (Peak area mL ng ⁻¹)
Acetaminophen	435189
Caffeine	263112
Reserpine	354877
Sulfadimethoxine	563987
Sulfaguanidine	145817
Terfenadine	1408605
Val-Tyr-Val	370978
AVERAGE	506081

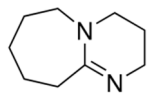
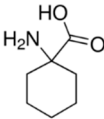
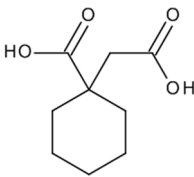
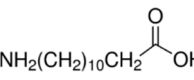
Table S3. Table of Log Kow vs Retention time (RT) of the analytical reference standards.

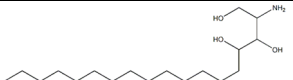
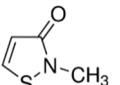
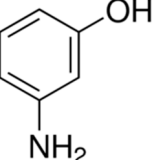
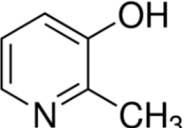
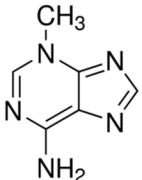
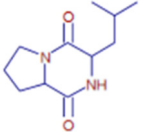
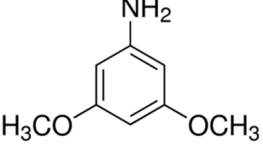
Analite	RT (min)	log Kow (log P)
L-Histidine	0.78	-1.26
Chlormequat	0.79	-3.80
3-hydroxy-2-methylpyridine	0.84	-0.29
Nicotine	0.84	0.72
3-methyladenine	0.80	-0.98
Triisopropanolamine	0.83	-0.07
Sulfaguanidine	0.85	-1.22
L-Pyroglutamic acid	0.94	-2.39
L-Tyrosine	0.97	0.38
Cotinine	1.03	-0.23
Dimethyldithiophosphate	1.20	0.65
Urocanic acid	1.29	0.01
Methamidophos	1.46	-0.82
Acephate	1.84	-0.85
Acetaminophen	1.95	0.46
Omethoate	2.25	0.06
Diethylthiophosphate	2.41	0.68
6-methoxyquinoline	2.79	2.17
5-hydroxy-thiabendazole	2.86	1.73
Carbendazim	2.90	1.52
Simazine 2-Hydroxy	2.92	-1.22
2-diethylamino-6-methyl pyrimidin-4-ol/one	2.96	1.11
Vancomycin	3.00	-1.44
PEG n5	3.08	-2.59
Caffeine	4.08	-0.07
Desisopropylatrazine	4.43	1.16
Val-Tyr-Val	4.86	0.80
6-Chloronicotinic acid	5.33	0.98
4-nitrophenol	5.77	1.57
acetamiprid-N-desmethyl	6.08	0.65
Cocaine	6.26	2.17
Cefoperazone	6.38	1.43
Salicylic acid	7.19	2.06
Sulfadimethoxine	7.67	1.63
Malathion dicarboxylic acid	7.78	1.48
Pyroquilon	10.00	1.40
Dichlorvos	10.15	0.71
Pyrimethanil	10.34	2.84
Bentazone	10.63	2.80
Trichlorfon (Dylox)	10.90	0.43
Phenytoin	11.08	2.29
Bromoxynil	11.25	2.95
Dibutyl phthalate	11.55	4.82
Diethyl phthalate	11.55	2.70
Pyrene	12.08	5.17
p-Toluenesulfonamide	12.15	0.79
Benodanil	12.20	3.23

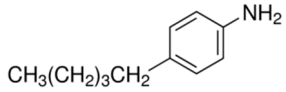
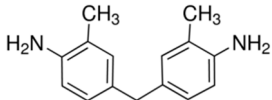
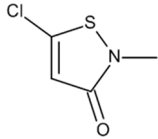
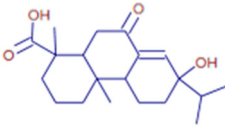
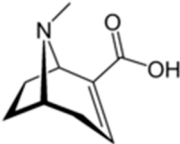
3,5,6-Trichloro-2-pyridinol	12.71	2.16
2,4-D	12.77	2.59
Isoproturon	12.86	2.32
N,N-diethyl-m-toluamide/DEET	13.17	1.96
Reserpine	13.19	3.32
MCPA	13.32	2.49
Inabenzfide	14.27	2.67
TCMTB	14.29	3.12
Acetochlor mercapturate	14.75	2.86
Alachlor mercapturate	14.75	2.86
N,N'-Dicyclohexylurea	14.79	3.10
Valproic acid	14.89	2.72
Flamprop	15.18	3.47
Mecoprop	15.19	2.84
Hydroxy-tebuconazole	15.42	2.50
3-phenoxybenzoic acid	15.64	3.91
4-Fluoro-3-phenoxybenzoic acid	15.83	4.05
D,L-Camphor	16.14	2.13
Methyl dihydrojasmonate	16.14	2.67
Tepraloxym	16.28	2.88
Fenhexamid	16.54	4.02
Benzophenone-3 (Oxybenzone)	16.59	3.64
Acetochlor	16.61	2.92
Fluopyram	16.68	4.36
Fenvalerate free acid	16.72	3.33
Triclosan glucuronide	16.72	2.53
Rifaximin	16.85	3.22
Metolachlor	16.89	3.00
Dimethyl sebacate	16.89	2.79
Benzoic acid	16.98	1.89
Prochloraz	17.15	3.80
Fipronil	17.66	4.76
Triclosan sulfate	17.71	4.66
Dinoterb	17.77	3.42
Spinosad A (Spinosyn A)	18.21	4.80
Butocarboxim	18.27	1.49
Chlorfenvinphos	18.43	4.51
3,5-ditert-butyl-4-hydroxybenzaldehyde	18.54	4.77
Fipronil sulfone	18.60	7.44
Hexadecanedioic acid	19.15	5.05
Dibutyl hexanodioate	19.29	4.22
Citroflex A-4	19.34	6.49
Benazol P	19.38	4.30
Monobutyl phthalate	19.53	2.72
Triclosan	19.65	5.17
Tributyl phosphate	19.86	4.26
Galaxolidone	19.96	5.50
Ethyl Oleate	20.25	8.69
4-tert-Butylcyclohexyl acetate	20.47	3.96

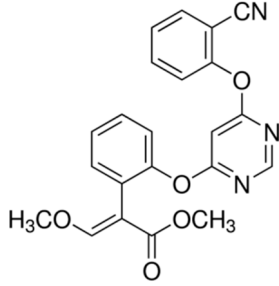
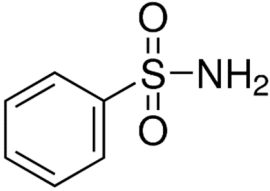
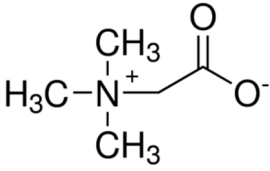
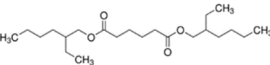
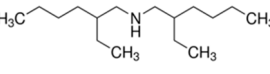
Dibutyl sebacate	20.89	5.97
Dipentyl phthalate	21.00	5.89
Palmitoyl ethanolamide	21.32	5.82
Hexadecanamide	21.48	6.84
Palmitoleic acid	21.51	6.64
Oleamide	21.56	7.07
Avermectin B1a (Abamectin)	21.57	6.51
Benzyl octyl adipate	21.58	6.50
Triethyleneglycol bis(2-ethylhexanoate)	21.66	5.57
Bis(2-ethylhexyl)adipate	22.04	7.85
Salinomycin	22.06	6.10
1-Stearoylglycerol	22.11	7.23
Ivermectin B1a	22.19	6.61
Nigericin	22.26	4.82
Octyl decyl phthalate	22.39	9.34
Stearamide	22.45	6.70
2,2-Methylenebis(4-ethyl-6-tert-butylphenol)	22.90	6.24
Dodecyl sulfate	22.92	5.39
Erucamide	22.93	9.74
Irgafos 168	25.10	12.56

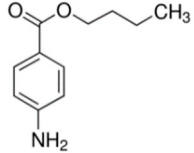
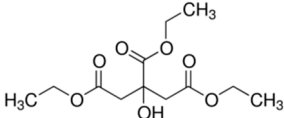
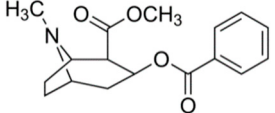
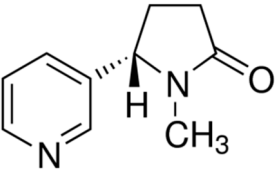
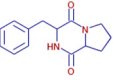
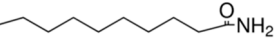
Table S4. Identified compounds and spectrometric and chromatographic criteria.

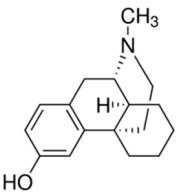
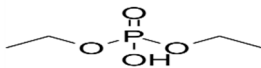
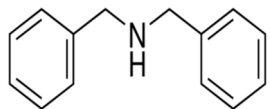
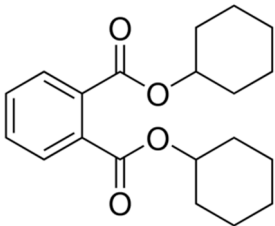
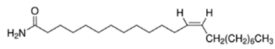
Compound (CAS number)	Structure	Δ Mass (ppm) ^a	Isotopic pattern (SFit %) ^b	MS ² match ^c	Rt _{exp} (min) ^d	Rt _{theo} (min) ^e	MS ³ Match ^f	Description [Reference]	Detected areas ^g	Maximum estimated concentration (pg m ⁻³) ^h
1,8-Diazabicyclo [5.4.0]undec-7-ene (6674-22-2)		0.01	95	77.1	3.32	5.75	f1, f2	Catalyst/Endogenous metabolite	U	15.68
1-aminocyclohexanecarboxylic acid (2756-85-6)		0.29	88	90.3	3.94	3.97	MS ³ (CD)	Aminoacid	R	38.38
1-(carboxymethyl)cyclohexanecarboxylic acid (67950-95-2)		0.05	70	80.1	4.71	5.87	MS ³ (CD)	Pharmaceutical Secondary Standard	U, R, I	94.36
12-Aminododecanoic acid (693-57-2)		0.12	86	82.8	13.66	13.16	MS ³ (CD)	Bacterial metabolite/corrosion inhibitor	R, I	157.13

2-Amino-1,3,4-octadecanetriol (13552-11-9)		-0.03	92	70.3	16.59	16.48	MS ³ (CD)	Antiasthmatics/ Endogenous metabolite	R	9.23
2-methyl-4-isothiazolin-3-one (2682-20-4)		0.14	92	98.4	1.44	1.67	n.a.	Biocide/ Extractable&Leachables	U, R, I	100.60
3-aminophenol (591-27-5)		0.12	78	97	0.79	1.87	n.a.	Pesticide/Industrial Chemicals	U, R, I	47.82
3-hydroxy-2-methylpyridine (1121-25-1)		0.1	81	98.9	0.85	0.85*	n.a.	Intermediate in vitamin B6 metabolism	U, R, I	40.40 ^{Ref st}
3-Methyladenine (5142-23-4)		-0.04	91	95.6	0.80	0.80*	MS ³ (CD)	Human metabolite/Endogenous metabolite	U, I	8.86 ^{Ref st}
3-(2-methylpropyl)-octahydro- pyrrolo[1,2-a]pyrazine-1,4-dione (2873-36-1)		0.06	81	96.6	6.12	6.91	MS ³ (CD)	Amino acid-Flavouring ingredient	U, I	50.46
3,5-dimethoxyaniline (10272-07-8)		-0.01	70	71.7	0.80	2.55	n.a.	Medication	U	9.75

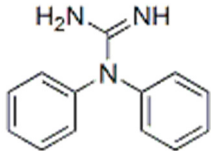
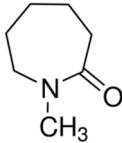
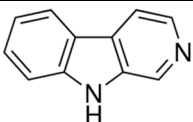
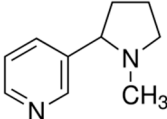
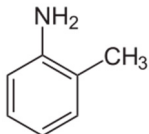
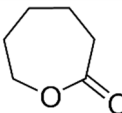
4-Pentylaniline (33228-44-3)		0.21	96	81.9	5.31	10.20	n.a.	Antimicrobial, colorant/ Extractables&Leachables	U, R, I	15.50
4,4'-Methylenebis(2-methylaniline) (838-88-0)		-0.07	70	73.1	2.96	5.70	n.a.	Primary aromatic amine (cosmetic, food, personal care)	I	16.56
5-Chloro-2-methyl-4-isothiazolin-3-one (26172-55-4)		0.11	90	78.6	10.57	10.05	f1, f2	Biocide/Excipients-additives-colorants	R	18.00
7-hydroxy-1,4a-dimethyl-9-oxo-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-1-carboxylic acid		-0.24	86	75	16.72	15.48	f2	Endogenous metabolite, natural product/medicine	U, R, I	173.34
Anhydroecgonine (127379-23-1)		0.08	78	71.9	0.88	1.70	MS ³ (CD)	Chemical intermediate from cocaine/Drugs of abuse/Illegal drugs	U, I	16.20

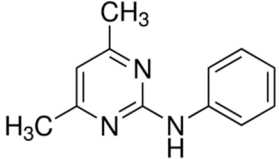
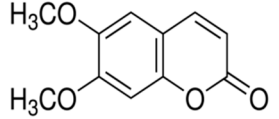
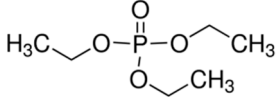
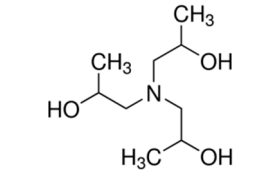
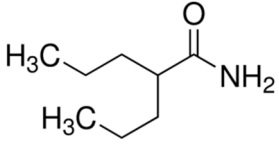
Azoxystrobin (131860-33-8)		0.18	88	94.3	15.10	15.10*	MS ³ (CD)	Pesticide/fungicide	U	36.25 ^{Ref st}
Benzenesulfonamide (98-10-2)		0.15	81	82.5	12.18	5.20	MS ³ (CD)	Inhibitor of human carbonic anhydrase B/Textile chemicals/auxiliary/dyes	R	17.41
Betaine (107-43-7)		-0.03	79	94.3	7.48	6.86	n.a.	Inhibitor/Endogenous metabolite/lipotropic drug	R	12.29
Bis(2-ethylhexyl)adipate (103-23-1)		0.03	83	88.1	22.55	22.66	MS ³ (CD)	Plasticizer/Industrial chemicals/Personal care products	U, R, I	374.79
Bis(2-ethylhexyl) amine (106-20-7)		0.1	86	94.5	15.87	23.30	MS ³ (CD)	Surfactant/Industrial chemicals	U	19.48

Butyl 4-aminobenzoate (94-25-7)		0.09	99	81.9	16.32	15.10	MS ³ (CD)	Local anaesthetic/Therapeutics/prescription drugs	R	14.45
Citroflex 2 (77-93-0)		0.09	73	97.8	10.87	8.50	MS ³ (CD)	Plasticizer/Industrial chemicals	U, R, I	42.38
Cocaine (50-36-2)		0.18	70	95.5	6.25	6.26	MS ³ (CD)	Drugs	U	28.13 ^{Ref st}
Cotinine (15569-85-4)		0.2	70	71.3	1.03	1.03	f2	Major metabolite of nicotine/Endogenous metabolite	U, I	67.48 ^{Ref st}
Cyclo(phenylalanyl-prolyl) (3705-26-8)		0.14	91	93.7	7.27	7.93	MS ³ (MzCloud)	Metabolite of organic compounds	U	12.20
Decanamide (2319-21-1)		0.15	84	91.3	17.07	16.68	f1, f2	Derives from decanoic acid	U, R, I	111.18

Dextrorphan (125-73-5)		0.33	93	90.1	14.57	14.28	f2	Pyschoactive drugs	R	21.67
Diethyl phosphate (598-02-7)		0.01	96	97.8	8.85	5.05	MS ³ (CD)	Metabolite of chlorpyrifos	U, R, I	24.36
Dibenzylamine (103-49-1)		0.01	77	98.4	5.88	8.72	MS ³ (CD)	Indirect additives food contact	U	86.46
Dicyclohexyl phthalate (84-61-7)		0.1	78	96.4	21.01	21.04	MS ³ (CD)	Adhesive/Industrial chemicals	R, I	121.70
Erucamide (112-84-5)		0.24	71	96.6	22.88	23.18	MS ³ (CD)	Slip promoter/Industrial chemicals	U, R, I	64.61

Ethoprophos (13194-48-4)		0.21	83	75.8	16.7 0	16.69	MS ³ (CD)	Nematicide/insecticide	U, I	37.67 ^{Ref st}
Imidacloprid (138261-41-3)		-0.09	71	97.8	5.32	5.32	MS ³ (MzClou d)	Insecticide	U	20.31 ^{Ref st}
L-Glutamic acid (617-65-5)		0.22	71	89.7	0.79	0.52	MS ³ (CD)	Peptide/Endogenous metabolite	R	11.25
Metalaxyl (57837-19-1)		0.2	89	97.1	13.3 7	13.37	MS ³ (CD)	Fungicide	U	14.24 ^{Ref st}
N-Benzylethanolamine (104-63-2)		0.03	84	85.2	2.00	3.01	MS ³ (CD)	Corrosion inhibitor	R	112.91
N,N-dimethyldecylamine-N-oxide (2605-79-0)		-0.17	84	94.5	13.7 0	14.17	f1, f2	Environmental contaminant/xenobiotic/I ndustrial chemicals	U, R, I	119.45

N,N'-Diphenylguanidine (20277-92-3)		-0.18	81	96.7	4.62	7.03	f1, f2	Complexing agent	U, R, I	251.29
N-Methylcaprolactam (2556-73-2)		-0.06	71	70.9	6.55	6.22	n.a.	Catalyst	R	32.16
Norharman (244-63-3)		0.17	86	96.8	4.21	5.29	f1, f2	Repellent/Endogenous metabolite	U, R, I	15.82
Nicotine (22083-74-5)		0.23	91	96.4	0.84	0.84	f2	Insecticide/drugs	U, I	55.67 ^{Ref st}
o-toluidine (1885-29-6)		-0.1	88	86.3	0.85	2.59	n.a.	Intermediate in the synthesis of the large-volume herbicides	R, U	68.51
Oxepanone (502-44-3)		0.01	94	94.4	7.48	6.86	n.a.	Lactone	R, I	13.19

Pyrimethanil (53112-28-0)		-0.03	89	98.5	10.36	10.34	f1, f2	Fungicide	U	21.84 ^{Ref st}
Scoparone (120-08-1)		0.2	90.1	98	7.59	7.90	MS ³ (MzCloud)	Natural organic compound	I	29.99
Triethyl phosphate (78-40-0)		0.04	87	98.7	8.85	7.89	MS ³ (CD)	Flame retardant	U, R, I	246.33
Triisopropanolamine (122-20-3)		-0.38	70	92.2	0.82	0.83	MS ³ (CD)	Amine/Employed in textiles and cosmetics	R	17.23 ^{Ref st}
Valpromide (2430-27-5)		0.26	76	93	10.57	10.05	n.a.	Metabolite from valproic acid/Prescription drug	R	19.39

^aΔmass (ppm): mass error

^bIsotopic pattern (SFit %): match between the experimental isotopic pattern and the theoretical one

^cMS² match: match between the experimental and the MS² spectra in the mzCloud library

^dRt_{exp}: experimental retention time;

^eRt_{pred}: predicted retention time based on log P

^fMS³ match: match between the experimental and the MS³ spectra in the mzCloud library: n.a. (MS³ not available in CD); f1 (mzCloud does not contain a MS³ spectra of this compound); f2 (the experimental MS³ spectra do not match with that stored in mzCloud or with the in-silico fragmentation)

^gDetected areas: I= Industrial; U=urban; R=rural

^hMaximum estimated concentration: Maximum concentration taking into account the maximum area detected and the average response factor of the seven substances employed in the QCRM (Ref st: semiquantification)

performed with its own reference standard)

Table S5. Compounds more probably present in industrial areas (Industrial-Rural).

Compound	Formula	Log2 Fold Change	p-value	Identified level
3-Methyladenine	C ₈ H ₇ N ₅	4.67	5.45 × 10 ⁻¹⁰	Level 1
Anhydroecgonine	C ₉ H ₁₃ NO ₂	4.06	4.11 × 10 ⁻⁷	Level 1
Nicotine	C ₁₀ H ₁₄ N ₂	3.58	2.49 × 10 ⁻⁹	Level 1
3-Hydroxy-2-methylpyridine	C ₆ H ₇ NO	3.56	2.29 × 10 ⁻⁹	Level 1
3-(3-pyridinyl)propanoic acid	C ₈ H ₉ NO ₂	4.10	1.50 × 10 ⁻⁹	Level 2 (ms3)
Nikethamide	C ₁₀ H ₁₄ N ₂ O	3.21	5.45 × 10 ⁻¹⁰	Level 2 (ms2)
Phenacetin	C ₁₀ H ₁₃ NO ₂	3.27	7.43 × 10 ⁻⁹	Level 2 (ms3)
2-Hydroxyphenylalanine	C ₉ H ₁₁ NO ₃	3.46	5.63 × 10 ⁻¹⁰	Level 2 (ms3)
3-(2,6-Dioxocyclohexyl)propanenitrile	C ₉ H ₁₁ NO ₂	4.53	5.76 × 10 ⁻¹⁰	Level 2 (ms3)
5-(Cyanomethyl)-1H-imidazole-4-carbonitrile	C ₆ H ₄ N ₄	5.59	1.26 × 10 ⁻⁷	Level 2 (ms3)
2,2,2-Trifluoro-1-(1-naphthyl)ethanol	C ₁₂ H ₉ F ₃ O	5.12	2.10 × 10 ⁻⁶	Level 2 (ms2)
4-Hydroxybenzaldehyde	C ₇ H ₆ O ₂	5.25	5.45 × 10 ⁻¹⁰	Level 2 (ms2)
ZV4	C ₅ H ₁₁ NO	5.60	3.07 × 10 ⁻⁶	Level 2 (ms2)
Ethyl 4-hydroxy-3-methoxyphenylacetate	C ₁₁ H ₁₄ O ₄	5.83	9.92 × 10 ⁻⁸	Level 2 (ms2)
Hydroferulic acid	C ₁₀ H ₁₂ O ₄	6.85	7.01 × 10 ⁻¹⁰	Level 2 (ms3)
3,5-Dimethoxy-4-hydroxybenzoate	C ₉ H ₁₀ O ₅	5.40	5.51 × 10 ⁻¹⁰	Level 2 (ms3)
Ethyl gallate	C ₉ H ₁₀ O ₅	4.41	5.2 × 10 ⁻¹⁰	Level 2 (ms3)
Pyroquilon	C ₁₁ H ₁₁ NO	3.01	5.77 × 10 ⁻¹⁰	Level 3
6-Methoxyquinoline	C ₁₀ H ₉ NO	3.18	5.45 × 10 ⁻¹⁰	Level 3
3-hydroxy-3-methylpentanedioic acid	C ₆ H ₁₀ O ₅	3.86	2.44 × 10 ⁻⁸	Level 3
4,6-Bis(1-aziridinyl)-N-(2,2-dimethyl-1,3-dioxan-5-yl)-1,3,5-triazin-2-amine	C ₁₃ H ₂₀ N ₆ O ₂	3.72	1.81 × 10 ⁻⁸	Level 3
Methyl 2-oxo-4-(trifluoromethyl)cyclohexanecarboxylate	C ₉ H ₁₁ F ₃ O ₃	3.92	1.06 × 10 ⁻⁹	Level 3
Diaminotoluene	C ₇ H ₁₀ N ₂	3.23	7.32 × 10 ⁻⁰⁹	Level 3
Ethyl 1-hydroxy-2,3,4,9-tetrahydro-1H-carbazole-6-carboxylate	C ₁₅ H ₁₇ NO ₃	3.90	5.45 × 10 ⁻¹⁰	Level 3
1-propylimidazole	C ₆ H ₁₀ N ₂	4.01	1.70 × 10 ⁻⁸	Level 3
3,3,3-Trifluoro-2-(2-furylmethyl)propanoic acid	C ₈ H ₇ F ₃ O ₃	3.74	5.54 × 10 ⁻¹⁰	Level 3
N'-[5-chloro-2-(4-chlorophenoxy)-4-(1H-pyrrol-1-yl)phenyl]-N,N-dimethyliminoforamide	C ₁₉ H ₁₇ Cl ₂ N ₃ O	5.08	5.45 × 10 ⁻¹⁰	Level 3
Methyl [5-methoxy-2-nitro-4-(trifluoromethyl)phenyl]acetate	C ₁₁ H ₁₀ F ₃ NO ₅	6.95	1.07 × 10 ⁻⁹	Level 3
6-Methylnicotinonitrile	C ₇ H ₆ N ₂	3.07	5.65 × 10 ⁻¹⁰	Level 3
5-acetyl-2,6-dimethyl-1,2,3,4-tetrahydropyridin-4-one	C ₉ H ₁₃ NO ₂	4.94	5.45 × 10 ⁻¹⁰	Level 3
1-(Diazidomethyl)-2-nitrobenzene	C ₇ H ₅ N ₇ O ₂	3.65	5.45 × 10 ⁻¹⁰	Level 3
5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,6-dimethoxy-4H-chromen-4-one	C ₁₈ H ₁₆ O ₈	3.81	5.45 × 10 ⁻¹⁰	Level 3

Compound	Formula	Log2 Fold Change	<i>p</i> -value	Identified level
4-Nitro-2-(1H-tetrazol-5-yl)aniline	C ₇ H ₆ N ₆ O ₂	5.02	5.62 × 10 ⁻¹⁰	Level 3
Xanthone	C ₁₃ H ₈ O ₂	3.18	5.45 × 10 ⁻¹⁰	Level 3
Fenuron	C ₉ H ₁₂ N ₂ O	3.26	5.45 × 10 ⁻¹⁰	Level 3
1,2,3,4-Tetramethyl-1,3-cyclopentadiene	C ₉ H ₁₄	3.16	5.10 × 10 ⁻⁶	Level 3
2,7-Difluoro-4,5-dimethoxy-2'H,5'H-spiro[fluorene-9,4'-i midazolidine]-2',5'-dione	C ₁₇ H ₁₂ F ₂ N ₂ O ₄	7.53	1.54 × 10 ⁻⁹	Level 3
3,5-Octadiyne	C ₈ H ₁₀	3.14	1.01 × 10 ⁻⁹	Level 3
N'-[(2,4-dihydroxyphenyl)methylene]-4-methylbenzene sulfonohydrazide	C ₁₄ H ₁₄ N ₂ O ₄ S	3.29	1.24 × 10 ⁻⁸	Level 3
1-Naphthylisocyanate	C ₁₁ H ₇ NO	4.43	5.65 × 10 ⁻¹⁰	Level 3
(1S,8S,9S,10S,13R)-6,9,10-trimethyl-2-oxo-4,14-dioxatetra cyclo[7.5.0.0Åa,ÅaÅ1.0ÅI,Å]tetradeca-3(7),5-dien-8-yl acetate	C ₁₇ H ₂₀ O ₅	3.46	5.45 × 10 ⁻¹⁰	Level 3
8-Hydroxyquinoline	C ₉ H ₇ NO	5.71	5.75 × 10 ⁻¹⁰	Level 3
Umbelliferone	C ₉ H ₆ O ₃	3.12	5.45 × 10 ⁻¹⁰	Level 3
S-(Allylcarbamothioyl)-L-cysteine	C ₇ H ₁₂ N ₂ O ₂ S ₂	3.20	5.45 × 10 ⁻¹⁰	Level 3
Dihydrothymine	C ₅ H ₈ N ₂ O ₂	4.21	3.97 × 10 ⁻⁷	Level 3
3-hydroxybenzylhydrazine	C ₇ H ₁₀ N ₂ O	4.11	5.79 × 10 ⁻¹⁰	Level 3
Serotonin	C ₁₀ H ₁₂ N ₂ O	4.44	5.55 × 10 ⁻¹⁰	Level 3
2-(5-Amino-1H-pyrazol-1-yl)ethanol	C ₅ H ₉ N ₃ O	4.45	1.17 × 10 ⁻⁹	Level 3
119183	C ₇ H ₇ N ₃	3.16	6.22 × 10 ⁻¹⁰	Level 3
(4-Methyl-1H-imidazol-5-yl)methanol	C ₅ H ₈ N ₂ O	3.38	2.07 × 10 ⁻⁹	Level 3
2-Methyl-2H-indazol-4-amine	C ₈ H ₉ N ₃	4.75	5.45 × 10 ⁻¹⁰	Level 3
6-Methyl-2-pyridinemethanol	C ₇ H ₉ NO	3.76	1.34 × 10 ⁻⁶	Level 3
Aminobenzodiazapine	C ₉ H ₁₁ N ₃ O	4.38	5.45 × 10 ⁻¹⁰	Level 3
11-Aminoundecanoic acid	C ₁₁ H ₂₃ NO ₂	4.94	5.45 × 10 ⁻¹⁰	Level 3
7-Amino-3,4-dihydro-2(1H)-quinoxalinone	C ₈ H ₉ N ₃ O	4.60	8.70 × 10 ⁻¹⁰	Level 3
4-[3-(5H-Tetrazol-5-ylidene)triazanyl]benzoic acid	C ₈ H ₇ N ₇ O ₂	4.27	5.45 × 10 ⁻¹⁰	Level 3
2-NP-AHD	C ₁₀ H ₈ N ₄ O ₄	4.62	5.48 × 10 ⁻¹⁰	Level 3
4,6-Diamino-1-(4-nitrophenyl)-1,3,5-triazin-2(1H)-one	C ₉ H ₈ N ₆ O ₃	4.95	2.82 × 10 ⁻⁶	Level 3
Methyl piperonyl ketone	C ₁₀ H ₁₀ O ₃	4.42	5.77 × 10 ⁻¹⁰	Level 3
4,7-dioxosebacic acid	C ₁₀ H ₁₄ O ₆	4.11	9.78 × 10 ⁻⁹	Level 3
6-Methoxy-2-methyl-3-(3-oxobutyl)-4(1H)-quinolinone	C ₁₅ H ₁₇ NO ₃	3.15	5.45 × 10 ⁻¹⁰	Level 3
4-[(E)-[(5-Amino-1H-tetrazol-1-yl)imino]methyl]benzaldehyde	C ₉ H ₈ N ₆ O	3.16	8.03 × 10 ⁻¹⁰	Level 3
NP-018817	C ₁₅ H ₂₄ O ₄	3.20	8.64 × 10 ⁻⁴	Level 3
Ethyl 5-formyl-2,4-dimethyl-1H-pyrrole-3-carboxylate	C ₁₀ H ₁₃ NO ₃	3.79	2.48 × 10 ⁻⁹	Level 3
Glutaric acid	C ₅ H ₈ O ₄	5.61	7.21 × 10 ⁻¹⁰	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
p-Xylylenediamine	C ₈ H ₁₂ N ₂	3.18	5.45 × 10 ⁻¹⁰	Level 3
6-Vinylnicotinonitrile	C ₈ H ₆ N ₂	4.30	5.45 × 10 ⁻¹⁰	Level 3
1-deoxy-1-(2,4-difluorophenyl)-β-D-ribofuranose	C ₁₁ H ₁₂ F ₂ O ₄	5.80	5.61 × 10 ⁻¹⁰	Level 3
(-)-Ecgonine methyl ester	C ₁₀ H ₁₇ NO ₃	3.90	1.59 × 10 ⁻⁹	Level 3
(2E)-3-(3,4-Dimethoxyphenyl)acrylic acid	C ₁₁ H ₁₂ O ₄	4.17	5.45 × 10 ⁻¹⁰	Level 3
NP-019992	C ₁₀ H ₁₂ O ₄	3.17	2.34 × 10 ⁻⁵	Level 3
1-propyl-1H-benzo[d]imidazole hydrobromide	C ₁₀ H ₁₂ N ₂	3.12	1.21 × 10 ⁻⁷	Level 3
Ethyl 4,4,4-trifluoro-3-hydroxy-3-methoxybutanoate	C ₇ H ₁₁ F ₃ O ₄	3.47	5.45 × 10 ⁻¹⁰	Level 3
Methyl 4-hydroxy-3-methoxy-5-(trifluoromethyl)benzoate	C ₁₀ H ₉ F ₃ O ₄	4.03	6.04 × 10 ⁻¹⁰	Level 3
4-Tolylurea	C ₈ H ₁₀ N ₂ O	3.87	1.13 × 10 ⁻⁹	Level 3
NP-020713	C ₂₀ H ₂₆ O ₄	4.20	5.45 × 10 ⁻¹⁰	Level 3
7-Aminoindole	C ₈ H ₈ N ₂	3.69	2.08 × 10 ⁻⁹	Level 3
2,3,5-Trimethoxy-1,4-benzenediol	C ₉ H ₁₂ O ₅	3.22	5.45 × 10 ⁻¹⁰	Level 3
Combretastatin	C ₁₈ H ₂₂ O ₆	3.55	5.45 × 10 ⁻¹⁰	Level 3
7β,12α-Dihydroxykaurenolide	C ₂₀ H ₂₈ O ₄	3.12	5.06 × 10 ⁻⁸	Level 3
Syringaldehyde	C ₉ H ₁₀ O ₄	4.40	5.46 × 10 ⁻¹⁰	Level 3
Penicillic Acid	C ₈ H ₁₀ O ₄	3.12	5.45 × 10 ⁻¹⁰	Level 3
4-Methoxysalicylic acid	C ₈ H ₈ O ₄	3.72	5.45 × 10 ⁻¹⁰	Level 3
4-Methylumbelliferone hydrate	C ₁₀ H ₈ O ₃	3.17	5.45 × 10 ⁻¹⁰	Level 3
1,3-Octadiyne	C ₈ H ₁₀	3.01	1.25 × 10 ⁻⁹	Level 3
3-[(4-Phenyl-2-butanyl)amino]propanenitrile	C ₁₃ H ₁₈ N ₂	3.29	2.06 × 10 ⁻⁹	Level 3
Metrafenone	C ₁₉ H ₂₁ BrO ₅	7.20	5.45 × 10 ⁻¹⁰	Level 3
(1R,2R)-1-(4-Hydroxy-3-methoxyphenyl)-1,2,3-propanetriol	C ₁₀ H ₁₄ O ₅	3.74	5.45 × 10 ⁻¹⁰	Level 3
4-(2-Methyl-2-propanyl)-2-(trifluoromethyl)cyclohexanone	C ₁₁ H ₁₇ F ₃ O	4.78	3.74 × 10 ⁻⁶	Level 3
Dimethyl (3-oxocyclohexyl)malonate	C ₁₁ H ₁₆ O ₅	4.29	5.45 × 10 ⁻¹⁰	Level 3
Radicinin	C ₁₂ H ₁₂ O ₅	3.74	5.45 × 10 ⁻¹⁰	Level 3
2-Methoxy-5-(trifluoromethoxy)benzyl alcohol	C ₉ H ₉ F ₃ O ₃	3.62	5.45 × 10 ⁻¹⁰	Level 3
2-deoxyglucose	C ₆ H ₁₂ O ₅	4.43	1.28 × 10 ⁻⁹	Level 3
4-Phenyl-2-(trifluoromethyl)-1,2,4-butanetriol	C ₁₁ H ₁₃ F ₃ O ₃	4.20	5.45 × 10 ⁻¹⁰	Level 3
1,1,2,2,3,3,4,4,5,5-Cyclopentanedecol	C ₅ H ₁₀ O ₁₀	4.73	5.45 × 10 ⁻¹⁰	Level 3
7-hydroxy-6-methoxy-2H-chromen-2-one	C ₁₀ H ₈ O ₄	4.49	5.45 × 10 ⁻¹⁰	Level 3
N4-(3-chloro-4-fluorophenyl)-6-methylpyrimidine-2,4-diamine hydrochloride	C ₁₁ H ₁₀ ClFN ₄	4.79	5.45 × 10 ⁻¹⁰	Level 3
5,6,7-Trimethoxy-2H-chromen-2-one	C ₁₂ H ₁₂ O ₅	4.02	2.36 × 10 ⁻⁷	Level 3
MW5143500	C ₉ H ₁₀ O ₄	3.69	5.45 × 10 ⁻¹⁰	Level 3
NP-002855	C ₁₂ H ₂₂ O ₄	3.19	5.45 × 10 ⁻¹⁰	Level 3
dihydralazine	C ₈ H ₁₀ N ₆	3.41	8.06 × 10 ⁻⁵	Level 3
3,4-Dimethoxy-5-(3,3,3-trifluoropropyl)benzoic acid	C ₁₂ H ₁₃ F ₃ O ₄	4.74	5.46 × 10 ⁻¹⁰	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
3964	C ₇ H ₈ N ₂ O	3.64	5.45 × 10 ⁻¹⁰	Level 3
(1S,4R,7S,8S,11S)-9-tert-butyl-7,9-dihydroxy-3,5,12-trioxatetracyclo[6.6.0.0.0]tetradecane-2,6,13-trione	C ₁₅ H ₁₈ O ₈	4.62	5.46 × 10 ⁻¹⁰	Level 3
6,7-Dihydro-8(5H)-quinolinone	C ₉ H ₉ NO	3.17	1.85 × 10 ⁻⁹	Level 3
2,2,2-Trifluoro-1-(3,4,5-trimethoxyphenyl)ethanol	C ₁₁ H ₁₃ F ₃ O ₄	3.53	5.45 × 10 ⁻¹⁰	Level 3
Aldicarb oxime	C ₅ H ₁₁ NOS	3.32	7.57 × 10 ⁻¹⁰	Level 3
Methyl 2-[[4-oxo-3,4-dihydrophthalazin-1-yl)methyl]thio]acetate	C ₁₂ H ₁₂ N ₂ O ₃ S	4.02	5.45 × 10 ⁻¹⁰	Level 3
NSC 131681	C ₈ H ₉ NO	4.06	7.30 × 10 ⁻¹⁰	Level 3
5-Ethylcyclohexane-1,3-dione	C ₈ H ₁₂ O ₂	4.79	2.29 × 10 ⁻⁹	Level 3
Cyclodecyl trifluoroacetate	C ₁₂ H ₁₉ F ₃ O ₂	3.51	5.45 × 10 ⁻¹⁰	Level 3
4,7-dihydroxy-4-(hydroxymethyl)-3,4a,8,8-tetramethyl-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-one	C ₁₅ H ₂₄ O ₄	4.01	3.30 × 10 ⁻⁸	Level 3
hymecromone	C ₁₀ H ₈ O ₃	3.09	5.45 × 10 ⁻¹⁰	Level 3
2-Diazonio-1-([2-(2,4-dinitrophenyl)amino]ethyl)aminoethenolate	C ₁₀ H ₁₀ N ₆ O ₅	4.73	5.45 × 10 ⁻¹⁰	Level 3
4-Nitro-N-(1H-tetrazol-5-yl)benzamide	C ₈ H ₆ N ₆ O ₃	3.87	5.45 × 10 ⁻¹⁰	Level 3
4-(3,4-DIMETHOXYPHENYL)BUTYRIC ACID	C ₁₂ H ₁₆ O ₄	4.06	5.45 × 10 ⁻¹⁰	Level 3
NP-019983	C ₂₀ H ₁₆ O ₆	4.20	5.49 × 10 ⁻¹⁰	Level 3
[(3S)-3-(5-Benzyl-1,3,4-oxadiazol-2-yl)-1-pyrrolidinyl](4-pyridinyl)methanone	C ₁₉ H ₁₈ N ₄ O ₂	3.48	5.45 × 10 ⁻¹⁰	Level 3
4-decyl-3-hydroxy-5-oxooxolane-2,3-dicarboxylic acid	C ₁₆ H ₂₆ O ₇	6.45	7.47 × 10 ⁻⁷	Level 3
ethyl 1-(3-nitro-2-thienyl)piperidine-4-carboxylate	C ₁₂ H ₁₆ N ₂ O ₄ S	5.49	5.46 × 10 ⁻¹⁰	Level 3
Prohexadione	C ₁₀ H ₁₂ O ₅	4.09	5.45 × 10 ⁻¹⁰	Level 3
N-(4-fluorophenyl)-2-methyl-5-(morpholinosulfonyl)-3-furamide	C ₁₆ H ₁₇ FN ₂ O ₅ S	7.44	6.30 × 10 ⁻¹⁰	Level 3
Cytidine	C ₉ H ₁₃ N ₃ O ₅	3.44	5.45 × 10 ⁻¹⁰	Level 3
DL-carvone	C ₁₀ H ₁₄ O	3.02	1.23 × 10 ⁻⁸	Level 3
Ethyl 3-hydroxy-4,4,4-trifluorobutyrate	C ₆ H ₉ F ₃ O ₃	5.23	5.75 × 10 ⁻⁷	Level 3
4-(tert-butyl)phenyl 3,5-dimethylisoxazole-4-carboxylate	C ₁₆ H ₁₉ NO ₃	3.66	5.45 × 10 ⁻¹⁰	Level 3
Ethyl orsellinate	C ₁₀ H ₁₂ O ₄	4.22	5.45 × 10 ⁻¹⁰	Level 3
3-Formylbenzoic acid	C ₈ H ₆ O ₃	3.50	5.45 × 10 ⁻¹⁰	Level 3
dl-Perillaldehyde	C ₁₀ H ₁₄ O	3.06	9.24 × 10 ⁻⁶	Level 3
NP-003553	C ₂₀ H ₃₄ O ₄	4.26	6.00 × 10 ⁻¹⁰	Level 3
LW8000000	C ₈ H ₈ O ₅	4.51	2.10 × 10 ⁻⁹	Level 3
8-[4-(3,4,5-Trifluorophenyl)cyclohexyl]-1,4-dioxaspiro[4.5]decane	C ₂₀ H ₂₅ F ₃ O ₂	3.06	2.64 × 10 ⁻⁶	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
6-anilino-2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carbonitrile	C ₁₁ H ₈ N ₄ O ₂	5.11	4.08 × 10 ⁻⁵	Level 3
(-)	C ₇ H ₁₅ N ₇ O ₂	8.28	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₆ F ₃ N ₆ O ₈ PS	7.60	5.15 × 10 ⁻⁹	Level 4
(-)	C ₁₂ H ₂₉ N ₄ O ₄ P	3.71	7.14 × 10 ⁻⁸	Level 4
(-)	C ₆ H ₇ F ₃ O ₄ P ₂	4.71	6.04 × 10 ⁻¹⁰	Level 4
(-)	C ₁₁ H ₁₅ F ₅ N ₄ OS	5.68	7.98 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₄ N ₇ P	8.61	4.62 × 10 ⁻⁸	Level 4
(-)	C ₉ H ₁₃ F ₃ O ₅	5.57	5.96 × 10 ⁻¹⁰	Level 4
(-)	C ₃ H ₄ N ₆ O ₃	7.11	1.46 × 10 ⁻⁹	Level 4
(-)	C ₄ H ₁₂ F ₂ N ₅ OPS	5.77	5.48 × 10 ⁻¹⁰	Level 4
(-)	C ₁₂ H ₉ N ₇ O ₄ P ₂	5.99	3.08 × 10 ⁻⁹	Level 4
(-)	C ₁₅ H ₁₆ FN ₂ P ₃ S	6.12	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₈ H ₁₀ N ₆ O ₆	5.55	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₄ N ₆ O ₃	4.22	3.91 × 10 ⁻⁴	Level 4
(-)	C ₄ H ₇ FN ₂ O ₅	7.11	4.23 × 10 ⁻⁹	Level 4
(-)	C ₆ H ₁₃ F ₂ N ₂ O ₅ P	6.07	2.51 × 10 ⁻⁶	Level 4
(-)	C ₁₂ H ₁₇ FN ₄ O ₄ S ₂	6.65	1.23 × 10 ⁻⁹	Level 4
(-)	C ₅ H ₁₂ O ₁₀	4.73	9.29 × 10 ⁻⁷	Level 4
(-)	C ₁₀ H ₂₂ F ₂ N ₄ OS ₃	5.64	6.64 × 10 ⁻¹⁰	Level 4
(-)	C ₂ H ₇ N ₁₀ O ₃ P	5.77	1.06 × 10 ⁻⁹	Level 4
(-)	C ₁₄ H ₂₂ N ₂ OP ₂ S	4.50	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₅ H ₁₆ FN ₄ P ₃	5.01	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₂₁ H ₃₀ ClO ₁₀ P	6.80	5.48 × 10 ⁻¹⁰	Level 4
(-)	C ₁₁ H ₁₆ F ₃ NO	3.00	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₁₃ F ₆ PS	3.65	5.63 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₁₃ FS	3.53	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₈ N ₁₀ P ₂	6.35	9.58 × 10 ⁻¹⁰	Level 4
(-)	C ₃ H ₅ Cl ₃ N ₂ O ₅	3.56	9.16 × 10 ⁻⁹	Level 4
(-)	C ₂₀ H ₂₁ F ₃ O	3.05	3.20 × 10 ⁻⁵	Level 4
(-)	C ₁₀ H ₁₁ F ₃ O ₄	4.53	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₇ H ₇ N ₂ O ₆ P	4.44	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₂₀ H ₂₀ F ₄ N ₂ O ₁₀	9.15	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₉ F ₃ O ₄	4.46	5.46 × 10 ⁻¹⁰	Level 4
(-)	C ₁₆ H ₂₅ FO ₃	4.45	5.47 × 10 ⁻¹⁰	Level 4
(-)	C ₁₀ H ₁₉ O ₂ P ₃	4.61	6.09 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₇ FN ₂ O ₃ P ₂	6.36	3.16 × 10 ⁻⁶	Level 4
(-)	C ₂₀ H ₂₁ F ₃ O ₃	4.84	5.45 × 10 ⁻¹⁰	Level 4

Compound	Formula	Log2 Fold Change	p-value	Identified level
(-)	C ₈ H ₁₅ FN ₄ O ₉ S	8.03	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₆ HBrCl ₂ N ₄ O	6.81	5.45 × 10 ⁻¹⁰	Level 4

(-) = No name described in CD

Table S6. Compounds more probably present in industrial areas (Industrial-Rural).

Compound	Formula	Log2 Fold Change	p-value	Identified level
Methcathinone	C ₁₀ H ₁₃ NO	-3.01	8.85 × 10 ⁻⁰⁴	Level 2 (ms2)
MHPG	C ₉ H ₁₂ O ₄	-3.25	5.35 × 10 ⁻¹⁰	Level 2 (ms3)
4-hydroxy-6-undecylpyran-2-one	C ₁₆ H ₂₆ O ₃	-3.12	5.46 × 10 ⁻¹⁰	Level 2 (ms3)
Euscaphic acid	C ₃₀ H ₄₈ O ₅	-3.30	5.23 × 10 ⁻¹⁰	Level 2 (ms3)
1-(3-Phenyl-prop-2-ynyl)-piperidine	C ₁₄ H ₁₇ N	-4.07	7.43 × 10 ⁻¹⁰	Level 2 (ms2)
5-Ethyl-5-(2-methylbutyl)-1,3-bis(2-oxiranylmethyl)-2,4-imidazolidindion	C ₁₆ H ₂₆ N ₂ O ₄	-3.40	5.46 × 10 ⁻¹⁰	Level 2 (ms3)
8-Amino-7-oxononanoic acid	C ₉ H ₁₇ NO ₃	-5.69	1.25 × 10 ⁻⁰⁴	Level 2 (ms3)
1-Aminocyclododecanecarboxylic acid	C ₁₃ H ₂₅ NO ₂	-3.22	5.95 × 10 ⁻¹⁰	Level 2 (ms2)
(2R,3R,4R,5S,6R)-2-(Hydroxymethyl)-6-propyl-3,4,5-piperidinetriol	C ₉ H ₁₉ NO ₄	-4.41	1.09 × 10 ⁻⁹	Level 2 (ms3)
2,2'-(1,7-Dioxa-4,10-diazacyclododecane-4,10-diyl)dietanol	C ₁₂ H ₂₆ N ₂ O ₄	-3.72	6.00 × 10 ⁻¹⁰	Level 2 (ms3)
DL-Carnitine	C ₇ H ₁₅ NO ₃	-4.13	5.45 × 10 ⁻¹⁰	Level 3
1,3-di-o-Tolylguanidine	C ₁₅ H ₁₇ N ₃	-7.60	5.45 × 10 ⁻¹⁰	Level 3
7-Hydroxycoumarinyl-γ-linolenate	C ₂₇ H ₃₄ O ₄	-3.08	2.83 × 10 ⁻⁰⁹	Level 3
Fenuron	C ₉ H ₁₂ N ₂ O	-3.33	5.45 × 10 ⁻¹⁰	Level 3
Metolachlor morpholinone	C ₁₄ H ₁₉ NO ₂	-3.71	5.45 × 10 ⁻¹⁰	Level 3
Diheptyl phthalate	C ₂₂ H ₃₄ O ₄	-4.48	2.25 × 10 ⁻⁴	Level 3
N-Boc-2-amino-2-methyl-1-propanol	C ₉ H ₁₉ NO ₃	-4.20	1.13 × 10 ⁻⁴	Level 3
4-Hydroxy-1-butanefulfonic acid	C ₄ H ₁₀ O ₄ S	-4.96	3.98 × 10 ⁻⁴	Level 3
Adipic acid dihydrazide	C ₆ H ₁₄ N ₄ O ₂	-3.13	1.35 × 10 ⁻⁹	Level 3
[2-(hydroxymethyl)-5,5,8a-trimethyl-1,4,4a,5,6,7,8,8a-occtahydronaphthalen-1-yl]methanol	C ₁₅ H ₂₆ O ₂	-3.27	8.35 × 10 ⁻¹⁰	Level 3
L-Pyroglutamic acid	C ₅ H ₇ NO ₃	-4.65	5.47 × 10 ⁻¹⁰	Level 3
Gabapentin	C ₉ H ₁₇ NO ₂	-4.23	5.42 × 10 ⁻⁹	Level 3
N-Acetylvaline	C ₇ H ₁₃ NO ₃	-3.51	4.79 × 10 ⁻⁴	Level 3
DL-Glutamine	C ₅ H ₁₀ N ₂ O ₃	-4.96	5.45 × 10 ⁻¹⁰	Level 3
2-Thiophenetellurol	C ₄ H ₄ STe	-5.53	5.55 × 10 ⁻⁰⁷	Level 3
2-Methyl-5,8,11-trioxa-2-azatetradecan-13-ol	C ₁₁ H ₂₅ NO ₄	-3.97	5.61 × 10 ⁻¹⁰	Level 3
5-Methyl-4-sulfanyl-2-(2,4,4-trimethyl-2-pentanyl)phenol	C ₁₅ H ₂₄ OS	-3.62	4.74 × 10 ⁻⁴	Level 3
Ethephon	C ₂ H ₆ ClO ₃ P	-3.23	5.35 × 10 ⁻⁰⁵	Level 3
(2E)-3-Ethoxy-N-[[3-hydroxy-4-(hydroxymethyl)cyclopentyl]carbonyl]acrylamide	C ₁₂ H ₂₀ N ₂ O ₅	-3.70	6.00 × 10 ⁻¹⁰	Level 3
8-(Dimethylamino)guanosine	C ₁₂ H ₁₈ N ₆ O ₅	-6.69	9.11 × 10 ⁻⁶	Level 3
11-Oxoetiocholanolone	C ₁₉ H ₂₈ O ₃	-4.24	5.45 × 10 ⁻¹⁰	Level 3
UNII:FD6L8T043R	C ₁₆ H ₂₆ N ₂ O ₄	-3.62	1.87 × 10 ⁻⁰⁴	Level 3
4-Nitro-2-(1H-tetrazol-5-yl)aniline	C ₇ H ₆ N ₆ O ₂	-3.16	8.46 × 10 ⁻⁹	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
2-Methyl-N-[3-(trifluoromethyl)phenyl]propanamide	C ₁₁ H ₁₂ F ₃ NO	-6.71	5.45 × 10 ⁻¹⁰	Level 3
3603307	C ₉ H ₁₉ NO ₃	-3.32	9.75 × 10 ⁻⁵	Level 3
2-Methyl-2-propanyl {2-[2-(2-hydroxyethoxy)ethoxy]ethyl}carbamate	C ₁₁ H ₂₃ NO ₅	-4.30	3.25 × 10 ⁻⁹	Level 3
2-Cyclohexylacetohydrazide	C ₈ H ₁₆ N ₂ O	-3.23	5.45 × 10 ⁻¹⁰	Level 3
(-)	C ₅ HF ₃ N ₂ OP ₂ S ₂	-7.18	8.74 × 10 ⁻¹⁰	Level 4
(-)	C ₅ H ₄ F ₄ N ₂ S ₃	-5.06	1.80 × 10 ⁻⁰⁹	Level 4
(-)	C ₄₅ H ₉₁ F ₂ N ₇ O ₆	-8.99	5.46 × 10 ⁻¹⁰	Level 4
(-)	C ₁₈ H ₂₉ N ₆ O ₂ P ₃	-3.07	5.46 × 10 ⁻¹⁰	Level 4
(-)	C ₈ H ₉ N ₇ O ₃	-3.05	2.13 × 10 ⁻⁹	Level 4
(-)	C ₄ HN ₃ O ₇ P ₂ S	-6.80	6.08 × 10 ⁻¹⁰	Level 4
(-)	C ₁₇ H ₂₇ F ₅ N ₇ P ₃	-8.36	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₆ HF ₇ N ₃ O ₃ P ₃ S ₃	-6.08	9.08 × 10 ⁻¹⁰	Level 4
(-)	C ₁₂ H ₂₄ F ₄ N ₄ O ₂	-3.73	6.61 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₄ ClF ₁₀ NO ₂ P ₂ S ₅	-7.82	5.64 × 10 ⁻¹⁰	Level 4
(-)	C ₂ H ₅ BrF ₄ N ₄ S ₂	-5.35	2.95 × 10 ⁻⁹	Level 4
(-)	C ₂₄ H ₃ F ₂ O ₁₇ P ₃ S ₅	-9.14	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₀ H ₂₀ FN ₇ O ₅	-4.38	1.15 × 10 ⁻⁵	Level 4
(-)	C ₅ H ₄ ClF ₄ N ₂ O ₅ P ₃	-5.77	3.23 × 10 ⁻⁸	Level 4
(-)	C ₅₆ H ₈₇ F ₁₆ N ₃ O ₁₈ P ₂ S ₃	-8.55	5.58 × 10 ⁻¹⁰	Level 4
(-)	C ₁₂ H ₂ F ₁₁ O ₄ P ₃ S ₃	-5.58	1.02 × 10 ⁻⁸	Level 4
(-)	C ₃ HF ₂ N ₅ O ₈ P ₂ S ₅	-6.41	9.16 × 10 ⁻⁸	Level 4
(-)	C ₄ H ₄ F ₃ NO ₄ P ₂ S ₃	-5.68	5.48 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₂ F ₃ N ₄ O ₁₄ P ₃ S ₃	-7.19	1.04 × 10 ⁻⁹	Level 4
(-)	C ₃ H ₃ N ₄ O ₈ PS ₃	-4.65	3.28 × 10 ⁻⁶	Level 4
(-)	C ₁₉ H ₂₅ F ₄ NOS	-3.31	2.01 × 10 ⁻⁹	Level 4
(-)	C ₂₀ H ₄₅ Cl ₂ F ₃ N ₈ O ₅	-9.32	9.25 × 10 ⁻⁹	Level 4
(-)	C ₂₆ H ₃₆ O ₄ S ₂	-3.57	1.01 × 10 ⁻⁹	Level 4
(-)	C ₁₆ H ₃₈ N ₈ O ₂ S	-6.04	1.42 × 10 ⁻⁹	Level 4
(-)	C ₄ H ₁₀ FN ₃ O ₄	-5.26	1.21 × 10 ⁻⁹	Level 4
(-)	C ₁₅ H ₃₂ FN ₂ O ₁₈ P	-3.21	7.16 × 10 ⁻⁸	Level 4
(-)	C ₅ HF ₆ O ₇ P ₃ S	-7.56	7.20 × 10 ⁻⁹	Level 4
(-)	C ₁₈ H ₃₅ FN ₂ O ₆ S	-6.71	8.47 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₂ F ₆ O ₁₈ S ₃	-6.56	5.76 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₉ F ₂ O ₁₇ P ₃ S ₃	-6.09	6.96 × 10 ⁻⁷	Level 4
(-)	C ₈ H ₁₀ F ₇ O ₁₄ P ₃ S ₄	-6.83	4.60 × 10 ⁻⁹	Level 4
(-)	C ₂₀ H ₃₉ FN ₂ O ₄	-6.51	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₇ HF ₄ O ₁₆ P ₃ S	-8.01	7.06 × 10 ⁻¹⁰	Level 4

Compound	Formula	Log2 Fold Change	p-value	Identified level
(-)	C ₁₀ H ₃ F ₁₀ N ₄ O ₁₂ PS ₅	-6.96	2.66 × 10 ⁻⁷	Level 4
(-)	C ₁₀ HFN ₄ O ₁₆ P ₂ S ₃	-7.26	7.91 × 10 ⁻⁴	Level 4
(-)	C ₉ H ₂ F ₅ O ₁₆ P ₃	-3.05	2.08 × 10 ⁻⁹	Level 4
(-)	C ₈ HF ₂ N ₄ O ₉ P ₃ S ₂	-8.39	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₈ H ₃₁ FS	-3.44	6.79 × 10 ⁻¹⁰	Level 4
(-)	C ₂₈ H ₅₉ F ₂ O ₅ P ₃ S ₄	-8.13	8.64 × 10 ⁻¹⁰	Level 4
(-)	C ₁₉ H ₄₇ ClN ₉ OP	-7.83	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₃ F ₄ N ₅ O ₂	-3.70	5.55 × 10 ⁻¹⁰	Level 4
(-)	C ₅ H ₆ F ₂ N ₂ O ₈ P ₃ S ₃	-3.33	1.42 × 10 ⁻⁹	Level 4
(-)	C ₃ H ₈ P ₂ S	-6.49	1.16 × 10 ⁻⁹	Level 4
(-)	C ₅ H ₁₄ FN ₂ O ₇ P ₃ S ₅	-3.16	7.14 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₂ F ₁₁ O ₄ P ₃ S ₂	-7.73	5.12 × 10 ⁻⁸	Level 4
(-)	C ₅ H ₅ N ₄ O ₁₁ P ₃ S ₃	-8.39	5.52 × 10 ⁻¹⁰	Level 4
(-)	C ₅ HF ₆ N ₈ O ₄ P ₃ S ₅	-8.72	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₈ H ₁₀ BrClN ₂ OS ₃	-6.65	5.61 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₄ F ₇ N ₂ O ₁₃ P ₃ S ₅	-10.96	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₈ H ₂₅ F ₃ N ₂ O ₈	-3.64	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₆ H ₂ ClF ₃ O ₄	-8.76	1.13 × 10 ⁻⁹	Level 4
(-)	C ₂ H ₂ F ₅ O ₂ PS	-6.95	5.23 × 10 ⁻⁷	Level 4
(-)	C ₃ H ₃ F ₃ N ₅ O ₈ P ₃ S ₃	-11.07	5.51 × 10 ⁻¹⁰	Level 4
(-)	C ₂ H ₄ Cl ₂ FN ₂ OPS ₂	-10.82	1.40 × 10 ⁻⁹	Level 4
(-)	C ₄ H ₂ F ₃ O ₂ P ₃	-5.55	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₂ F ₃ O ₇ P ₃ S	-4.55	1.74 × 10 ⁻⁷	Level 4
(-)	C ₃ H ₆ Cl ₂ P ₂ S ₂	-8.68	1.39 × 10 ⁻⁶	Level 4
(-)	C ₁₄ H ₂₉ FO ₃	-4.28	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₄ HF ₂ O ₈ P	-5.49	1.45 × 10 ⁻⁹	Level 4
(-)	C ₆ H ₂ F ₃ P	-7.30	2.63 × 10 ⁻⁹	Level 4
(-)	C ₆ H ₃ F ₁₄ O ₇ P ₃ S ₅	-8.44	6.24 × 10 ⁻¹⁰	Level 4
(-)	C ₁₅ H ₆ F ₉ O ₈ P ₃ S ₅	-8.59	5.52 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₇ F ₃ N ₂ O ₆ S ₂	-4.16	1.40 × 10 ⁻⁹	Level 4
(-)	C ₁₃ H ₂₉ NO ₅	-3.79	5.92 × 10 ⁻⁷	Level 4
(-)	C ₄₄ H ₉₀ F ₃ N ₈ P	-7.19	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₆ HClF ₅ N ₂ O ₄ P ₃ S	-6.22	5.46 × 10 ⁻¹⁰	Level 4
(-)	C ₉ HO ₇ PS ₃	-5.40	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₀ H ₁₇ F ₃ N ₂ O ₂ S ₃	-3.32	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₅ H ₂ Cl ₂ F ₃ N ₃ S ₂	-3.92	9.44 × 10 ⁻⁶	Level 4
(-)	C ₈ HClF ₁₂ N ₃ O ₁₁ P ₃ S ₄	-9.27	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₈ HCl ₂ F ₅ N ₆ OS ₄	-8.29	5.55 × 10 ⁻¹⁰	Level 4

Compound	Formula	Log2 Fold Change	p-value	Identified level
(-)	C ₁₄ H ₂₁ F ₃ O ₅	-5.16	1.29 × 10 ⁻⁶	Level 4
(-)	C ₄₉ H ₉₉ N ₄ P ₃	-6.31	5.74 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₅ N ₂ PS ₂	-3.31	3.12 × 10 ⁻⁸	Level 4
(-)	C ₁₁ H ₂₉ F ₅ N ₈ O ₁₇ P ₂ S	-9.79	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₅₃ H ₉₇ F ₂ NO ₂ S	-9.29	5.48 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂ F ₂ O ₁₄ P ₂ S ₃	-4.70	6.08 × 10 ⁻⁹	Level 4
(-)	C ₃ H ₂ F ₂ O ₇ P ₂ S	-7.04	4.90 × 10 ⁻⁸	Level 4
(-)	C ₃ H ₂ BrF ₂ N ₉ O ₃ S ₃	-9.99	2.09 × 10 ⁻⁹	Level 4
(-)	C ₁₀ H ₂₀ F ₂ N ₆ O ₂ S	-4.92	1.46 × 10 ⁻⁸	Level 4
(-)	C ₆ H ₉ F ₃ N ₂ S ₂	-5.42	5.45 × 10 ⁻¹⁰	Level 4
(-)	(-) (m/z=115.97859)	-3.88	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=863.69976)	-8.70	5.49 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=647.43803)	-8.40	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=656.10704)	-8.60	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=123.96857)	-3.05	4.82 × 10 ⁻⁹	Level 5
(-)	(-) (m/z=436.51015)	-8.26	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=777.39584)	-8.06	5.53 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=734.40917)	-8.29	5.47 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=119.97166)	-7.93	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=793.72866)	-9.03	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=840.69745)	-8.22	5.53 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=489.83934)	-8.47	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=820.71495)	-8.82	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=735.07365)	-9.01	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=821.71117)	-7.78	6.01 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=547.83043)	-7.81	1.97 × 10 ⁻⁵	Level 5
(-)	(-) (m/z=609.80086)	-7.55	2.91 × 10 ⁻⁶	Level 5
(-)	(-) (m/z=696.42571)	-8.63	6.02 × 10 ⁻⁵	Level 5
(-)	(-) (m/z=541.81348)	-8.14	8.20 × 10 ⁻⁶	Level 5
(-)	(-) (m/z=539.80515)	-8.05	6.63 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=517.14610)	-8.36	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=442.51360)	-8.03	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=983.67282)	-8.16	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=609.78801)	-8.05	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=723.75475)	-8.61	2.51 × 10 ⁻⁶	Level 5
(-)	(-) (m/z=778.39331)	-8.04	5.74 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=820.38066)	-8.71	5.46 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=817.69453)	-8.50	6.09 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=538.80125)	-10.88	1.33 × 10 ⁻⁹	Level 5
(-)	(-) (m/z=482.83147)	-10.69	5.50 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=723.75762)	-6.55	1.21 × 10 ⁻⁹	Level 5
(-)	(-) (m/z=603.78429)	-9.24	5.45 × 10 ⁻¹⁰	Level 5
(-)	(-) (m/z=117.97467)	-3.34	3.23 × 10 ⁻⁸	Level 5
(-)	(-) (m/z=102.94277)	-3.47	3.74 × 10 ⁻⁵	Level 5
(-)	(-) (m/z=835.70505)	-10.14	7.70 × 10 ⁻⁹	Level 5
(-)	(-) (m/z=101.96297)	-5.42	1.59 × 10 ⁻⁴	Level 5
(-)	(-) (m/z=119.97352)	-3.78	7.21 × 10 ⁻⁹	Level 5
(-)	(-) (m/z=129.95791)	-7.44	1.60 × 10 ⁻⁶	Level 5
(-)	(-) (m/z=133.98920)	-3.76	5.45 × 10 ⁻¹⁰	Level 5

(-)	(-) (m/z=147.96855)	-3.33	1.67×10^{-6}	Level 5
(-)	(-) (m/z=133.98922)	-6.54	5.54×10^{-10}	Level 5
(-)	(-) (m/z=473.81270)	-6.52	5.45×10^{-10}	Level 5
(-)	(-) (m/z=119.97166)	-7.93	2.07×10^{-8}	Level 5
(-)	(-) (m/z=668.76319)	-10.25	5.60×10^{-10}	Level 5
(-)	(-) (m/z=690.75736)	-8.86	5.45×10^{-10}	Level 5
(-)	(-) (m/z=547.81046)	-8.80	1.10×10^{-9}	Level 5
(-)	(-) (m/z=105.95588)	-3.26	1.15×10^{-7}	Level 5
(-)	(-) (m/z=777.06124)	-9.46	5.46×10^{-10}	Level 5
(-)	(-) (m/z=117.98287)	-3.36	5.45×10^{-10}	Level 5
(-)	(-) (m/z=690.42275)	-9.38	5.46×10^{-10}	Level 5
(-)	(-) (m/z=647.10355)	-9.70	5.45×10^{-10}	Level 5
(-)	(-) (m/z=784.72349)	-9.41	5.45×10^{-10}	Level 5
(-)	(-) (m/z=671.77350)	-7.24	4.14×10^{-9}	Level 5
(-)	(-) (m/z=475.83582)	-6.43	2.32×10^{-8}	Level 5
(-)	(-) (m/z=668.76323)	-7.81	1.86×10^{-9}	Level 5
(-)	(-) (m/z=546.46825)	-9.17	5.46×10^{-10}	Level 5
(-)	(-) (m/z=798.72096)	-9.26	5.50×10^{-10}	Level 5
(-)	(-) (m/z=492.78803)	-3.29	9.19×10^{-10}	Level 5
(-)	(-) (m/z=479.82963)	-8.57	5.45×10^{-10}	Level 5
(-)	(-) (m/z=737.74217)	-11.3	5.45×10^{-10}	Level 5
(-)	(-) (m/z=485.83283)	-8.38	5.45×10^{-10}	Level 5
(-)	(-) (m/z=483.33303)	-8.93	5.81×10^{-10}	Level 5
(-)	(-) (m/z=436.50843)	-7.72	6.65×10^{-10}	Level 5
(-)	(-) (m/z=442.51392)	-8.01	5.96×10^{-10}	Level 5
(-)	(-) (m/z=734.40977)	-8.42	5.45×10^{-10}	Level 5
(-)	(-) (m/z=509.78710)	-8.83	5.59×10^{-10}	Level 5
(-)	(-) (m/z=566.80270)	-8.34	5.45×10^{-10}	Level 5

(-) = No name/No formula described in CD

Table S7. Compounds more probably present in urban areas (Urban–Rural).

Compound	Formula	Log2 Fold Change	<i>p</i> -value	Identified level
Cocaine	C ₁₇ H ₂₁ NO ₄	4.68	6.15 × 10 ⁻¹⁰	Level 1
Azoxystrobin	C ₂₂ H ₁₇ N ₃ O ₅	8.02	5.43 × 10 ⁻¹⁰	Level 1
Cotinine	C ₁₀ H ₁₂ N ₂ O	4.20	5.40 × 10 ⁻¹⁰	Level 1
Anhydroecgonine	C ₉ H ₁₃ NO ₂	4.31	1.67 × 10 ⁻⁷	Level 1
3-Methyladenine	C ₆ H ₇ N ₅	6.46	5.45 × 10 ⁻⁵	Level 1
3-Hydroxy-2-methylpyridine	C ₆ H ₇ NO	3.66	2.06 × 10 ⁻⁹	Level 1
Imidacloprid	C ₉ H ₁₀ ClN ₅ O ₂	6.57	5.47 × 10 ⁻¹⁰	Level 1
Metalaxyl	C ₁₅ H ₂₁ NO ₄	3.78	5.42 × 10 ⁻¹⁰	Level 1
Nicotine	C ₁₀ H ₁₄ N ₂	10.37	2.36 × 10 ⁻⁶	Level 1
Ethoprophos	C ₈ H ₁₉ O ₂ PS ₂	4.24	5.43 × 10 ⁻¹⁰	Level 1
1,8-Diazabicyclo [5.4.0]undec-7-ene	C ₉ H ₁₆ N ₂	4.01	2.73 × 10 ⁻⁹	Level 1
Pyrimethanil	C ₁₂ H ₁₃ N ₃	3.03	5.17 × 10 ⁻¹⁰	Level 1
Nikethamide	C ₁₀ H ₁₄ N ₂ O	6.40	5.45 × 10 ⁻¹⁰	Level 2 (ms2)
Melamine	C ₃ H ₆ N ₆	4.64	4.08 × 10 ⁻⁵	Level 2 (ms2)
Phenacetin	C ₁₀ H ₁₃ NO ₂	4.62	1.19 × 10 ⁻⁹	Level 2 (ms3)
3-(2,6-Dioxocyclohexyl)propanenitrile	C ₉ H ₁₁ NO ₂	6.21	5.33 × 10 ⁻¹⁰	Level 2 (ms3)
2-Hydroxyphenylalanine	C ₉ H ₁₁ NO ₃	4.98	5.26 × 10 ⁻¹⁰	Level 2 (ms3)
3-(3-pyridinyl)propanoic acid	C ₈ H ₉ NO ₂	5.11	7.72 × 10 ⁻¹⁰	Level 2 (ms2)
Fenuron	C ₉ H ₁₂ N ₂ O	5.12	5.45 × 10 ⁻¹⁰	Level 2 (ms2)
1-propylimidazole	C ₆ H ₁₀ N ₂	6.53	1.02 × 10 ⁻⁹	Level 2 (ms2)
Hydroferulic acid	C ₁₀ H ₁₂ O ₄	5.30	1.51 × 10 ⁻⁹	Level 2 (ms2)
Dihydrothymine	C ₅ H ₈ N ₂ O ₂	5.21	4.74 × 10 ⁻⁸	Level 2 (ms2)
(4-Methyl-1H-imidazol-5-yl)methanol	C ₅ H ₈ N ₂ O	6.63	5.48 × 10 ⁻¹⁰	Level 2 (ms2)
(Butylamino)acetonitrile	C ₆ H ₁₂ N ₂	6.29	5.45 × 10 ⁻¹⁰	Level 2 (ms2)
Benzocaine	C ₉ H ₁₁ NO ₂	5.13	4.04 × 10 ⁻⁴	Level 2 (ms2)
N-Methyloctan-1-amine	C ₉ H ₂₁ N	5.82	5.42 × 10 ⁻¹⁰	Level 2 (ms2)
Ropivacaine	C ₁₇ H ₂₆ N ₂ O	6.26	5.46 × 10 ⁻¹⁰	Level 2 (ms2)
Cardiopetalidine	C ₂₁ H ₃₃ NO ₄	5.14	5.45 × 10 ⁻¹⁰	Level 2 (ms3)
Pyroquilon	C ₁₁ H ₁₁ NO	3.35	5.41 × 10 ⁻¹⁰	Level 3
Norfenefrine	C ₈ H ₁₁ NO ₂	4.13	1.24 × 10 ⁻⁸	Level 3
Ethyl 4-hydroxy-3-methoxyphenylacetate	C ₁₁ H ₁₄ O ₄	3.74	4.02 × 10 ⁻⁶	Level 3
Diaminotoluene	C ₇ H ₁₀ N ₂	5.22	8.00 × 10 ⁻¹⁰	Level 3
NP-019811	C ₆ H ₇ NO ₂	4.02	5.45 × 10 ⁻¹⁰	Level 3
3h-1,2,3-triazolo[4,5-c]pyridin-4-amine	C ₅ H ₅ N ₅	3.85	5.44 × 10 ⁻¹⁰	Level 3
6-Methylnicotinonitrile	C ₇ H ₆ N ₂	3.80	5.46 × 10 ⁻¹⁰	Level 3
5-acetyl-2,6-dimethyl-1,2,3,4-tetrahydropyridin-4-one	C ₉ H ₁₃ NO ₂	3.29	6.25 × 10 ⁻¹⁰	Level 3
2,2,2-Trifluoro-1-(1-naphthyl)ethanol	C ₁₂ H ₉ F ₃ O	4.39	8.95 × 10 ⁻⁶	Level 3
Methyl piperonyl ketone	C ₁₀ H ₁₀ O ₃	3.16	1.10 × 10 ⁻⁹	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
Methyl [5-methoxy-2-nitro-4-(trifluoromethyl)phenyl]acetate	C ₁₁ H ₁₀ F ₃ NO ₅	4.81	7.86 × 10 ⁻⁹	Level 3
8-Hydroxyquinoline	C ₉ H ₇ NO	5.12	6.38 × 10 ⁻¹⁰	Level 3
1-Naphthylisocyanate	C ₁₁ H ₇ NO	5.45	5.46 × 10 ⁻¹⁰	Level 3
3-methyl-5-phenylpyridazine	C ₁₁ H ₁₀ N ₂	3.93	5.58 × 10 ⁻¹⁰	Level 3
Xanthone	C ₁₃ H ₈ O ₂	3.09	5.45 × 10 ⁻¹⁰	Level 3
2-(Diethylamino)ethanol	C ₆ H ₁₅ NO	3.50	5.45 × 10 ⁻¹⁰	Level 3
Duloxetine	C ₁₈ H ₁₉ NOS	3.05	1.23 × 10 ⁻⁹	Level 3
4-Hexyl-1H-pyrazole	C ₉ H ₁₆ N ₂	3.76	1.38 × 10 ⁻⁹	Level 3
2,7-Difluoro-4,5-dimethoxy-2'H,5'H-spiro[fluorene-9,4'-imidazolidine]-2',5'-dione	C ₁₇ H ₁₂ F ₂ N ₂ O ₄	6.21	3.98 × 10 ⁻⁹	Level 3
(2Z)-2-(2,2,2-Trifluoro-1-hydroxyethylidene)cycloheptanone	C ₉ H ₁₁ F ₃ O ₂	3.30	9.63 × 10 ⁻⁶	Level 3
Mepivacaine	C ₁₅ H ₂₂ N ₂ O	6.25	5.45 × 10 ⁻¹⁰	Level 3
3-(Octylamino)propanenitrile	C ₁₁ H ₂₂ N ₂	3.42	5.45 × 10 ⁻¹⁰	Level 3
Propylhexedrine	C ₁₀ H ₂₁ N	3.28	5.48 × 10 ⁻¹⁰	Level 3
Detomidine	C ₁₂ H ₁₄ N ₂	3.43	5.45 × 10 ⁻¹⁰	Level 3
(-)-Ecgonine methyl ester	C ₁₀ H ₁₇ NO ₃	5.58	6.25 × 10 ⁻¹⁰	Level 3
Ethyl 5-formyl-2,4-dimethyl-1H-pyrrole-3-carboxylate	C ₁₀ H ₁₃ NO ₃	4.79	9.57 × 10 ⁻¹⁰	Level 3
2,2'-(1,2-Phenylene)bis(1,1,3,3-tetramethylguanidine)	C ₁₆ H ₂₈ N ₆	3.20	2.02 × 10 ⁻⁵	Level 3
119183	C ₇ H ₇ N ₃	4.51	5.45 × 10 ⁻¹⁰	Level 3
7-Amino-3,4-dihydro-2(1H)-quinoxalinone	C ₈ H ₉ N ₃ O	6.00	5.77 × 10 ⁻¹⁰	Level 3
Epinephrine	C ₉ H ₁₃ NO ₃	3.59	5.55 × 10 ⁻¹⁰	Level 3
5-(Cyanomethyl)-1H-imidazole-4-carbonitrile	C ₆ H ₄ N ₄	6.22	3.09 × 10 ⁻⁸	Level 3
2-Methyl-2H-indazol-4-amine	C ₈ H ₉ N ₃	6.25	5.45 × 10 ⁻¹⁰	Level 3
Aminobenzodiazapine	C ₉ H ₁₁ N ₃ O	5.72	5.45 × 10 ⁻¹⁰	Level 3
11-Aminoundecanoic acid	C ₁₁ H ₂₃ NO ₂	5.95	5.45 × 10 ⁻¹⁰	Level 3
ZV4	C ₅ H ₁₁ NO	3.30	2.14 × 10 ⁻⁴	Level 3
6-anilino-2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carbonitrile	C ₁₁ H ₈ N ₄ O ₂	4.36	1.21 × 10 ⁻⁴	Level 3
KK9000000	C ₄ H ₇ F ₃ O ₂	3.52	6.24 × 10 ⁻¹⁰	Level 3
Anabasine	C ₁₀ H ₁₄ N ₂	3.98	1.40 × 10 ⁻⁴	Level 3
Gramine	C ₁₁ H ₁₄ N ₂	3.34	2.27 × 10 ⁻⁴	Level 3
2-(5-Amino-1H-pyrazol-1-yl)ethanol	C ₅ H ₉ N ₃ O	6.74	5.57 × 10 ⁻¹⁰	Level 3
Glutaric acid	C ₅ H ₈ O ₄	5.45	7.65 × 10 ⁻¹⁰	Level 3
p-Xylylenediamine	C ₈ H ₁₂ N ₂	5.62	5.45 × 10 ⁻¹⁰	Level 3
4-(2-Aminopropyl)-N,N-dimethylaniline	C ₁₁ H ₁₈ N ₂	4.26	5.45 × 10 ⁻¹⁰	Level 3
N,N-Diethyltryptamine	C ₁₄ H ₂₀ N ₂	3.34	5.45 × 10 ⁻¹⁰	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
Iprovalicarb	C ₁₈ H ₂₈ N ₂ O ₃	6.08	8.27 × 10 ⁻¹⁰	Level 3
1-(Cyclohexylmethyl)piperazine	C ₁₁ H ₂₂ N ₂	3.34	5.45 × 10 ⁻¹⁰	Level 3
6-Vinylnicotinonitrile	C ₈ H ₆ N ₂	5.89	5.45 × 10 ⁻¹⁰	Level 3
(3-aminobenzyl)diethylamine	C ₁₁ H ₁₈ N ₂	3.56	5.45 × 10 ⁻¹⁰	Level 3
1-deoxy-1-(2,4-difluorophenyl)-β-D-ribofuranose	C ₁₁ H ₁₂ F ₂ O ₄	5.07	6.18 × 10 ⁻¹⁰	Level 3
3-hydroxybenzylhydrazine	C ₇ H ₁₀ N ₂ O	5.25	5.46 × 10 ⁻¹⁰	Level 3
Dodecanedinitrile	C ₁₂ H ₂₀ N ₂	4.26	5.45 × 10 ⁻¹⁰	Level 3
Serotonin	C ₁₀ H ₁₂ N ₂ O	6.93	5.45 × 10 ⁻¹⁰	Level 3
L-Tyrosine	C ₉ H ₁₁ NO ₃	3.38	5.45 × 10 ⁻¹⁰	Level 3
Ethyl 4,4,4-trifluoro-3-hydroxy-3-methoxybutanoate	C ₇ H ₁₁ F ₃ O ₄	3.39	5.45 × 10 ⁻¹⁰	Level 3
4-Tolylurea	C ₈ H ₁₀ N ₂ O	4.77	6.71 × 10 ⁻¹⁰	Level 3
3-Methoxytyramine	C ₉ H ₁₃ NO ₂	4.14	5.45 × 10 ⁻¹⁰	Level 3
4,4'-Bipyridine	C ₁₀ H ₈ N ₂	3.44	5.45 × 10 ⁻¹⁰	Level 3
2,2-Diethoxy-N,N-diethylethanamine	C ₁₀ H ₂₃ NO ₂	3.46	5.45 × 10 ⁻¹⁰	Level 3
2-Methoxy-5-methylaniline	C ₈ H ₁₁ NO	4.01	5.45 × 10 ⁻¹⁰	Level 3
7-Aminoindole	C ₈ H ₈ N ₂	4.57	1.01 × 10 ⁻⁹	Level 3
2,2,6,6-Tetramethyl-4-piperidinol	C ₉ H ₁₉ NO	6.37	5.58 × 10 ⁻¹⁰	Level 3
Pyrene	C ₁₆ H ₁₀	9.58	1.94 × 10 ⁻⁴	Level 3
NP-020713	C ₂₀ H ₂₆ O ₄	3.03	5.47 × 10 ⁻¹⁰	Level 3
3-[(4-Phenyl-2-butanyl)amino]propanenitrile	C ₁₃ H ₁₈ N ₂	7.18	5.46 × 10 ⁻¹⁰	Level 3
Skatole	C ₉ H ₉ N	3.11	5.45 × 10 ⁻¹⁰	Level 3
Metrafenone	C ₁₉ H ₂₁ BrO ₅	5.89	5.46 × 10 ⁻¹⁰	Level 3
3-hydroxy-3-methylpentanedioic acid	C ₆ H ₁₀ O ₅	3.14	1.24 × 10 ⁻⁷	Level 3
1-Azaspiro[5.7]tridecane	C ₁₂ H ₂₃ N	4.51	5.45 × 10 ⁻¹⁰	Level 3
2-deoxyglucose	C ₆ H ₁₂ O ₅	3.53	2.71 × 10 ⁻⁹	Level 3
4-hydroxy-3-(3-methylbut-2-en-1-yl)benzoic acid	C ₁₂ H ₁₄ O ₃	3.63	1.51 × 10 ⁻⁹	Level 3
2-aminododecanol	C ₁₂ H ₂₇ NO	3.82	5.45 × 10 ⁻¹⁰	Level 3
7-hydroxy-6-methoxy-2H-chromen-2-one	C ₁₀ H ₈ O ₄	5.99	5.45 × 10 ⁻¹⁰	Level 3
6-(Diethylamino)-1-hexanol	C ₁₀ H ₂₃ NO	3.26	5.45 × 10 ⁻¹⁰	Level 3
7beta,12alpha-Dihydroxykaurenolide	C ₂₀ H ₂₈ O ₄	6.68	7.07 × 10 ⁻¹⁰	Level 3
Paraxanthine	C ₇ H ₈ N ₄ O ₂	4.30	5.72 × 10 ⁻¹⁰	Level 3
(4-Methoxybenzyl)(phenyl)phosphine	C ₁₄ H ₁₅ OP	3.05	5.51 × 10 ⁻¹⁰	Level 3
16-Heptadecyne-1,2,4-triol	C ₁₇ H ₃₂ O ₃	3.01	5.45 × 10 ⁻¹⁰	Level 3
MFCD00995440	C ₁₀ H ₂₀ N ₂	3.68	5.45 × 10 ⁻¹⁰	Level 3
3964	C ₇ H ₈ N ₂ O	4.33	5.45 × 10 ⁻¹⁰	Level 3
Triethylamine	C ₆ H ₁₅ N	3.46	5.86 × 10 ⁻¹⁰	Level 3
1,3-Phenylenediamine	C ₆ H ₈ N ₂	3.73	5.45 × 10 ⁻¹⁰	Level 3
6,7-Dihydro-8(5H)-quinolinone	C ₉ H ₉ NO	4.67	6.55 × 10 ⁻¹⁰	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
4,6-Bis(1-aziridinyl)-N-(2,2-dimethyl-1,3-dioxan-5-yl)-1,3,5-triazin-2-amine	C ₁₃ H ₂₀ N ₆ O ₂	4.45	7.98 × 10 ⁻¹⁰	Level 3
NSC 131681	C ₈ H ₉ NO	6.08	5.46 × 10 ⁻¹⁰	Level 3
5-Ethylcyclohexane-1,3-dione	C ₈ H ₁₂ O ₂	6.60	8.16 × 10 ⁻¹⁰	Level 3
3-CYCLOHEXYLAMINOPROPIONITRILE	C ₉ H ₁₆ N ₂	3.26	5.45 × 10 ⁻¹⁰	Level 3
CM3599500	C ₈ H ₁₃ NO ₂	3.35	5.46 × 10 ⁻¹⁰	Level 3
6-Methyl-2-pyridinemethanol	C ₇ H ₉ NO	3.06	3.47 × 10 ⁻⁴	Level 3
Creatinine	C ₄ H ₇ N ₃ O	3.45	1.06 × 10 ⁻⁹	Level 3
N-(4-fluorophenyl)-2-methyl-5-(morpholin-sulfonyl)-3-furamide	C ₁₆ H ₁₇ FN ₂ O ₅ S	4.54	2.89 × 10 ⁻⁹	Level 3
8-[4-(3,4,5-Trifluorophenyl)cyclohexyl]-1,4-dioxaspiro[4.5]decane	C ₂₀ H ₂₅ F ₃ O ₂	6.56	4.23 × 10 ⁻⁹	Level 3
N-5-(Diaminomethylene)-L-ornithyl-L-valyl-L-alanine	C ₁₄ H ₂₈ N ₆ O ₄	3.51	5.45 × 10 ⁻¹⁰	Level 3
9-Amino-1-nonanol	C ₉ H ₂₁ NO	3.36	5.45 × 10 ⁻¹⁰	Level 3
2,2-Dimethoxy-1-(1-piperidinyl)ethanone	C ₉ H ₁₇ NO ₃	3.39	5.45 × 10 ⁻¹⁰	Level 3
1,3-diazaspiro[4.4]nonane-2,4-dione 5,5-TETRAMETHYLENEHYDANTOIN	C ₇ H ₁₀ N ₂ O ₂	3.11	5.07 × 10 ⁻⁰⁹	Level 3
2-dimethylaminomethyl-1-methylpyrrole	C ₈ H ₁₄ N ₂	3.49	5.45 × 10 ⁻¹⁰	Level 3
Ethyl 3-hydroxy-4,4,4-trifluorobutyrate	C ₆ H ₉ F ₃ O ₃	3.15	1.52 × 10 ⁻⁵	Level 3
1-propyl-1H-benzo[d]imidazole hydrobromide	C ₁₀ H ₁₂ N ₂	3.56	6.53 × 10 ⁻⁷	Level 3
Disperse Yellow 3	C ₁₅ H ₁₅ N ₃ O ₂	3.90	5.89 × 10 ⁻⁸	Level 3
3-Hydroxyanthranilic acid	C ₇ H ₇ NO ₃	3.53	5.45 × 10 ⁻¹⁰	Level 3
2,2,2-Trifluoro-N-(5-hexen-1-yl)-N-methylacetamide	C ₉ H ₁₄ F ₃ NO	3.47	5.45 × 10 ⁻¹⁰	Level 3
1-Nitrosocyclohexyl trifluoroacetate	C ₈ H ₁₀ F ₃ NO ₃	3.21	4.66 × 10 ⁻⁷	Level 3
Andrographolide	C ₂₀ H ₃₀ O ₅	3.86	5.49 × 10 ⁻¹⁰	Level 3
(-)	C ₁₈ H ₃₁ F ₅ O ₃ S	3.44	5.43 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₆ F ₃ N ₆ O ₈ PS	6.09	6.55 × 10 ⁻⁸	Level 4
(-)	C ₁₂ H ₉ N ₇ O ₄ P ₂	5.09	1.15 × 10 ⁻⁸	Level 4
(-)	C ₅ H ₁₆ FN ₄ P ₃	4.70	5.47 × 10 ⁻¹⁰	Level 4
(-)	C ₂₁ H ₃₀ ClO ₁₀ P	5.38	5.96 × 10 ⁻¹⁰	Level 4
(-)	C ₁₅ H ₂₆ FN ₇ O ₄	3.30	5.47 × 10 ⁻¹⁰	Level 4
(-)	C ₇ H ₇ N ₂ O ₆ P	3.12	9.71 × 10 ⁻¹⁰	Level 4
(-)	C ₆ H ₇ F ₃ O ₄ P ₂	3.31	1.36 × 10 ⁻⁹	Level 4
(-)	C ₁₀ H ₁₆ F ₃ NO ₅	4.08	5.47 × 10 ⁻¹⁰	Level 4
(-)	C ₁₁ H ₁₅ F ₅ N ₄ OS	5.42	8.56 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₄ N ₇ P	7.57	2.50 × 10 ⁻⁷	Level 4
(-)	C ₁₇ H ₃₂ FNO ₅	4.24	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₄ H ₁₀ F ₄ N ₈ O ₃	6.03	1.29 × 10 ⁻⁹	Level 4
(-)	C ₉ H ₁₃ F ₃ O ₅	4.49	8.31 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₇ N ₆ O ₃ P	5.51	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₃ H ₄ N ₆ O ₃	5.28	1.09 × 10 ⁻⁸	Level 4
(-)	C ₄ H ₁₂ F ₂ N ₅ OPS	3.59	9.49 × 10 ⁻¹⁰	Level 4
(-)	C ₅ H ₁₂ O ₁₀	4.03	3.79 × 10 ⁻⁶	Level 4
(-)	C ₁₀ H ₂₂ F ₂ N ₄ OS ₃	4.48	1.15 × 10 ⁻⁹	Level 4
(-)	C ₁₇ H ₃₅ F ₃ N ₄ O ₁₂ P ₂	5.26	2.06 × 10 ⁻⁸	Level 4
(-)	C ₆ H ₁₃ F ₂ N ₂ O ₅ P	5.13	3.04 × 10 ⁻⁵	Level 4
(-)	C ₂₁ H ₂₈ F ₄ N ₂ O ₁₃	3.71	5.78 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₁₃ FS	3.61	5.45 × 10 ⁻¹⁰	Level 4

(-)	$C_{28}H_{51}F_2N_2O_3P$	3.58	1.51×10^{-9}	Level 4
(-)	$C_{12}H_{17}FN_4O_4S_2$	5.13	5.92×10^{-9}	Level 4
(-)	$C_{15}H_{16}FN_2P_3S$	5.53	5.45×10^{-10}	Level 4
(-)	$C_8H_{10}N_6O_6$	5.39	5.45×10^{-10}	Level 4
(-)	$C_{17}H_{29}N_4O_4P$	4.20	1.46×10^{-7}	Level 4
(-)	$C_4H_7FN_2O_5$	5.13	1.10×10^{-7}	Level 4
(-)	$C_6H_{14}FN_3OS$	4.00	3.45×10^{-4}	Level 4
(-)	$C_{13}H_{32}F_2N_6OS$	3.87	1.34×10^{-9}	Level 4
(-)	$C_8H_{14}F_3NO_4$	3.32	5.45×10^{-10}	Level 4
(-)	$C_{20}H_{20}F_4N_2O_{10}$	8.10	5.45×10^{-10}	Level 4
(-)	$C_{16}H_{25}FO_3$	3.32	6.30×10^{-10}	Level 4
(-)	$C_{12}H_{16}F_4NO_9P$	4.01	6.12×10^{-10}	Level 4
(-)	$C_{19}H_{31}F_3N_4O$	3.19	3.77×10^{-9}	Level 4
(-)	$C_8H_{15}FN_4O_9S$	7.10	5.45×10^{-10}	Level 4
(-)	$C_{17}H_{34}N_6O_5$	3.39	3.87×10^{-7}	Level 4
(-)	$C_8H_8N_8O_3S$	5.89	5.45×10^{-10}	Level 4
(-)	$C_{20}H_{21}F_3O_3$	4.38	5.45×10^{-10}	Level 4

Table S8. Compounds more probably present in rural areas (Urban–Rural).

Compound	Formula	Log2 Fold Change	<i>p</i> -value	Identified level
Triisopropanolamine	C ₉ H ₂₁ NO ₃	-6.87	2.80 × 10 ⁻⁵	Level 1
N,N,N',N'-Tetramethyl-2,5-disulfanyhexanediamide	C ₁₀ H ₂₀ N ₂ O ₂ S ₂	-5.15	5.76 × 10 ⁻¹⁰	Level 2 (ms2)
NP-021797	C ₁₂ H ₂₂ O ₃	-5.19	8.66 × 10 ⁻¹⁰	Level 2 (ms2)
2,2'-(1,7-Dioxa-4,10-diazacyclododecane-4,10-diyl)diethanol	C ₁₂ H ₂₆ N ₂ O ₄	-11.00	5.45 × 10 ⁻¹⁰	Level 2 (ms2)
Quingestanol	C ₂₅ H ₃₄ O ₂	-6.08	1.09 × 10 ⁻⁹	Level 2 (ms3)
Prolinol	C ₅ H ₁₁ NO	-7.84	5.46 × 10 ⁻¹⁰	Level 2 (ms2)
N-(2-Aminoethyl)-9-pentofuranosyl-9H-purin-6-amine	C ₁₂ H ₁₈ N ₆ O ₄	-6.22	5.43 × 10 ⁻¹⁰	Level 2 (ms3)
8-Amino-7-oxononanoic acid	C ₉ H ₁₇ NO ₃	-7.81	1.32 × 10 ⁻⁵	Level 2 (ms3)
1,2,3,4-Tetramethyl-1,3-cyclopentadiene	C ₉ H ₁₄	-5.05	7.02 × 10 ⁻⁵	Level 2 (ms2)
(2R,3R,4R,5S,6R)-2-(Hydroxymethyl)-6-propyl-3,4,5-piperidinetriol	C ₉ H ₁₉ NO ₄	-9.18	5.5 × 10 ⁻¹⁰	Level 2 (ms3)
Dicirenone	C ₂₆ H ₃₆ O ₅	-6.38	1.44 × 10 ⁻⁹	Level 2 (ms3)
Heptanophenone	C ₁₃ H ₁₈ O	-7.56	5.60 × 10 ⁻¹⁰	Level 2 (ms3)
3-(2-Oxocyclododecyl)propanenitrile	C ₁₅ H ₂₅ NO	-13.51	5.46 × 10 ⁻¹⁰	Level 2 (ms3)
2-(2-Aminoethyl)-3-oxotetradecanoic acid	C ₁₆ H ₃₁ NO ₃	-5.33	5.45 × 10 ⁻¹⁰	Level 2 (ms2)
2,2-Methylenebis(4-ethyl-6-tert-butylphenol)	C ₂₅ H ₃₆ O ₂	-5.55	6.67 × 10 ⁻⁵	Level 3
2-Thiophenellurol	C ₄ H ₄ STe	-3.06	2.44 × 10 ⁻⁴	Level 3
N-(9-Decen-1-yl)-2,2,2-trifluoroacetamide	C ₁₂ H ₂₀ F ₃ NO	-3.22	5.46 × 10 ⁻¹⁰	Level 3
Di-1-tetradecen-1-yl hydrogen phosphate	C ₂₈ H ₅₅ O ₄ P	-4.00	7.50 × 10 ⁻⁵	Level 3
7-Hydroxycoumarinyl-γ-linolenate	C ₂₇ H ₃₄ O ₄	-7.23	5.45 × 10 ⁻¹⁰	Level 3
(1E)-1-Nitro-1-tridecene	C ₁₃ H ₂₅ NO ₂	-5.35	9.85 × 10 ⁻⁹	Level 3
Sorbicillin	C ₁₄ H ₁₆ O ₃	-3.25	5.91 × 10 ⁻¹⁰	Level 3
5-[3-(ethoxycarbonyl)-4-piperidinoanilino]-3,3-dimethyl-5-oxopentanoic acid	C ₂₁ H ₃₀ N ₂ O ₅	-5.68	2.81 × 10 ⁻⁷	Level 3
NP-021050	C ₃₀ H ₄₈ O ₄	-3.38	5.45 × 10 ⁻¹⁰	Level 3
1-Aminocyclododecanecarboxylic acid	C ₁₃ H ₂₅ NO ₂	-4.33	5.46 × 10 ⁻¹⁰	Level 3
(2R,9R,10R,15S)-14-(furan-3-yl)-2,6,6,10,15-pentamethyl-5,13-dioxotetracyclo[8.7.0.0.0]heptadeca-3,11-dien-9-yl acetate	C ₂₈ H ₃₄ O ₅	-7.22	5.45 × 10 ⁻¹⁰	Level 3
1,3-di-o-Tolylguanidine	C ₁₅ H ₁₇ N ₃	-5.10	5.45 × 10 ⁻¹⁰	Level 3
Viloxazine	C ₁₃ H ₁₉ NO ₃	-4.42	6.60 × 10 ⁻¹⁰	Level 3
10-Hydroxycarbazepine	C ₁₅ H ₁₄ N ₂ O ₂	-6.22	6.03 × 10 ⁻¹⁰	Level 3
3-Amino-3-(3,4,5-trimethoxyphenyl)propanoic acid	C ₁₂ H ₁₇ NO ₅	-3.03	5.62 × 10 ⁻¹⁰	Level 3
Oxymatrine	C ₁₅ H ₂₄ N ₂ O ₂	-4.28	5.45 × 10 ⁻¹⁰	Level 3
NP-015980	C ₁₄ H ₂₄ O ₆	-3.83	1.09 × 10 ⁻⁹	Level 3
2-[(4-Fluorophenyl)imino]-3-(2-oxo-2-phenylethyl)-2,3-dihydro-4H-1,3-benzoxazin-4-one	C ₂₂ H ₁₅ FN ₂ O ₃	-7.44	5.45 × 10 ⁻¹⁰	Level 3
8-(Dimethylamino)guanosine	C ₁₂ H ₁₈ N ₆ O ₅	-5.00	2.83 × 10 ⁻⁵	Level 3
11-Oxoetiocholanolone	C ₁₉ H ₂₈ O ₃	-3.52	5.45 × 10 ⁻¹⁰	Level 3
16α-Hydroxydehydroepiandrosterone	C ₁₉ H ₂₈ O ₃	-5.20	5.47 × 10 ⁻¹⁰	Level 3
DL-Glutamine	C ₅ H ₁₀ N ₂ O ₃	-4.26	5.45 × 10 ⁻¹⁰	Level 3
Metolachlor morpholinone	C ₁₄ H ₁₉ NO ₂	-5.10	5.45 × 10 ⁻¹⁰	Level 3
2-(3-Phenylpropyl)tetrahydrofuran	C ₁₃ H ₁₈ O	-4.12	5.97 × 10 ⁻⁴	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
4-(4-methoxyphenyl)-6-pyridin-4-yl-1,3,5-triazin-2(3H)-one	C ₁₅ H ₁₂ N ₄ O ₂	-5.53	5.45 × 10 ⁻¹⁰	Level 3
MFCDD11502269	C ₁₆ H ₃₃ NO ₂	-3.08	8.33 × 10 ⁻¹⁰	Level 3
Betaxolol	C ₁₈ H ₂₉ NO ₃	-3.63	5.45 × 10 ⁻¹⁰	Level 3
DL-Carnitine	C ₇ H ₁₅ NO ₃	-4.34	5.45 × 10 ⁻¹⁰	Level 3
4-(Cyclooctylamino)-4-oxobutanoic acid	C ₁₂ H ₂₁ NO ₃	-3.30	8.19 × 10 ⁻¹⁰	Level 3
Fingolimod	C ₁₉ H ₃₃ NO ₂	-3.10	6.68 × 10 ⁻¹⁰	Level 3
2,5-Bis(5-tert-butyl-benzoxazol-2-yl)thiophene	C ₂₆ H ₂₆ N ₂ O ₂ S	-4.71	2.18 × 10 ⁻⁶	Level 3
UNII:W9EN9DLM98	C ₉ H ₂₁ NO ₃	-8.38	1.89 × 10 ⁻⁴	Level 3
N-Boc-2-amino-2-methyl-1-propanol	C ₉ H ₁₉ NO ₃	-7.64	7.17 × 10 ⁻⁷	Level 3
Diheptyl phthalate	C ₂₂ H ₃₄ O ₄	-5.22	4.96 × 10 ⁻⁵	Level 3
PB2275000	C ₄ H ₁₀ O ₃ S	-6.62	1.40 × 10 ⁻⁶	Level 3
MFCDD08144705	C ₇ H ₁₅ NO ₂	-5.74	1.37 × 10 ⁻⁵	Level 3
4-Hydroxy-1-butanefulfonic acid	C ₄ H ₁₀ O ₄ S	-5.00	2.65 × 10 ⁻⁴	Level 3
Gabapentin	C ₉ H ₁₇ NO ₂	-4.52	3.08 × 10 ⁻⁹	Level 3
5-[5-hydroxy-3-(hydroxymethyl)pentyl]-8a-(hydroxymethyl)-5,6-dimethyl-3,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid	C ₂₀ H ₃₄ O ₅	-3.41	5.45 × 10 ⁻¹⁰	Level 3
Pramocaine	C ₁₇ H ₂₇ NO ₃	-5.22	5.45 × 10 ⁻¹⁰	Level 3
Diethyl 3-(trifluoromethyl)pentanedioate	C ₁₀ H ₁₅ F ₃ O ₄	-3.06	5.69 × 10 ⁻¹⁰	Level 3
Benzyl				
{{(2S)-1-(methyl[(2-methyl-2-propanyl)oxy]carbonyl)amino)-3-[(3R)-tetrahydro-2H-pyran-3-yl]-2-propanyl}carbamate	C ₂₂ H ₃₄ N ₂ O ₅	-5.88	1.17 × 10 ⁻⁸	Level 3
8-[4-(2-Hydroxyethyl)-1-piperazinyl]-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione	C ₁₃ H ₂₀ N ₆ O ₃	-3.57	2.37 × 10 ⁻⁵	Level 3
3-(Methylsulfonyl)-1-propanol	C ₄ H ₁₀ O ₃ S	-6.95	2.79 × 10 ⁻⁷	Level 3
[2-(hydroxymethyl)-5,5,8a-trimethyl-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-yl]methanol	C ₁₅ H ₂₆ O ₂	-4.09	5.91 × 10 ⁻¹⁰	Level 3
L-Pyroglutamic acid	C ₅ H ₇ NO ₃	-3.99	5.64 × 10 ⁻¹⁰	Level 3
2-Methyl-2-propanyl				
4-(1-amino-2,2,2-trifluoroethyl)-1-piperidinecarboxylate	C ₁₂ H ₂₁ F ₃ N ₂ O ₂	-3.27	5.46 × 10 ⁻¹⁰	Level 3
Dropropizine	C ₁₃ H ₂₀ N ₂ O ₂	-3.87	6.01 × 10 ⁻¹⁰	Level 3
2,2,2-Trifluoro-N-octylacetamide	C ₁₀ H ₁₈ F ₃ NO	-3.19	5.45 × 10 ⁻¹⁰	Level 3
NP-004917	C ₁₅ H ₂₆ O ₃	-5.28	5.45 × 10 ⁻¹⁰	Level 3
Anapheline	C ₁₃ H ₂₄ N ₂ O	-4.18	5.45 × 10 ⁻¹⁰	Level 3
Dinotefuran-metabolite-UF	C ₇ H ₁₄ N ₂ O ₂	-3.95	5.45 × 10 ⁻¹⁰	Level 3
2-oxa-4-azatetracyclo[6.3.1.1~6,10~.0~1,5~]tridecan-3-one	C ₁₁ H ₁₅ NO ₂	-3.18	5.63 × 10 ⁻¹⁰	Level 3
2-morpholino-1-phenyl-1-ethanol	C ₁₂ H ₁₇ NO ₂	-4.01	1.06 × 10 ⁻⁹	Level 3
Tolmetin	C ₁₅ H ₁₅ NO ₃	-4.98	5.45 × 10 ⁻¹⁰	Level 3
N,N'-1,2-Ethanediybis(3-sulfanylpropanamide)	C ₈ H ₁₆ N ₂ O ₂ S ₂	-6.20	1.28 × 10 ⁻⁷	Level 3
(3beta,16alpha)-3,16-Dihydroxy-13,28-epoxyoleanan-30-al	C ₃₀ H ₄₈ O ₄	-3.47	5.45 × 10 ⁻¹⁰	Level 3
N,N-Dibutyl-4-morpholinesulfonamide	C ₁₂ H ₂₆ N ₂ O ₃ S	-8.98	5.49 × 10 ⁻¹⁰	Level 3
1-Aminocycloundecanecarboxylic acid	C ₁₂ H ₂₃ NO ₂	-3.35	5.45 × 10 ⁻¹⁰	Level 3
4-oxosebacic acid	C ₁₀ H ₁₆ O ₅	-3.61	5.45 × 10 ⁻¹⁰	Level 3

2-Methyl-5,8,11-trioxa-2-azatetradecan-13-ol	C ₁₁ H ₂₅ NO ₄	-11.86	5.45 × 10 ⁻¹⁰	Level 3
1-Aminocyclodecanecarboxylic acid	C ₁₁ H ₂₁ NO ₂	-4.60	5.45 × 10 ⁻¹⁰	Level 3
2,4-Bis-(octylmercapto)-6-(4-hydroxy-3,5-di-tert-butylanilino)-1,3,5-triazine	C ₃₃ H ₅₆ N ₄ OS ₂	-6.42	5.58 × 10 ⁻⁵	Level 3

Compound	Formula	Log2 Fold Change	p-value	Identified level
5-Methyl-4-sulfanyl-2-(2,4,4-trimethyl-2-pentanyl)phenol	C ₁₅ H ₂₄ OS	-9.97	2.85 × 10 ⁻⁷	Level 3
S-Isobutyl ethyl(2-((isobutylsulfanyl)carbonyl)amino)ethyl)carbamothioate	C ₁₄ H ₂₈ N ₂ O ₂ S ₂	-8.16	5.45 × 10 ⁻¹⁰	Level 3
N-Decyl-2,2,2-trifluoroacetamide	C ₁₂ H ₂₂ F ₃ NO	-4.54	5.45 × 10 ⁻¹⁰	Level 3
512173	C ₄ H ₂ Cl ₄ O ₃	-5.22	6.19 × 10 ⁻¹⁰	Level 3
N-(1-Hydroxy-2-butanyl)undecanamide	C ₁₅ H ₃₁ NO ₂	-3.66	5.45 × 10 ⁻¹⁰	Level 3
1-Trifluoroacetyl Piperidine	C ₇ H ₁₀ F ₃ NO	-7.17	1.84 × 10 ⁻⁴	Level 3
N-Acetylvaline	C ₇ H ₁₃ NO ₃	-5.06	2.45 × 10 ⁻⁵	Level 3
Ethyl 2,4-dioxohexanoate	C ₈ H ₁₂ O ₄	-3.98	5.45 × 10 ⁻¹⁰	Level 3
NP-018660	C ₁₃ H ₂₂ O ₃	-3.13	1.04 × 10 ⁻⁷	Level 3
N-HYDROXYETHYL-N-METHYLCAPRAMIDE	C ₁₃ H ₂₇ NO ₂	-3.55	5.45 × 10 ⁻¹⁰	Level 3
UNII:FD6L8T043R	C ₁₆ H ₂₆ N ₂ O ₄	-8.36	5.45 × 10 ⁻¹⁰	Level 3
euscaphic acid	C ₃₀ H ₄₈ O ₅	-3.71	5.45 × 10 ⁻¹⁰	Level 3
5,5-dimethyl-3-morpholinocyclohex-2-en-1-one	C ₁₂ H ₁₉ NO ₂	-4.28	5.45 × 10 ⁻¹⁰	Level 3
Isoetharine	C ₁₃ H ₂₁ NO ₃	-4.53	5.45 × 10 ⁻¹⁰	Level 3
3,3'-(1,12-Dodecanediyl)bis(1,2,4-oxadiazol-5-amine)	C ₁₆ H ₂₈ N ₆ O ₂	-5.77	3.32 × 10 ⁻⁷	Level 3
Jervine	C ₂₇ H ₃₉ NO ₃	-5.61	4.05 × 10 ⁻⁷	Level 3
N-Cyclohexyl-4-(2,2,2-trifluoroethoxy)cyclohexanamine	C ₁₄ H ₂₄ F ₃ NO	-5.71	5.45 × 10 ⁻¹⁰	Level 3
Aldicarb oxime	C ₅ H ₁₁ NOS	-3.56	6.64 × 10 ⁻¹⁰	Level 3
UNII:W9EN9DLM98	C ₉ H ₂₁ NO ₃	-9.06	1.77 × 10 ⁻⁷	Level 3
Butyl 2,2,2-trifluoro-N-hydroxyethanimidothioate	C ₆ H ₁₀ F ₃ NOS	-5.94	1.34 × 10 ⁻⁹	Level 3
1-(2-Amino-ethyl)-N-Boc-cyclohexylamine	C ₁₃ H ₂₆ N ₂ O ₂	-4.26	5.45 × 10 ⁻¹⁰	Level 3
4-Octylphenol	C ₁₄ H ₂₂ O	-4.64	4.42 × 10 ⁻⁶	Level 3
6,7,8-trimethoxy-2H-chromen-2-one	C ₁₂ H ₁₂ O ₅	-7.52	1.62 × 10 ⁻⁹	Level 3
N-Hexadecyl-1,4-dihydroxy-2-naphthamide	C ₂₇ H ₄₁ NO ₃	-4.25	8.41 × 10 ⁻⁵	Level 3
Diethyl sulfate	C ₄ H ₁₀ O ₄ S	-8.85	1.40 × 10 ⁻⁹	Level 3
2-Cyclohexylacetohydrazide	C ₈ H ₁₆ N ₂ O	-3.09	5.45 × 10 ⁻¹⁰	Level 3
Mazindol	C ₁₆ H ₁₃ ClN ₂ O	-4.28	5.45 × 10 ⁻¹⁰	Level 3
2-Methyl-N-[3-(trifluoromethyl)phenyl]propanamide	C ₁₁ H ₁₂ F ₃ NO	-5.92	5.51 × 10 ⁻¹⁰	Level 3
3603307	C ₉ H ₁₉ NO ₃	-8.82	2.93 × 10 ⁻⁸	Level 3
N-(9-oxodecyl)acetamide	C ₁₂ H ₂₃ NO ₂	-3.31	5.45 × 10 ⁻¹⁰	Level 3
2-HYDROXYLAURYLDIMETHYL BETAINE	C ₁₆ H ₃₃ NO ₃	-5.24	9.30 × 10 ⁻¹⁰	Level 3
2-Methyl-2-propanyl {2-[2-(2-hydroxyethoxy)ethoxy]ethyl}carbamate	C ₁₁ H ₂₃ NO ₅	-6.76	7.32 × 10 ⁻¹⁰	Level 3
(-)	C ₂₇ H ₅₁ F ₃ N ₂ O ₃	-5.11	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₀ H ₂₀ F ₂ N ₆ OS	-3.49	5.47 × 10 ⁻¹⁰	Level 4
(-)	C ₁₃ H ₂₅ N ₉ O	-6.58	5.75 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₅ NO ₄ P ₂	-3.33	1.13 × 10 ⁻⁹	Level 4
(-)	C ₂₀ H ₃₅ F ₃ O ₃	-3.08	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₈ H ₁₉ FN ₈	-4.13	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₂₃ F ₃ N ₆ O	-7.58	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₇ F ₃ N ₂ O ₆ S ₂	-7.23	5.50 × 10 ⁻¹⁰	Level 4
(-)	C ₁₂ H ₂₄ F ₂ N ₆ S	-3.18	6.51 × 10 ⁻¹⁰	Level 4
(-)	C ₁₈ H ₂₉ FS	-3.14	5.55 × 10 ⁻¹⁰	Level 4
(-)	C ₁₅ H ₂₇ N ₅ O ₃	-3.94	1.34 × 10 ⁻⁹	Level 4

(-)

$C_{21}H_{45}N_3O_2S_2$

-5.94

1.86×10^{-7}

Level 4

Compound	Formula	Log2 Fold Change	p-value	Identified level
(-)	C ₄ H ₂ F ₁₁ O ₄ P ₃ S ₂	-7.60	9.22 × 10 ⁻⁸	Level 4
(-)	C ₁₆ H ₃₈ N ₈ O ₂ S	-6.27	1.18 × 10 ⁻⁹	Level 4
(-)	C ₄ H ₁₀ FN ₃ O ₄	-5.50	9.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₈ H ₃₅ FN ₂ O ₆ S	-6.64	8.32 × 10 ⁻¹⁰	Level 4
(-)	C ₂₀ H ₃₉ FN ₂ O ₄	-6.59	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₇ HF ₄ O ₁₆ P ₃ S	-3.55	7.33 × 10 ⁻⁴	Level 4
(-)	C ₉ H ₁₆ F ₂ N ₂ O ₄ S ₂	-3.26	5.47 × 10 ⁻¹⁰	Level 4
(-)	C ₁₆ H ₂₈ F ₄ NP	-4.09	6.51 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₂₄ N ₅ O ₃ P	-6.61	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₂ H ₂₄ F ₄ N ₄ O ₂	-3.45	7.83 × 10 ⁻¹⁰	Level 4
(-)	C ₂₆ H ₃₆ O ₄ S ₂	-4.27	6.52 × 10 ⁻¹⁰	Level 4
(-)	C ₃₁ H ₄₈ N ₄ S ₂	-3.63	3.69 × 10 ⁻⁹	Level 4
(-)	C ₁₂ H ₂₅ ClN ₄ O ₈	-6.38	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₅ H ₂₈ F ₃ N	-3.60	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₃ H ₃₁ FN ₈ OS ₂	-5.94	2.04 × 10 ⁻⁸	Level 4
(-)	C ₁₁ H ₂₈ N ₄ O ₂ P ₂ S	-9.28	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₃ H ₄ N ₆ O ₂ S ₂	-7.26	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₁ F ₃ O ₅	-6.09	2.53 × 10 ⁻⁷	Level 4
(-)	C ₁₃ H ₂₄ F ₃ NO	-3.32	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₇ H ₃₀ FNO	-8.13	2.09 × 10 ⁻⁹	Level 4
(-)	C ₁₄ H ₂₁ F ₃ O ₄	-6.89	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₀ H ₁₇ F ₃ N ₂ S ₂	-5.39	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₁ F ₃	-3.93	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₈ H ₃₆ N ₂ O ₂ S ₂	-5.34	3.00 × 10 ⁻⁸	Level 4
(-)	C ₅ HF ₂ O ₂ P ₃ S	-5.22	9.54 × 10 ⁻¹⁰	Level 4
(-)	C ₁₄ H ₂₉ FO ₃	-3.56	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₀ H ₂₀ F ₂ N ₆ O ₂ S	-4.77	2.25 × 10 ⁻⁸	Level 4
(-)	C ₁₂ H ₂₁ F ₃ N ₂ S ₂	-7.81	5.49 × 10 ⁻¹⁰	Level 4
(-)	C ₆ H ₉ F ₃ N ₂ S ₂	-5.70	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₉ H ₁₉ FN ₃ O ₄ P	-5.03	1.53 × 10 ⁻⁹	Level 4
(-)	C ₁₀ H ₁₇ F ₃ N ₂ O ₂ S ₃	-7.81	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₃ H ₂₂ F ₃ NO	-5.43	3.87 × 10 ⁻⁹	Level 4
(-)	C ₁₇ H ₃₇ N ₃ O ₂ S ₂	-6.03	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₀ H ₂₀ F ₂ N ₃ OP	-4.74	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₃ H ₂₉ NO ₅	-6.94	2.69 × 10 ⁻⁹	Level 4
(-)	C ₁₀ H ₉ F ₅ N ₂ O ₃	-4.19	5.45 × 10 ⁻¹⁰	Level 4
(-)	C ₁₉ H ₃₄ F ₃ NO	-4.32	5.45 × 10 ⁻¹⁰	Level 4
(-)	(-) (m/z=609.80086)	-6.51	1.29 × 10 ⁻⁵	Level 5
(-)	(-) (m/z=541.81345)	-3.58	8.61 × 10 ⁻⁴	Level 5
(-)	(-) (m/z=671.77315)	-6.79	5.31 × 10 ⁻⁹	Level 5

(-) = No name/No formula described in CD

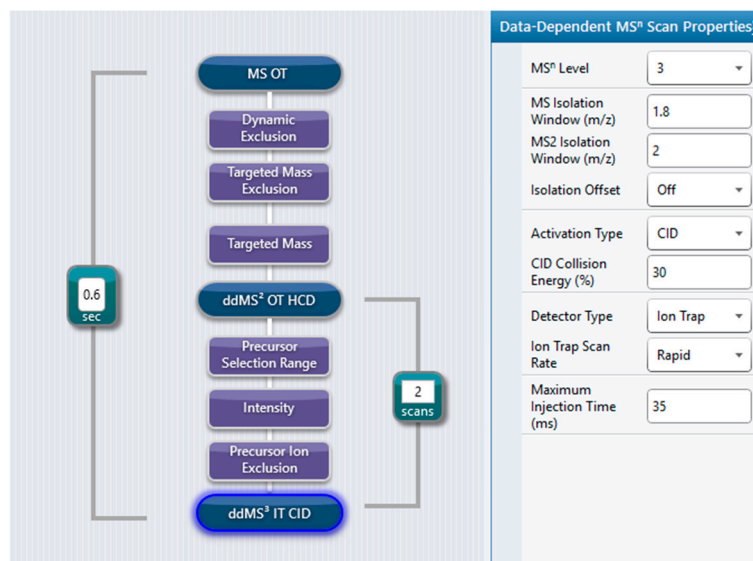
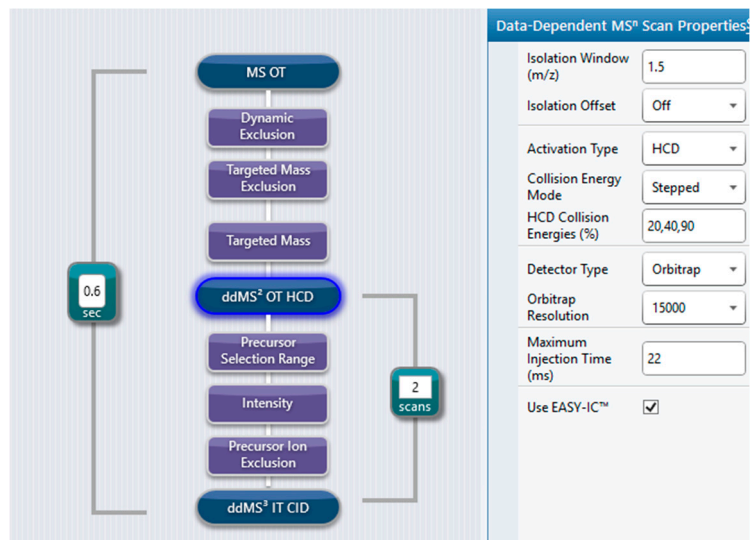
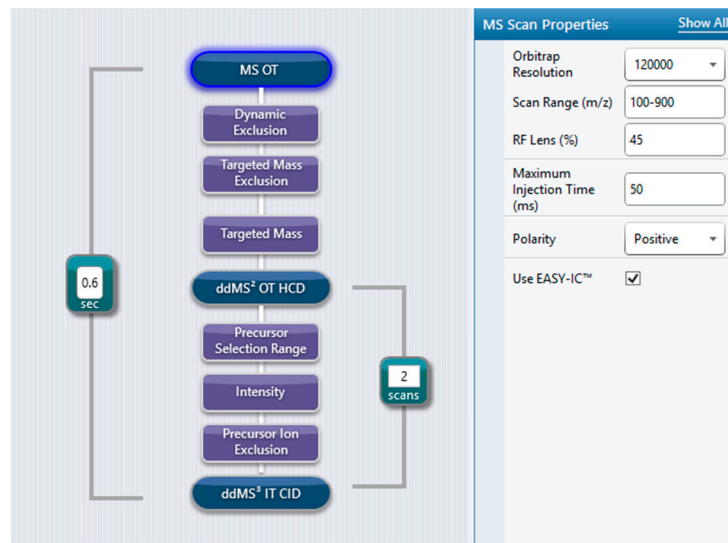


Figure S1. Workflow used in AcquireX Deep Scan Mode–MS³.

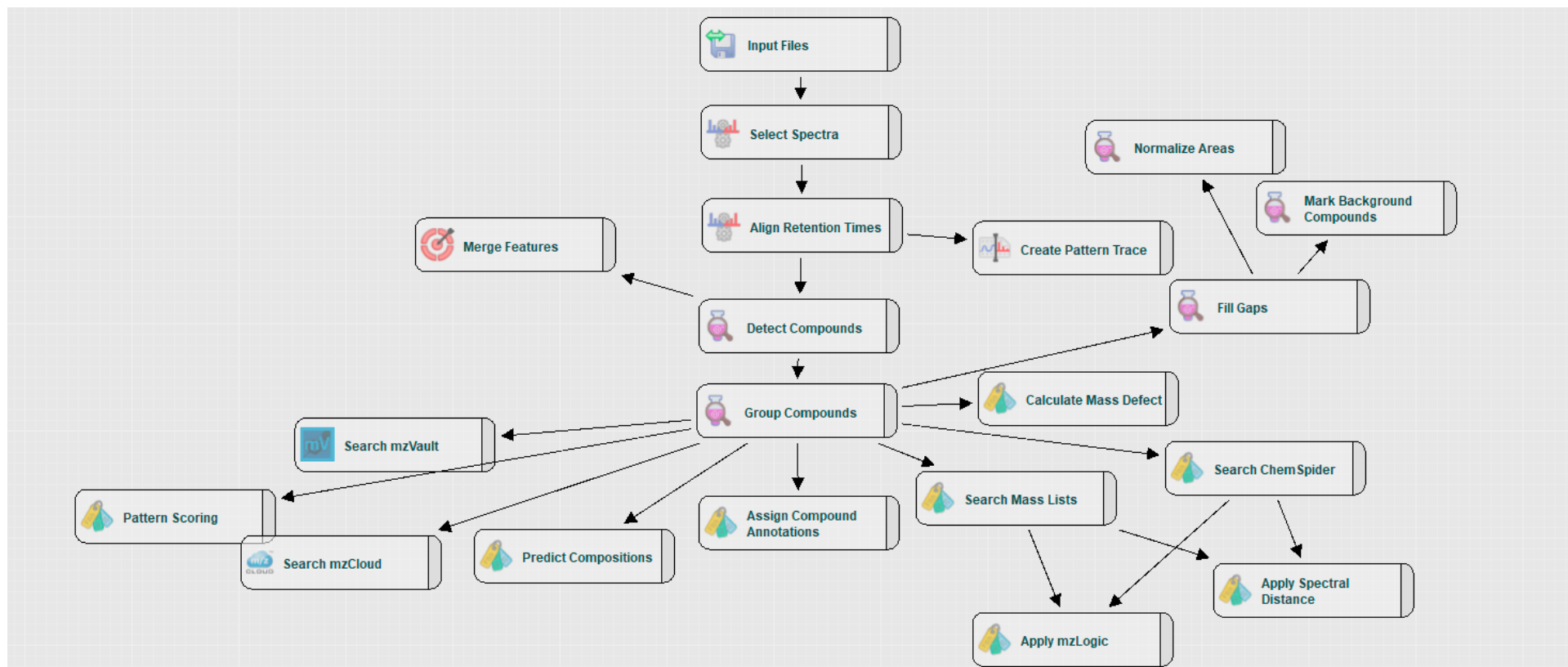


Figure S2. Workflow used in Compound Discoverer™ (CD) data processing.

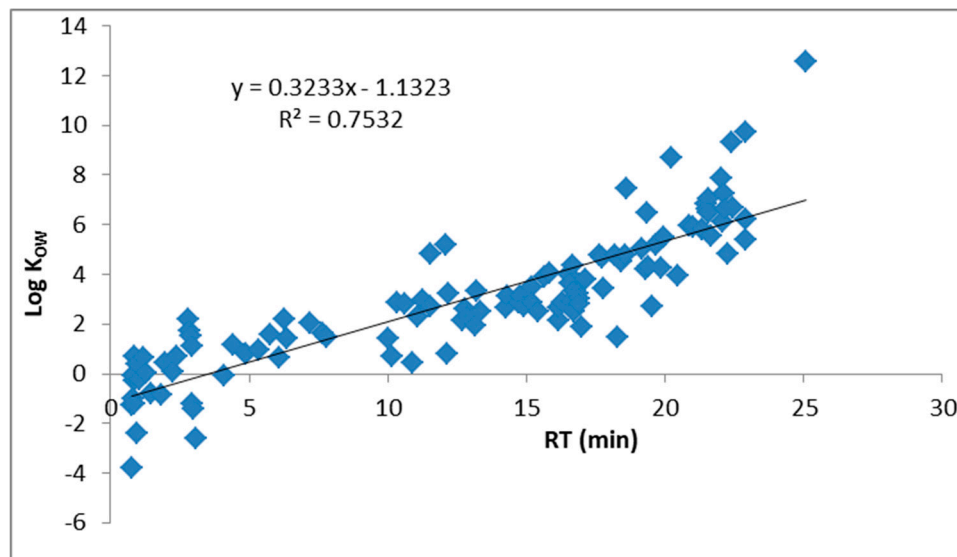


Figure S3. Graphic of Log K_{ow} vs Retention time (RT) of the analytical reference standards.

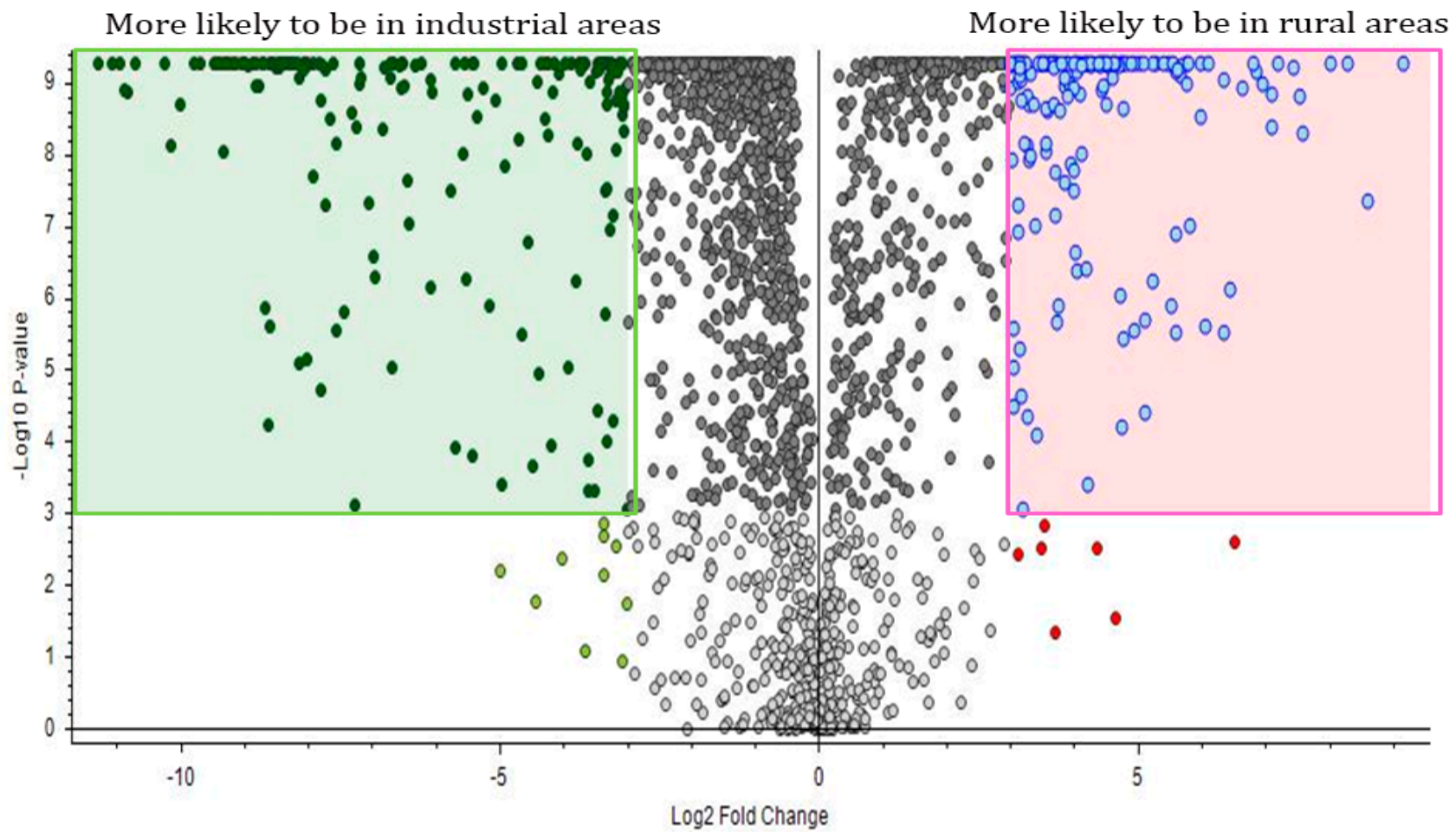


Figure S4. Volcano plot for identification of discriminating substances between industrial and rural areas (employed parameters: $p\text{-value}=0.001$ and $\text{log}_2\text{Fold}=3$).

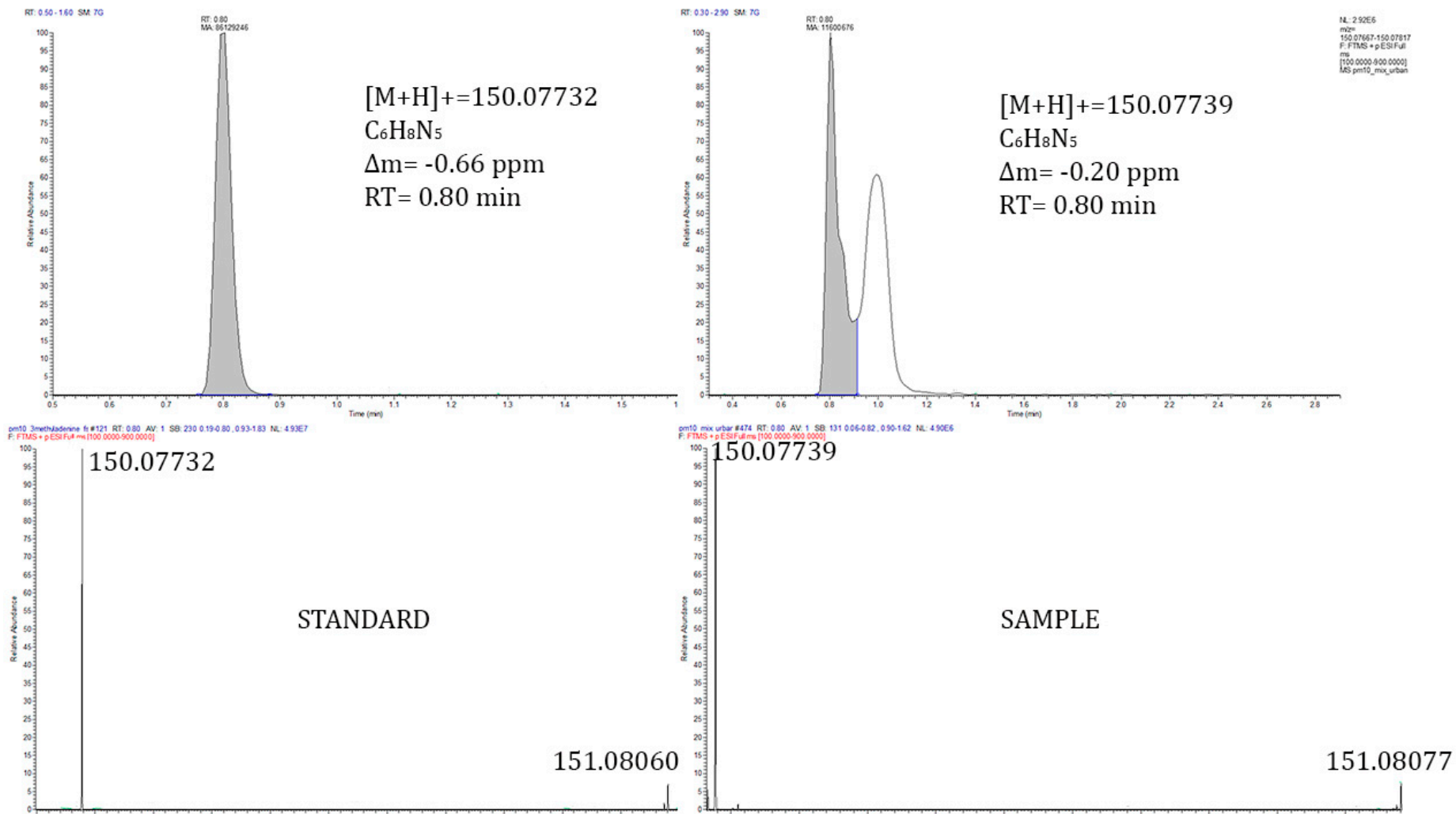


Figure S5. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of 3-methyladenine in a standard (left) and a real sample (right).

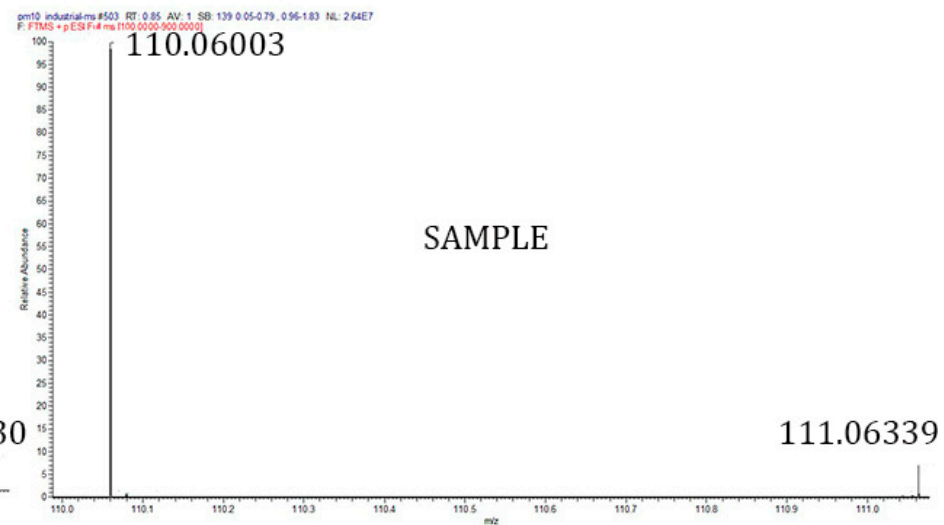
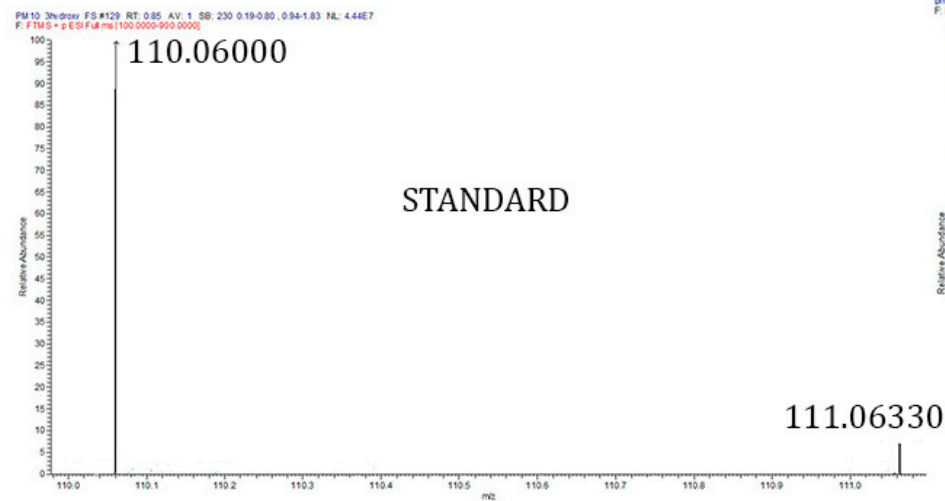
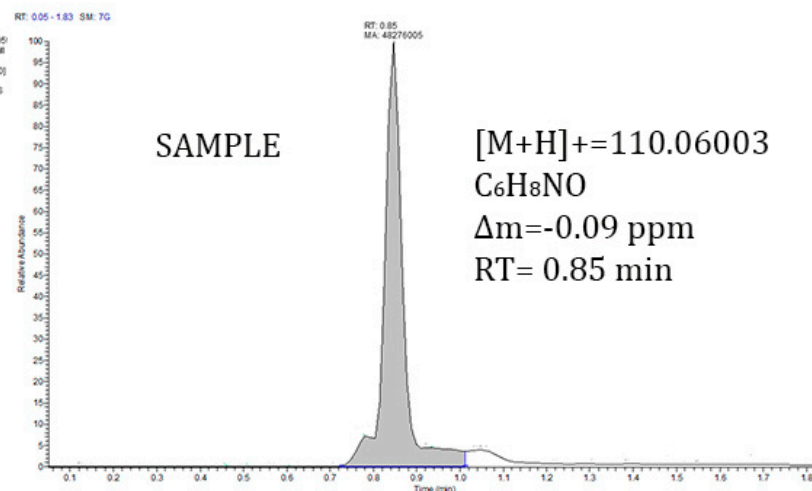
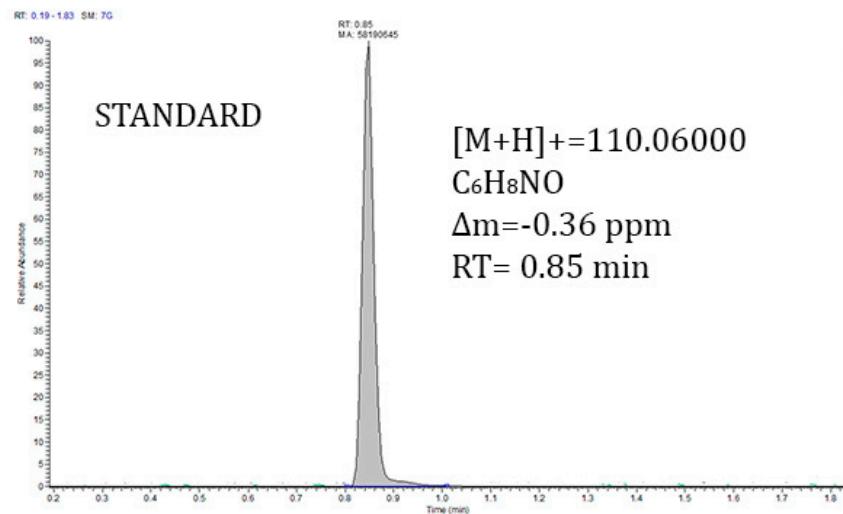


Figure S6. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of 3-hydroxy-2-methylpyridine in a standard (left) and a real sample (right).

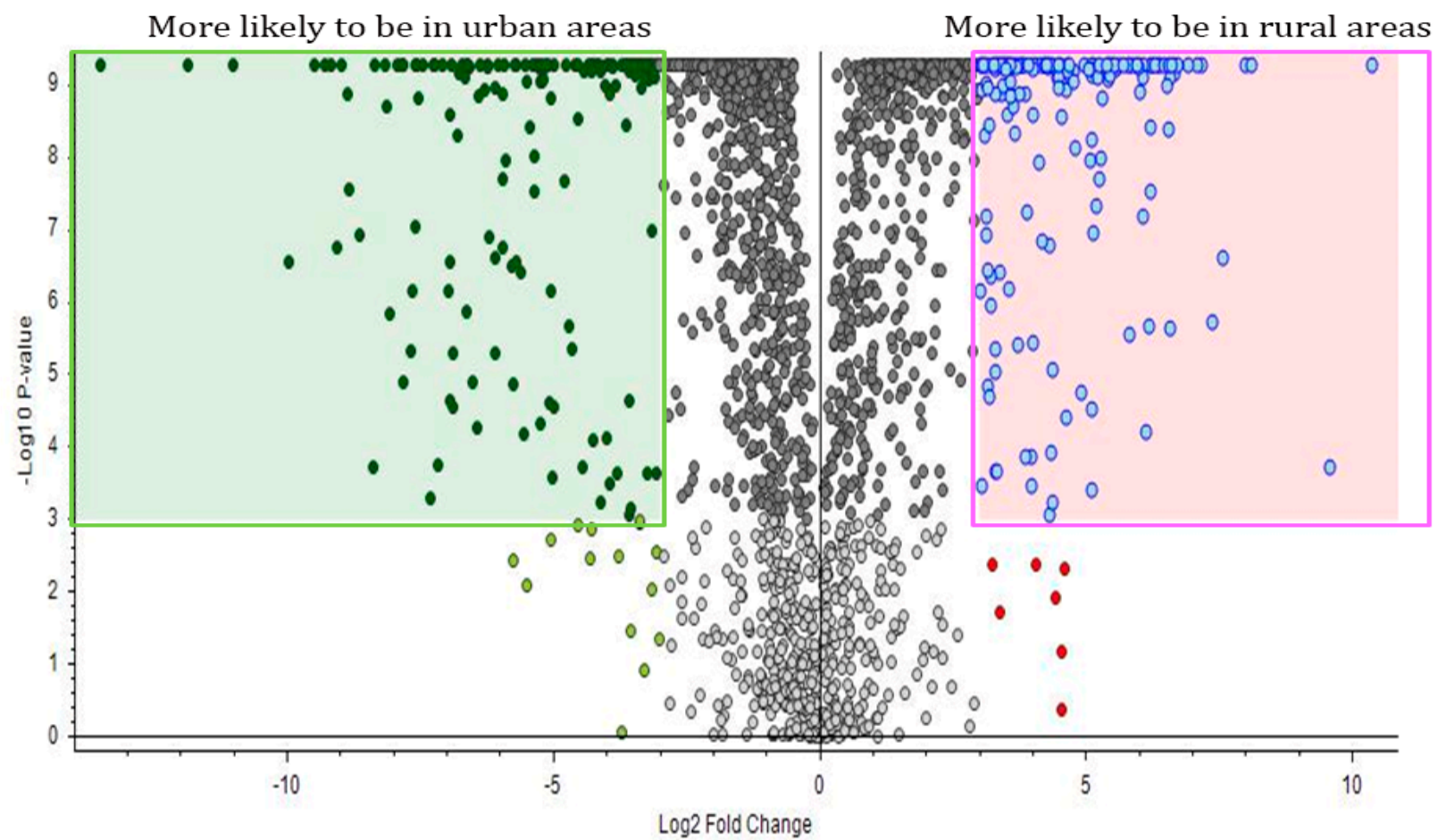
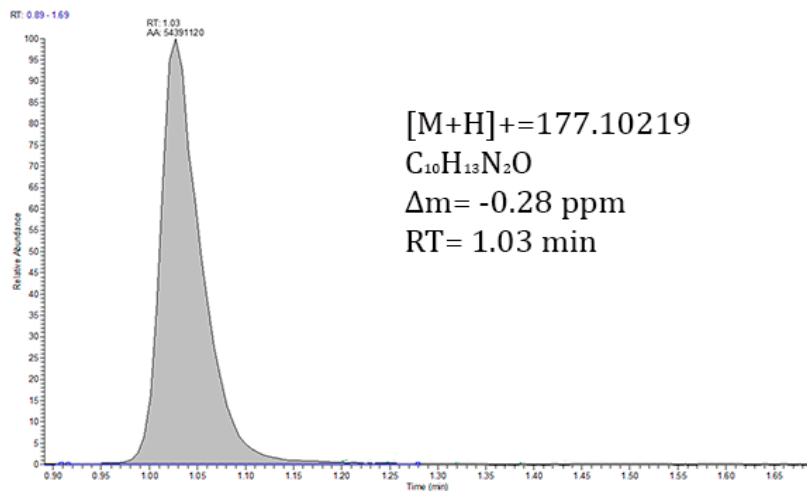
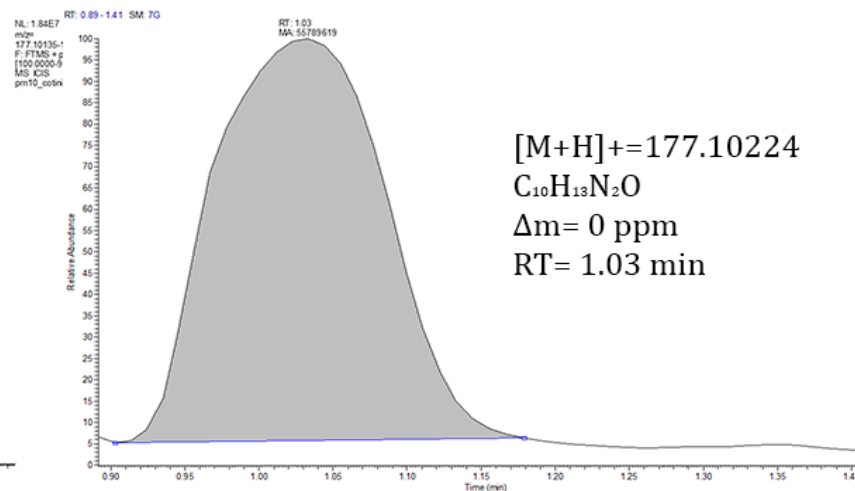


Figure S7. Volcano plot for identification of discriminating substances between urban and rural areas (employed parameters: $p\text{-value}=0.001$ and $\log_2\text{Fold}=3$).



$[M+H]^+=177.10219$
 $C_{10}H_{13}N_2O$
 $\Delta m = -0.28$ ppm
 RT = 1.03 min



$[M+H]^+=177.10224$
 $C_{10}H_{13}N_2O$
 $\Delta m = 0$ ppm
 RT = 1.03 min

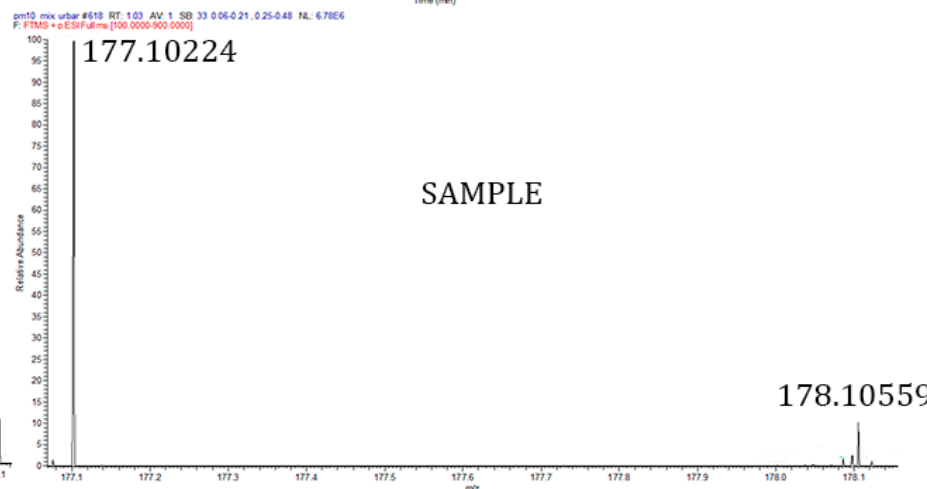
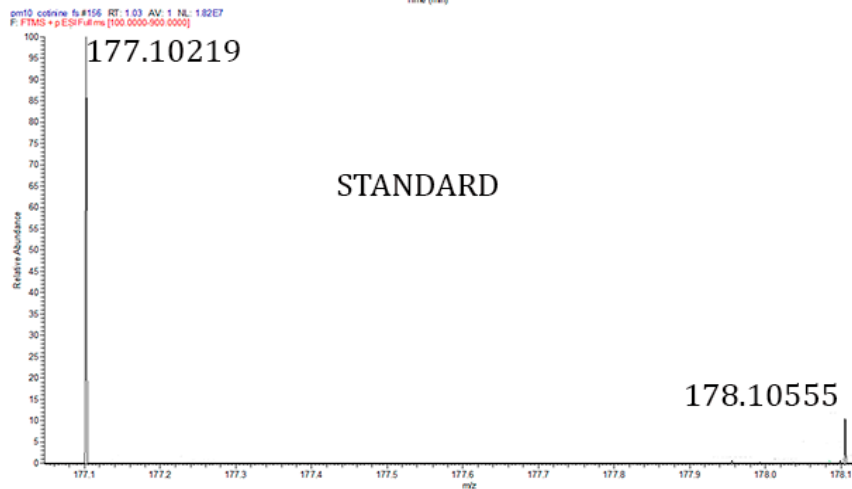


Figure S8. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of cotinine in a standard (left) and a real sample (right).

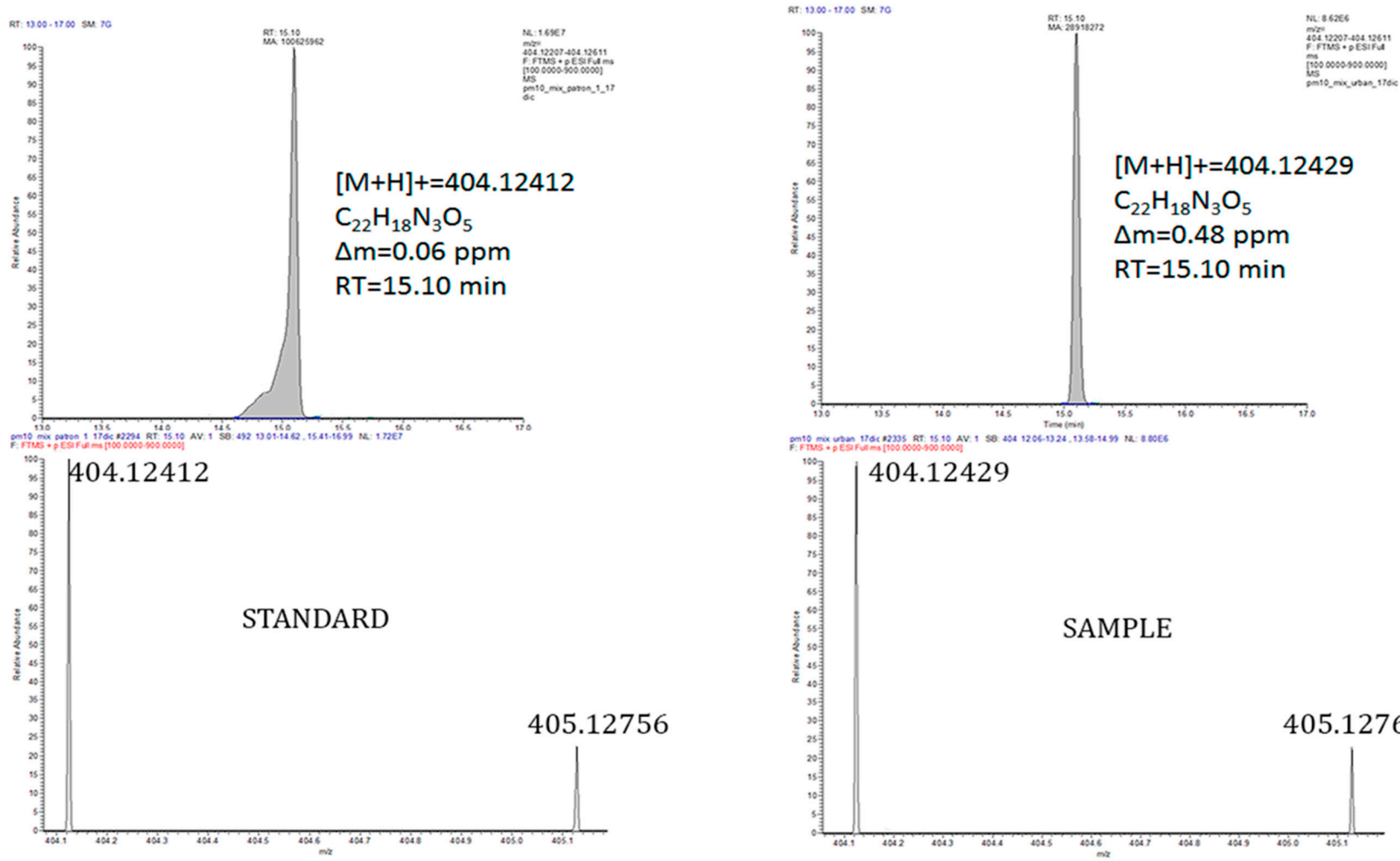


Figure S9. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of azoxystrobin in a standard (left) and a real sample (right).

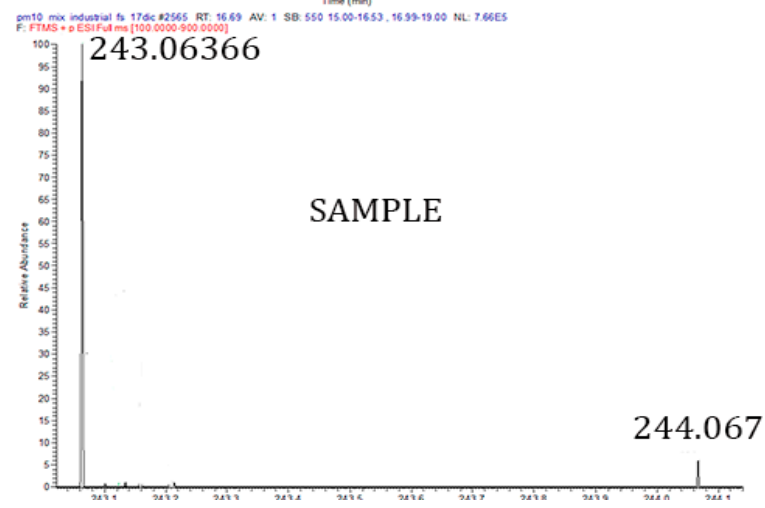
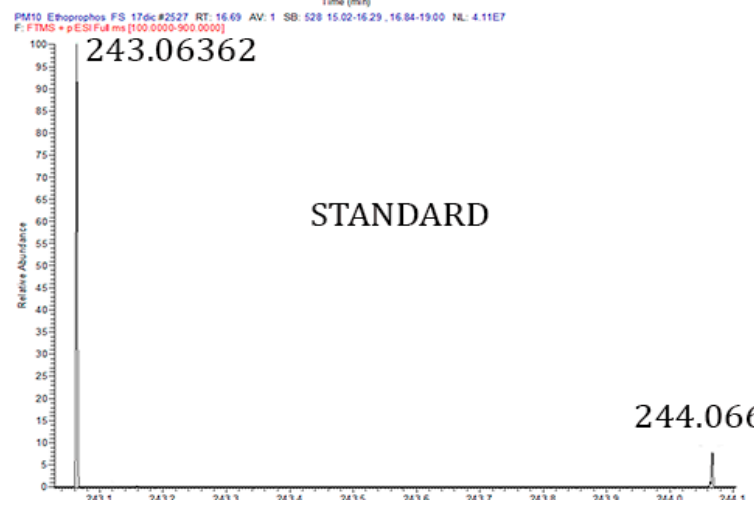
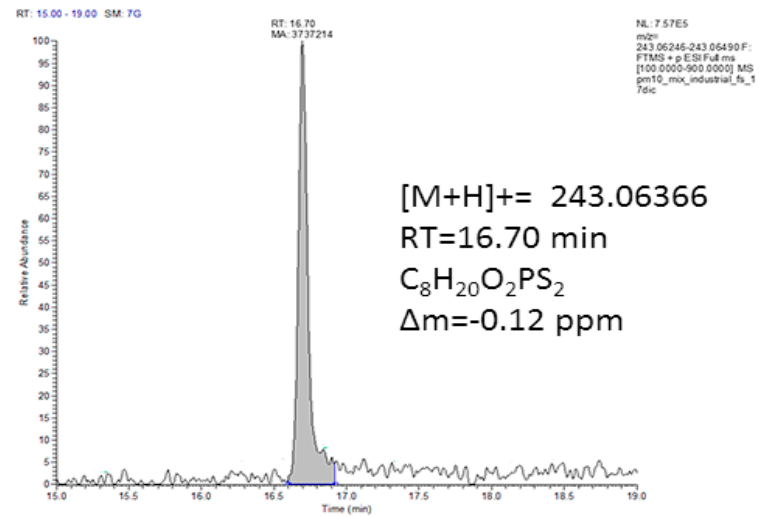
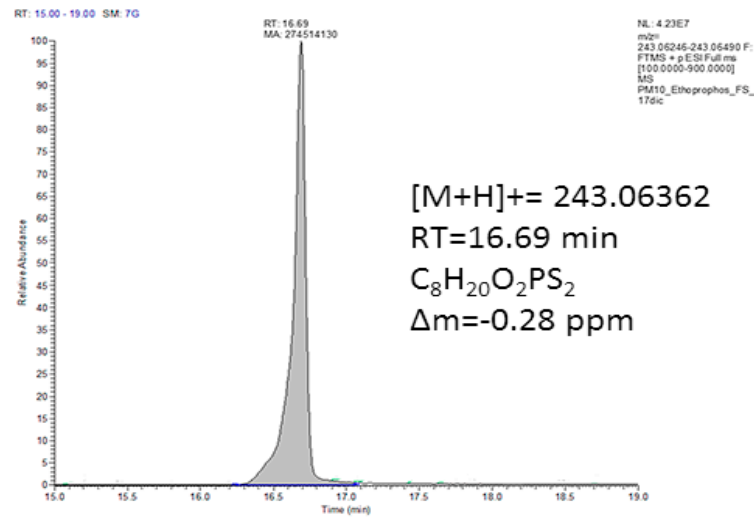


Figure S10. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of ethoprophos in a standard (left) and a real sample (right).

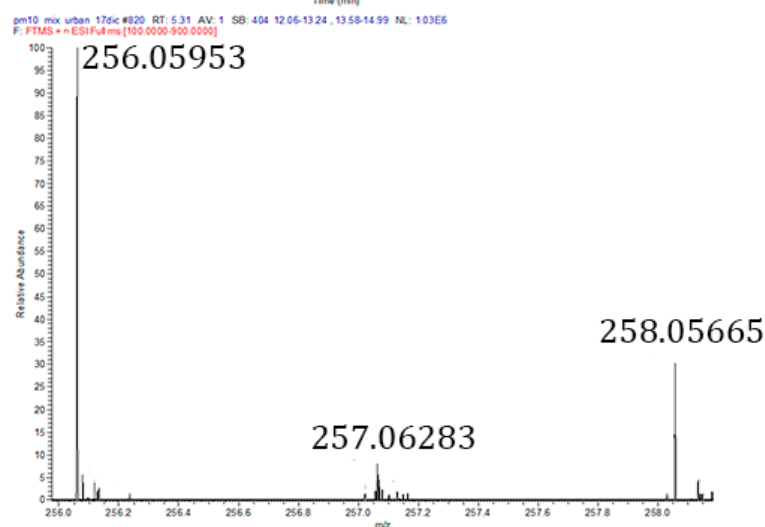
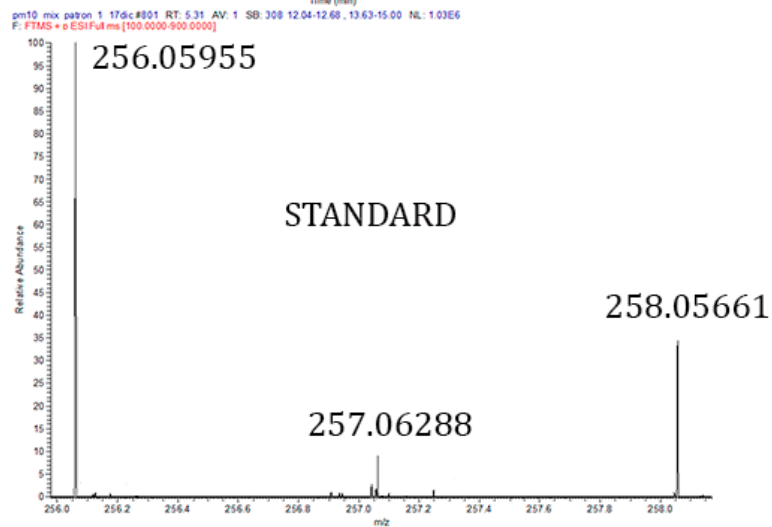
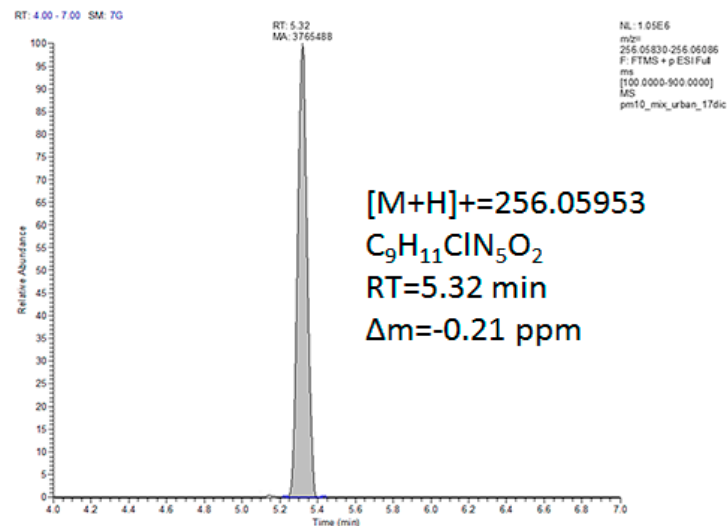
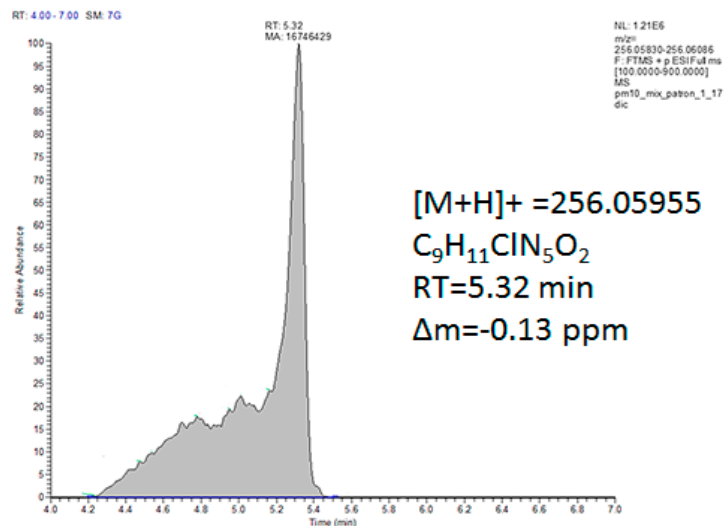


Figure S11. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of imidacloprid in a standard (left) and a real sample (right).

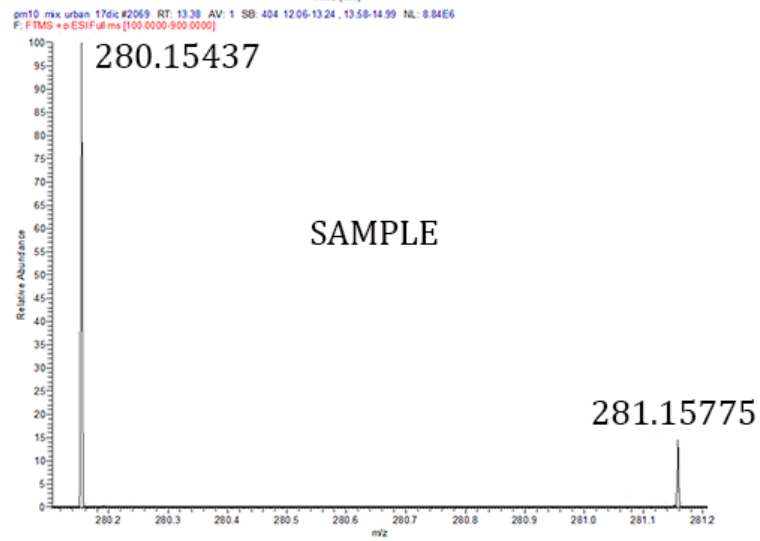
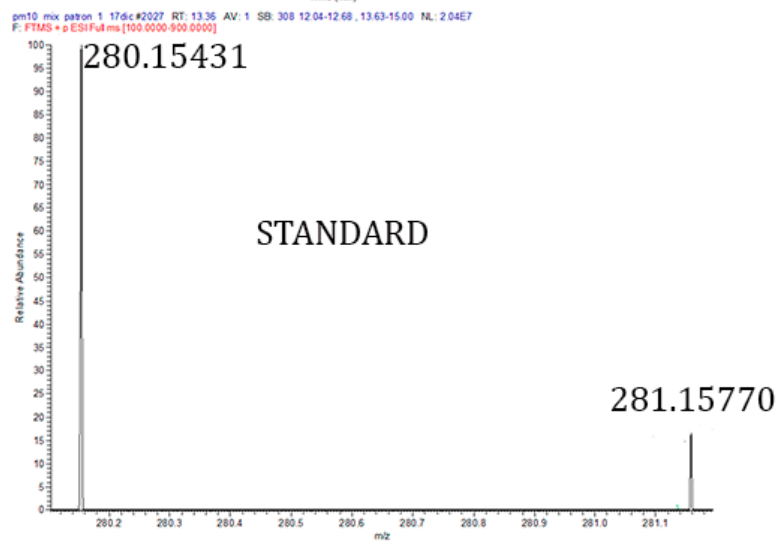
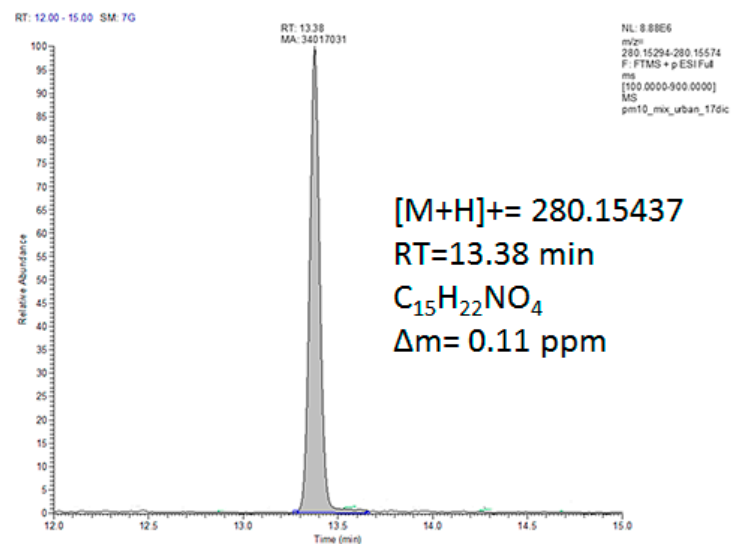
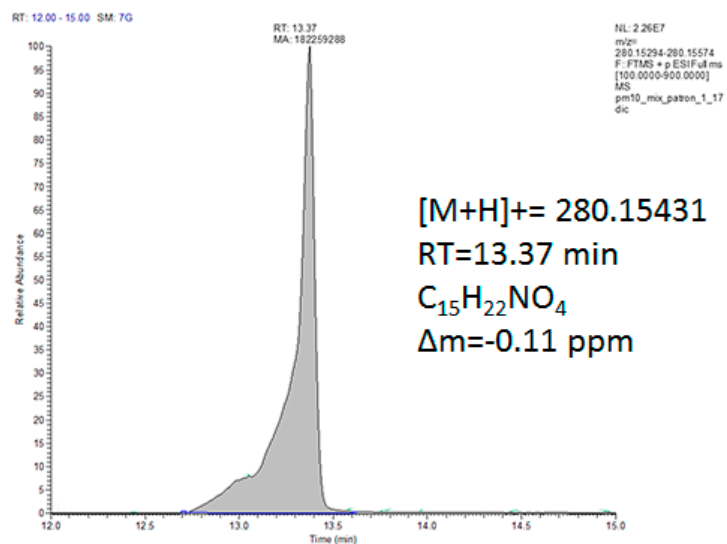


Figure S12. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of metalaxyl in a standard (left) and a real sample (right).

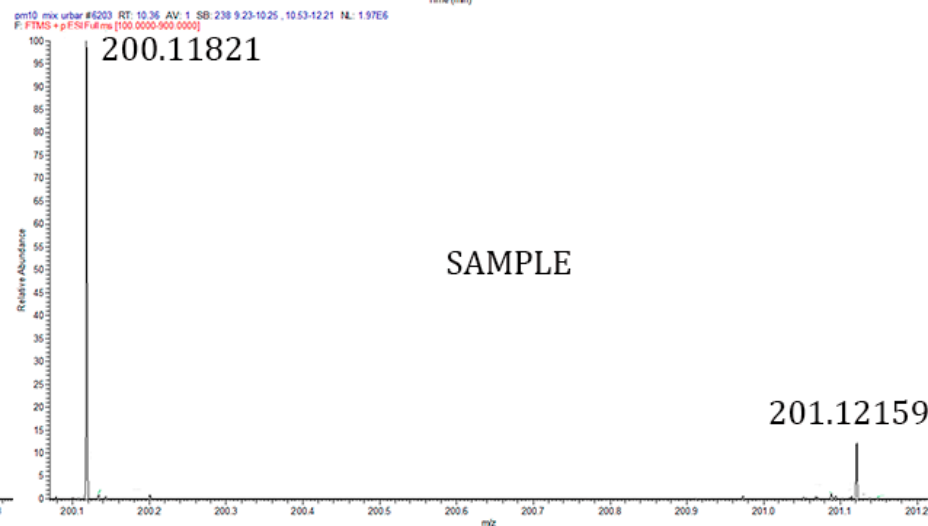
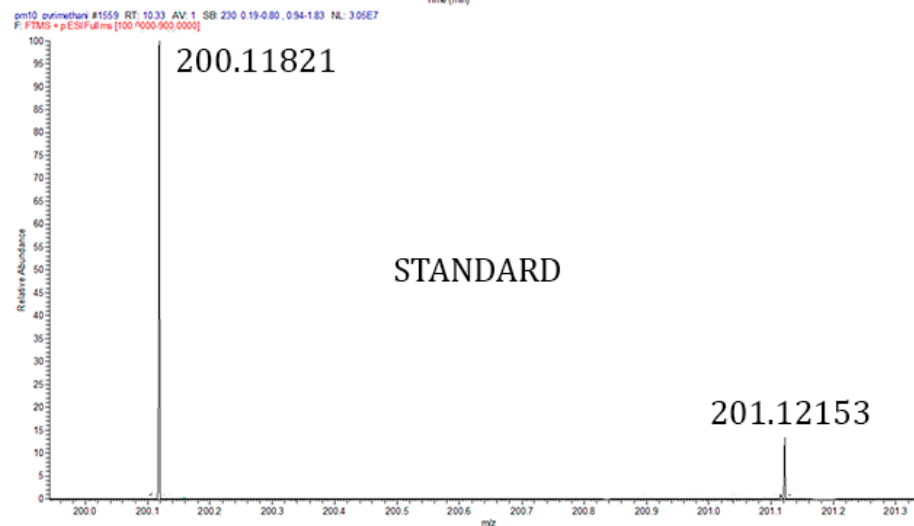
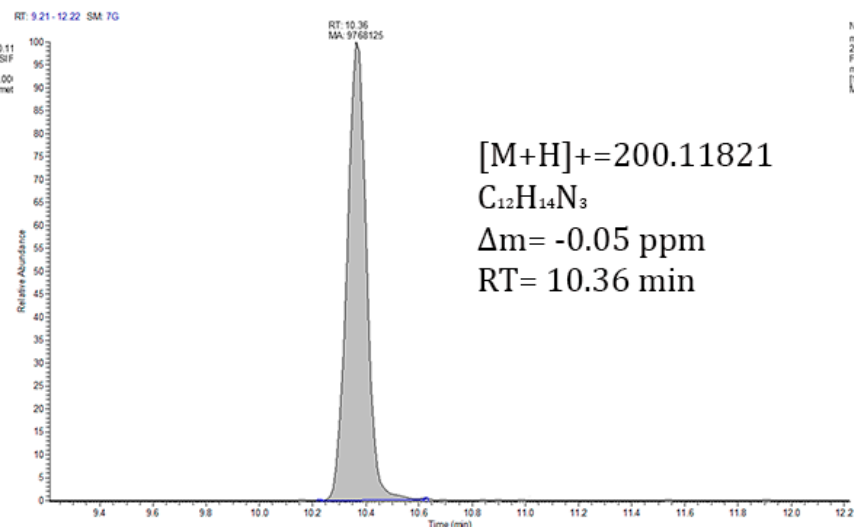
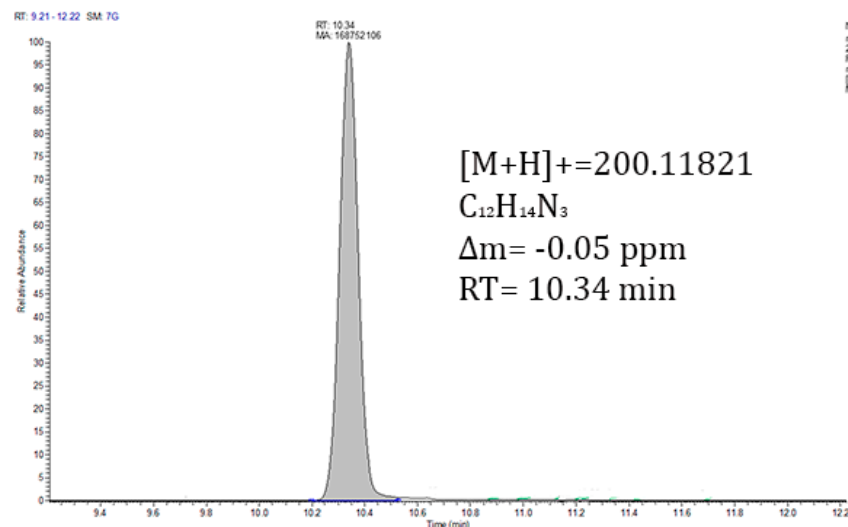
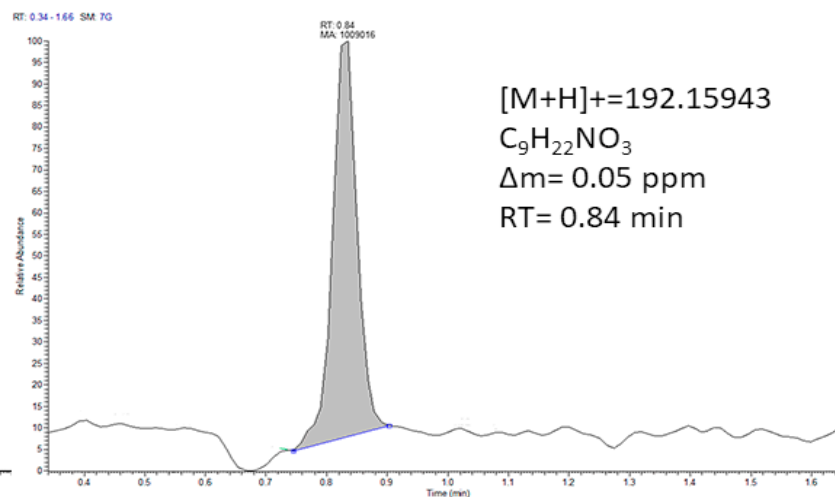
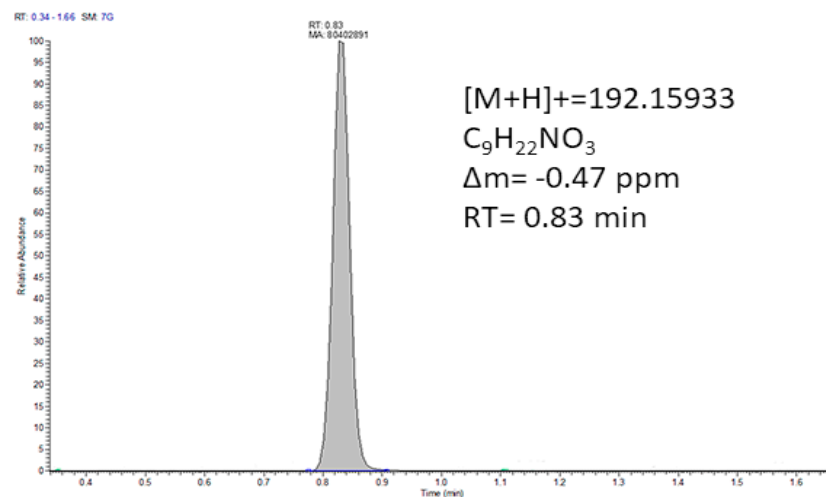


Figure S13. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of pyrimethanil in a standard (left) and a real sample (right).



NL: 3.87E5
 m/z: 192.15846-192.16038
 F: FTMS + p ESI Full
 ms [100.0000-900.0000]
 MS pm10_mx_urban

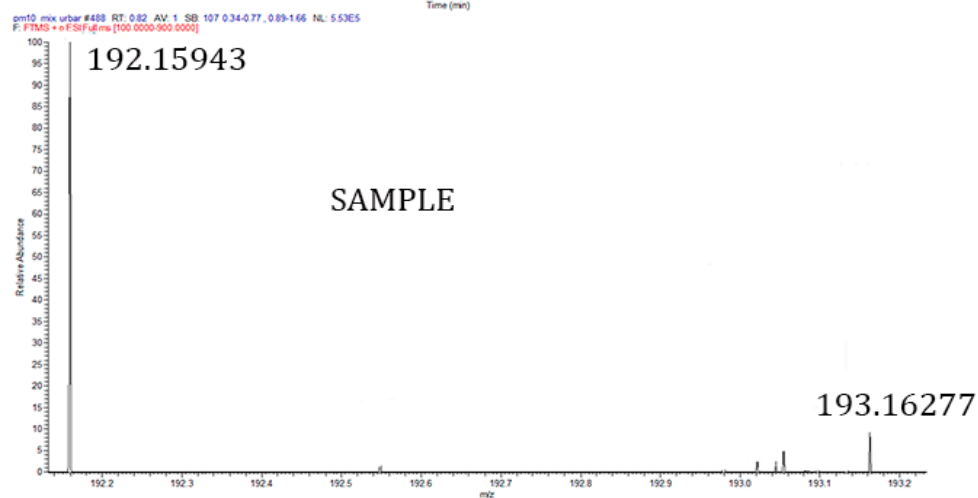
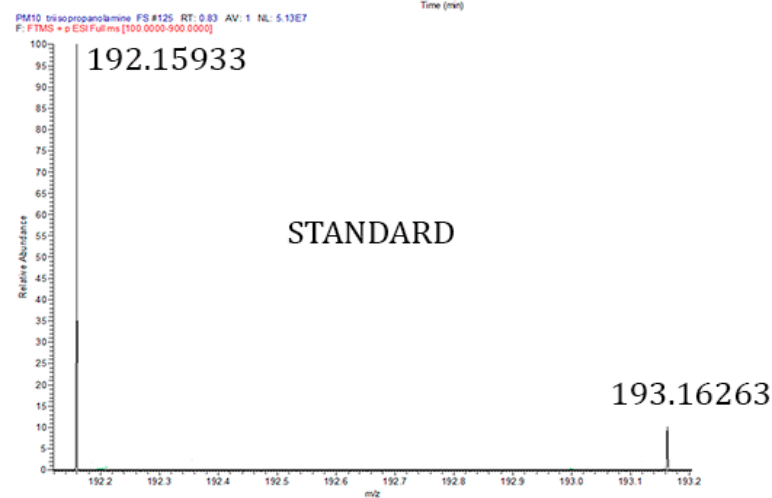


Figure S14. Extracted ion chromatogram (top) and isotopic profile (bottom) corresponding to the protonated molecule of triisopropanolamine in a standard (left) and a real sample (right)