OPTIONS FOR A STRATEGIC APPROACH TO ESTABLISH THE PATTERN AND RISK OF PHARMACEUTICALS IN THE ENVIRONMENT: THE CASE STUDY OF SAUDI ARABIA

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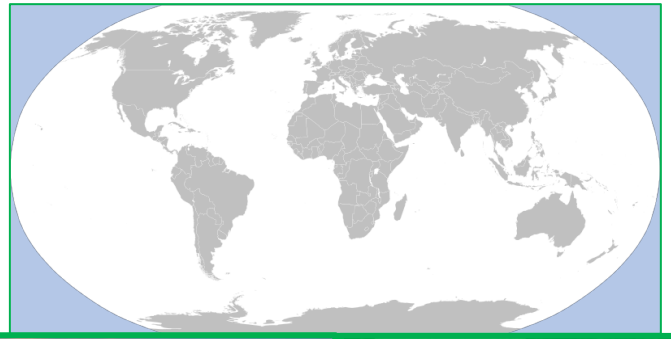
Sources

Agriculture

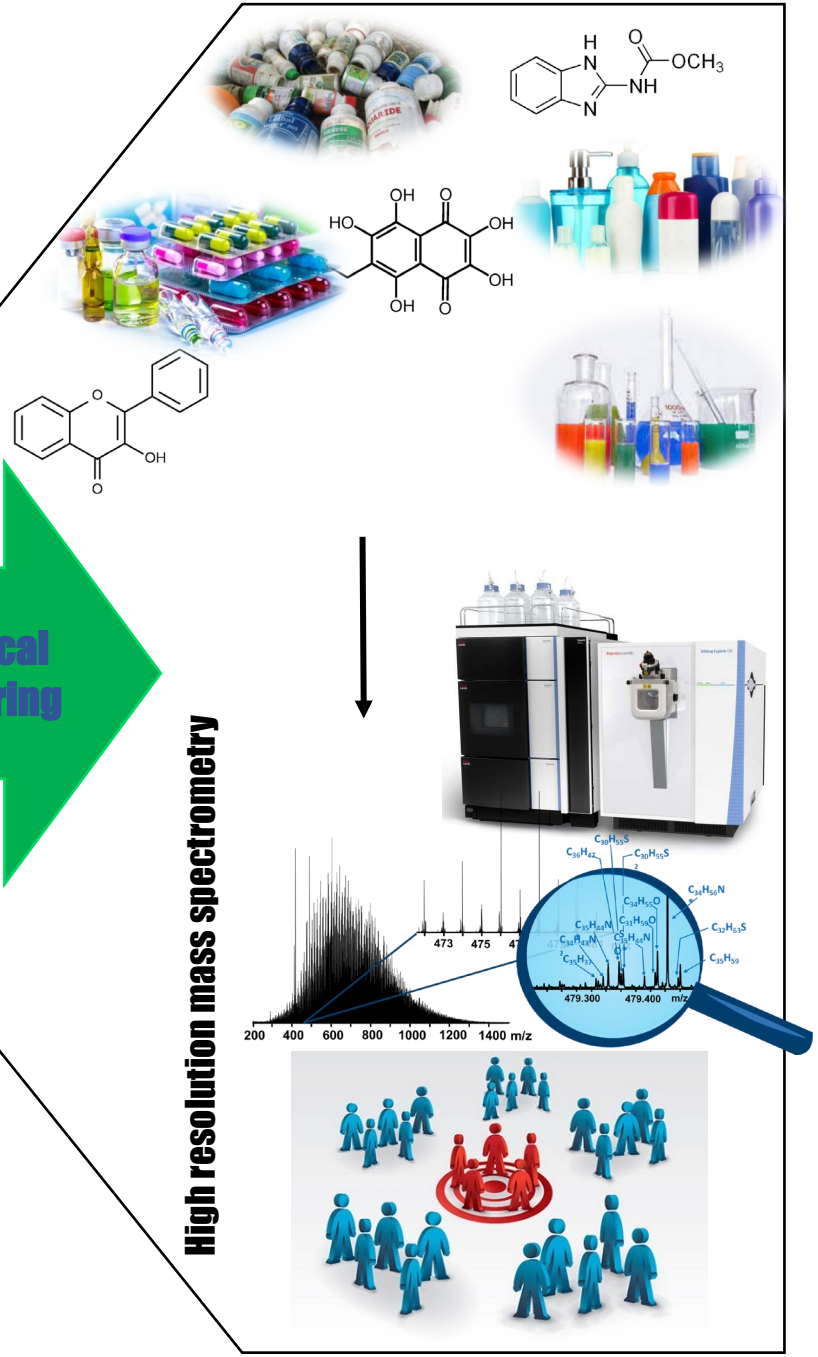
Industry

Urban

Anthropogenic pollution



Chemical Monitoring



AIM OF THE STUDY

TO EXPLORE THE FATE AND DISTRIBUTION OF A RANGE OF PHARMACEUTICALS IN THE ENVIRONMENT OF SAUDI ARABIA

TO ESTABLISH THE UPTAKE IN WILD AND RUDERAL PLANTS UNDER REALISTIC ENVIRONMENTAL CONDITIONS.

To this end, ultra-high performance liquid chromatography with high resolution mass spectrometry (orbitrap) were used together to different software, to achieve quantification as well as data interpretation and structure elucidation.

Determination by LC-HRMS

Thermo Scientific™ Vanquish™ UHPLC system:

- Vanquish Binary Pump
- Vanquish Column Compartment

Kinetex Core-Shell Biphenyl from Phenomenex (Torrance, CA, USA) (2.1 x 50 mm, 1.7 µm).

Mobile phases:

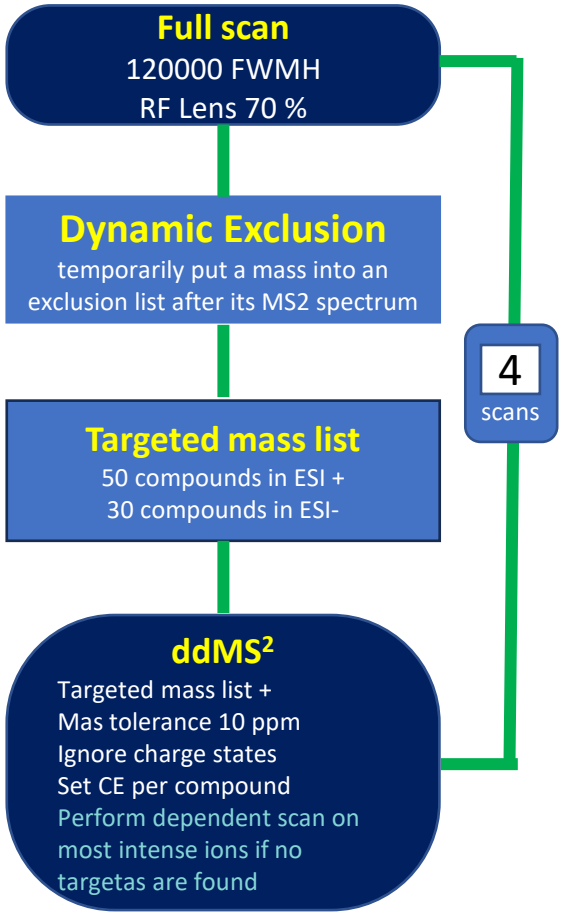
HESI+: (A) H2O/0.1 formic acid and (B) methanol/ 0.1 % formic acid/ 5 mM ammonium formate.

HESI-: (A) H2O 2mM ammonium fluride and (B) methanol 2 mM in ammonium fluoride.

Flow rate of 0.4 mL/min and column temperature of 30 ºC

Thermo Scientific™ Orbitrap Exploris™ 120 mass spectrometer equipped with a Thermo Scientific™ OptaMax™ NG ion source

- Ionization mode: ESI positive & negative
- Scan range (Full MS) (m/z): 80-1000
- Spray voltage positive (KV): +3.5
- Spray voltage negative (KV): -2.5
- Capillary temp (ºC): 320
- S-lens RF level: 70
- Heater temp (ºC): 350
- Sheath gas (units/N2): 50
- Aux gas (units/N2): 10
- Sweep gas (units/N2): 1



PPCPs	35
Acetaminophen	Ketoprofene
Allopurinol	Lamotrigine
Alprazolam	Loratadine
Atenolol	Lorazepam
Atorvastatin	Metformin
Caffeine	Metoprolol
Codeine	Norfloxacin
Carbamazepine	Ofloxacin
Chlorpromazine	Ranitidine
Citalopram	Sinvastatin
Clarythromycin	Sulfadiazine
Diazepam	Sulfamethoxazole
Etoricoxib	Tramadol
Erythromycin	Trimethroprim
Fluconazole	Velanfaxine
Flumequine	Verapamide
Fluoxetine	Zolpidem
Furazolidone	

Full scan
120000 FWMH
RF Lens 70 %

Dynamic Exclusion
temporarily put a mass into an exclusion list after its MS2 spectrum

Targeted mass list
50 compounds in ESI +
30 compounds in ESI-

ddMS²
Targeted mass list +
Mas tolerance 10 ppm
Ignore charge states
Set CE per compound
Perform dependent scan on most intense ions if no targetas are found

4 scans

Compound	24
Atorvastatin	*Ibuprofen*
Bisphenol A	*Indometacin*
Benzafibrate	Ketoprofene
Butylparaben	Mephenamic acid
Clofibric acid	Methylparaben
Chloramphenicol	Naproxen
Diclofenac	Propylparaben
Ethylparaben	Salicylic Acid
Fenofibrate	Thiamphenicol
Furosemide	Triclocarban
Gemfibrozil	Triclosan
Hydrochlorothiazide	Warfarine

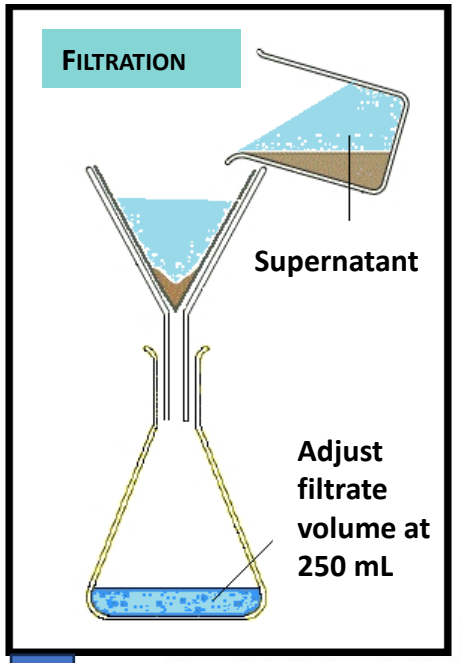
Extraction procedure – POLAR CONTAMINANTS

SOIL & PLANTS

Lyophylized soil or plant (2 g)

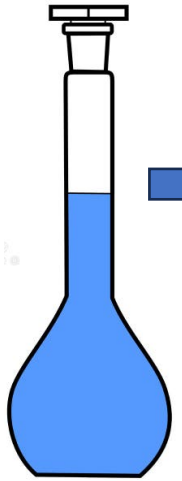
5 mL Mc Ilvain buffer (pH = 5.6) +0.2 M EDTA
5 mL methanol

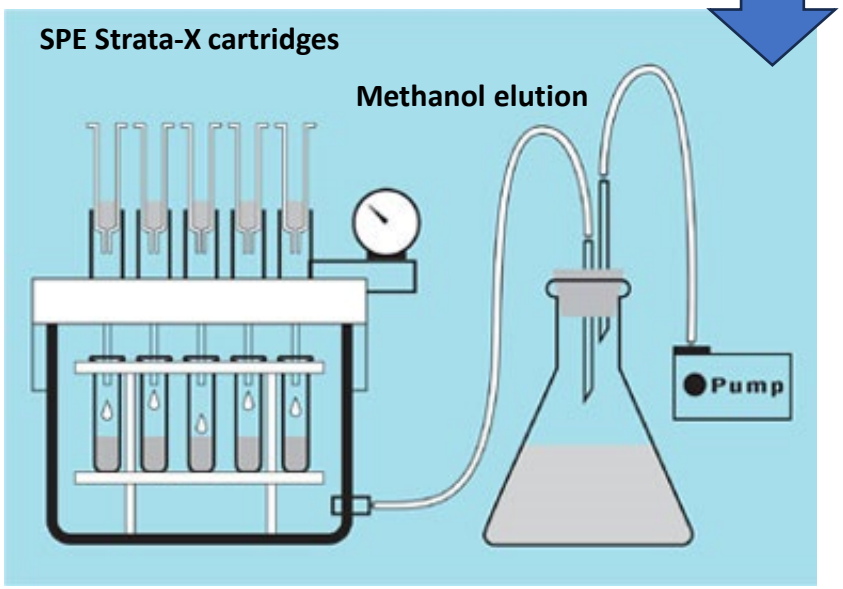
ULTRASOUNDS
5 min



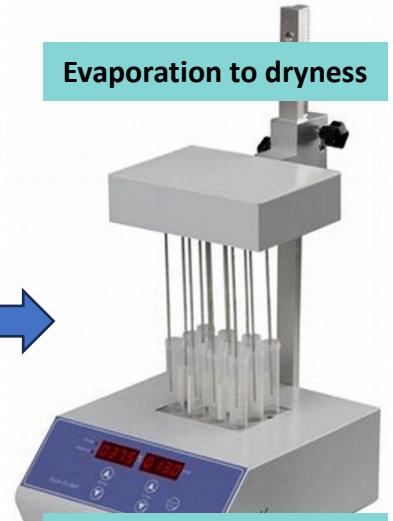
WATER

250 mL of filtrated water



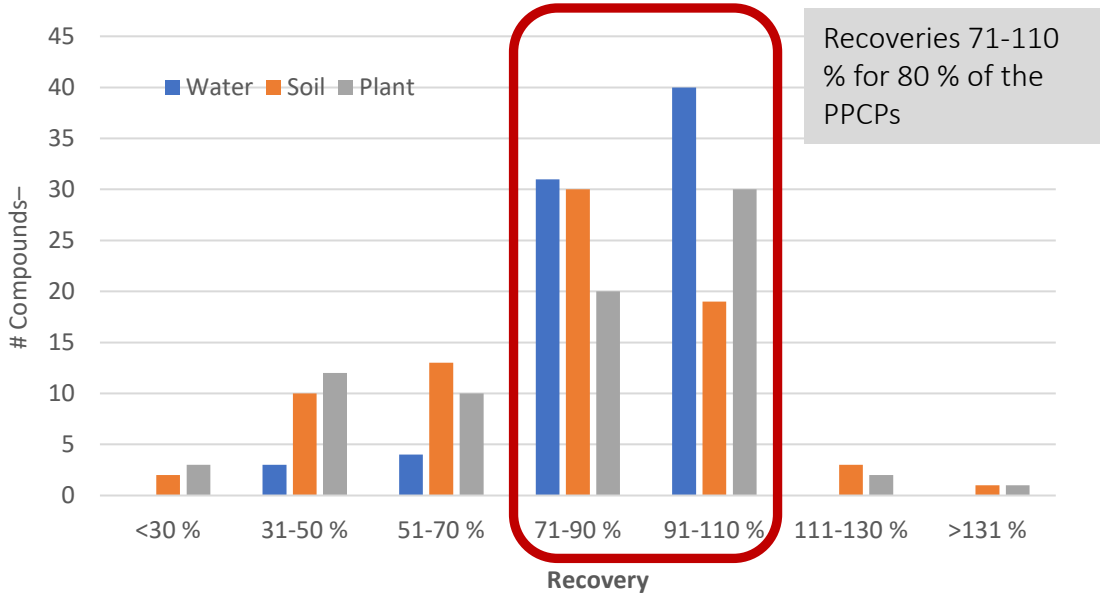


Evaporation to dryness

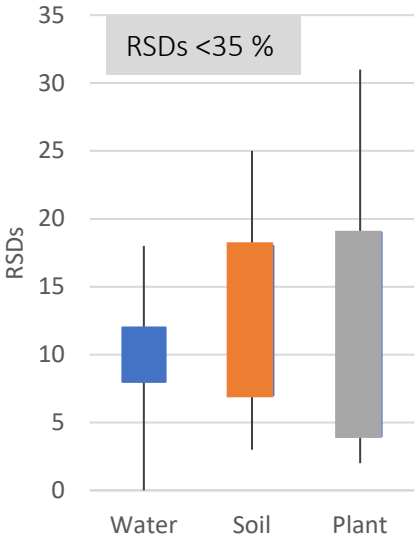


Redissolve in 1 mL of mobile phase

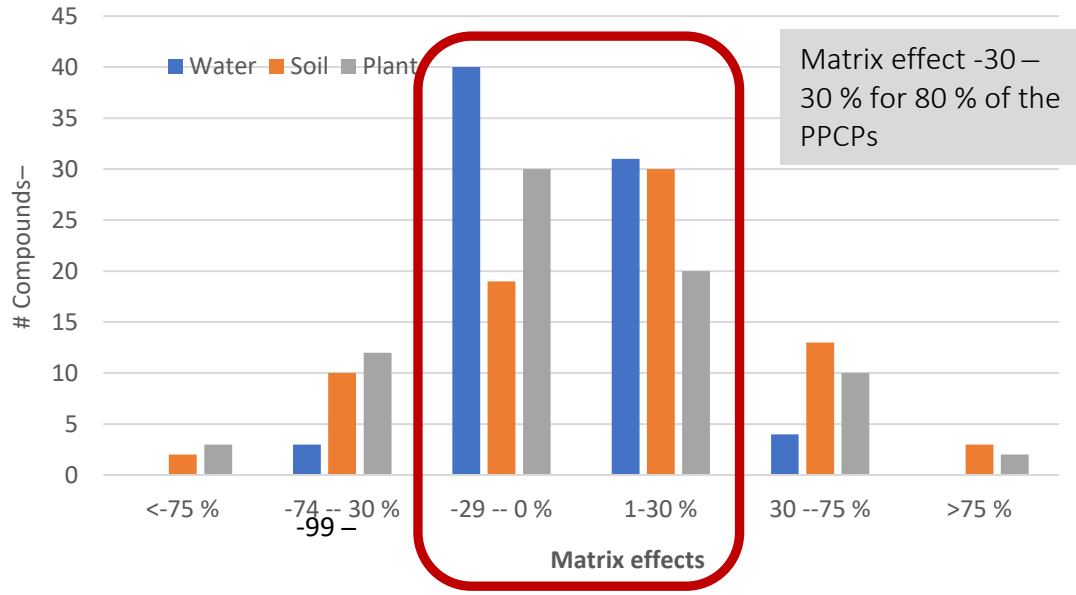
Results and discussion



Recoveries 71-110 % for 80 % of the PPCPs



RSDs <35 %



Matrix effect -30 – 30 % for 80 % of the PPCPs

Sensitivity:
LOQs
0.1 -1 ng L^{-1} water 80 % PPCPs
0.1-1 ng g^{-1} soil 75 % PPCPs
0.1-1 ng g^{-1} plants 70 % PPCPs

>1 -10 ng L^{-1} water 20 % PPCPs
>1-10 ng g^{-1} soil 20 % PPCPs
>1-10 ng g^{-1} plants 20 % PPCPs

>10 ng g^{-1} soil 10 % PPCPs
> 10 ng g^{-1} soil 10 % PPCPs

Analysis

Batch View
- Samples
- Reference Sample
- Threshold Samples

Data Review
- Sample View
- Compound View
- Comparative View

Report View

Local Method
- Acquisition
- Quantitation
  - Processing
  - Compounds
  - QAQC
  - Groups
- Reports

Acquisition
Analysis
Method Development

Data Review - Saudis_Pharma_pos [Quan] *

Compounds

	Flags	Compound	RT	Type
1	⚠	Acetaminophen (Paracetamol)	1.29	Target Compound
2	⚠	Acetaminophen d3	1.29	Internal Standard
3	⚠	Alprazolam	6.00	Target Compound
4	⚠	Amoxicillin	1.65	Target Compound
5	⚠	Atenolol	1.13	Target Compound
6	⚠	Atenolol d7	1.15	Internal Standard
7	⚠	Atorvastatin	5.87	Target Compound
8	⚠	Caffeine	2.80	Target Compound
9	⚠	Carbamazepine	4.42	Target Compound
10	⚠	Carbamazepine d2	4.46	Internal Standard
11	⚠	Codeine	1.36	Target Compound
12	⚠	Enalapril	3.32	Target Compound
13	⚠	Etoricoxib	5.05	Target Compound
14	⚠	Lorazepam	4.74	Target Compound
15	⚠	Metformin	1.59	Target Compound
16		Norfloxacin	7.53	Target Compound
17		Ofloxacin	6.27	Target Compound
18	⚠	Omeprazole	4.11	Target Compound

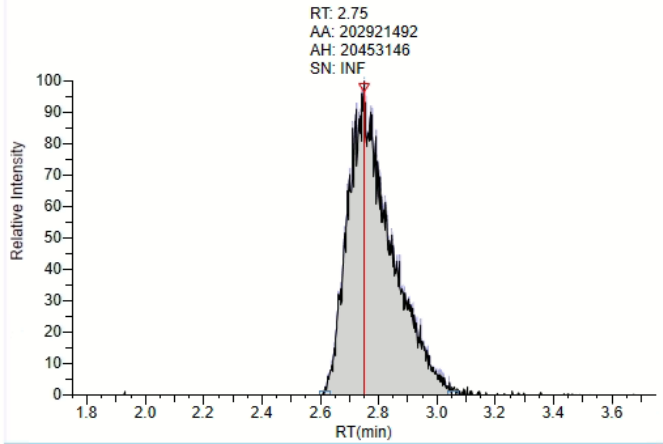
Sample Results

	Sele	Filename	Flag Details	Status	Sample Type	Level	Area	Actual RT	Sample Amt	Type	Height	RT	RT Delta	al Amt	Std Add A
1	☑	5ppb pos 2	A,CV,R		Cal Std	L1	65516898	2.71	22.666	Sample	7795251	2.80	-0.09		N/A
2	☑	5ppb pos	A,CV,R		Cal Std	L1	19410396	3.08	6.715	Sample	4154192	2.80	0.28		N/A
3	☑	10ppb pos 2	A,CV,R		Cal Std	L2	87685500	2.67	30.335	Sample	10582671	2.80	-0.13		N/A
4	☑	10ppb pos	A,CV,R		Cal Std	L2	46244651	3.02	15.999	Sample	6945976	2.80	0.22		N/A
5	☑	25ppb pos 2	A,CV,R		Cal Std	L3	50399525	2.74	17.436	Sample	11531239	2.80	-0.06		N/A
6	☑	25ppb pos	CV,R		Cal Std	L3	68457054	2.86	23.683	Sample	9606946	2.80	0.06		N/A
7	☑	50ppb pos 2	CV,R		Cal Std	L4	164591700	2.73	56.942	Sample	29239387	2.80	-0.07		N/A
8	☑	50ppb pos	CV,R		Cal Std	L4	116099242	2.81	40.165	Sample	15726625	2.80	0.01		N/A
9	☑	100ppg pos 2	R		Cal Std	L5	304277523	2.67	105.267	Sample	61630404	2.80	-0.13		N/A
10	☑	100ppg pos	R		Cal Std	L5	233514104	2.80	80.786	Sample	34675476	2.80	0.00		N/A
11	☑	200ppb pos 2	R		Cal Std	L6	316613270	2.69	109.535	Sample	76290140	2.80	-0.11		N/A
12	☑	200ppb pos	R		Cal Std	L6	502341749	2.71	173.789	Sample	84211520	2.80	-0.09		N/A
13	☑	400ppb pos 2	R,FI,CPF		Cal Std	L7	1130799663	2.69	391.209	Sample	183636548	2.80	-0.11		N/A
14	☑	400ppb pos	R,FI,CPF		Cal Std	L7	600666778	2.82	207.805	Sample	140437977	2.80	0.02		N/A
15	☑	500ppb pos 2	R		Cal Std	L8	1429193691	2.68	494.441	Sample	192465125	2.80	-0.12		N/A
16	☑	500ppb pos	R		Cal Std	L8	1488641498	2.80	515.007	Sample	161649824	2.80	0.00		N/A
17	☑	alhaeer A bottom b s1	FI,CPF		Unknown		1231788	2.77	0.426	Sample	4235358	2.80	-0.03		N/A

Compound Details

Quan Peak

Alhaeer B Bshager s3 Caffeine m/z: 195.0877



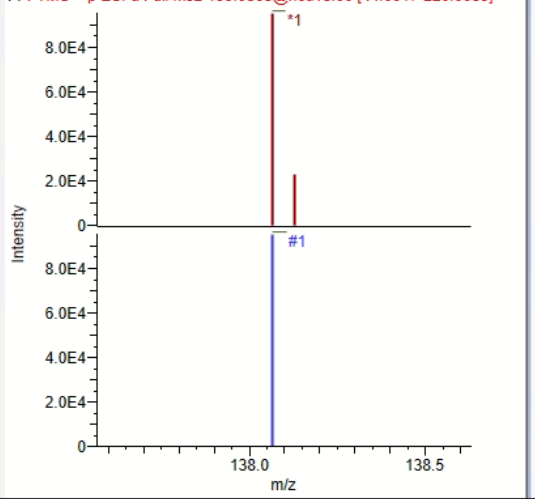
m/z: 195.0877
Apex RT: 2.75 Left RT: 2.61 Right RT: 3.05

Fragments

All Fragments
#1: 138.0657

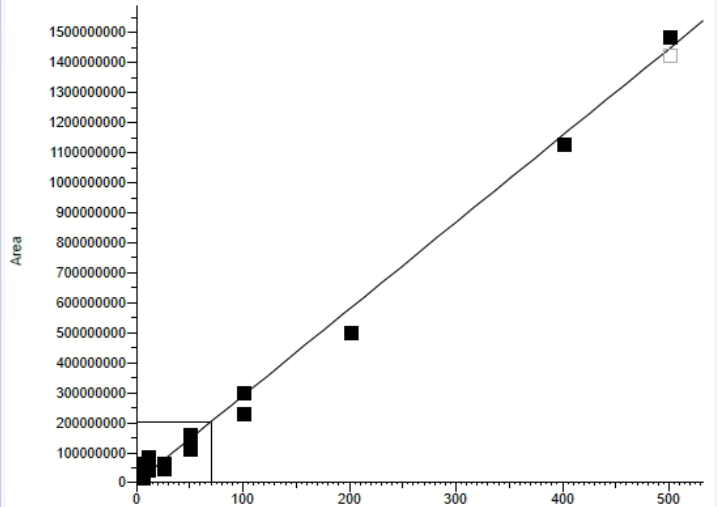
Minimum # of fragments needed: 1

Alhaeer B Bshager s3 #: 1289 RT: 2.77
F: FTMS + p ESI d Full ms2 195.0868@hcd18.00 [44.0017-220.0085]



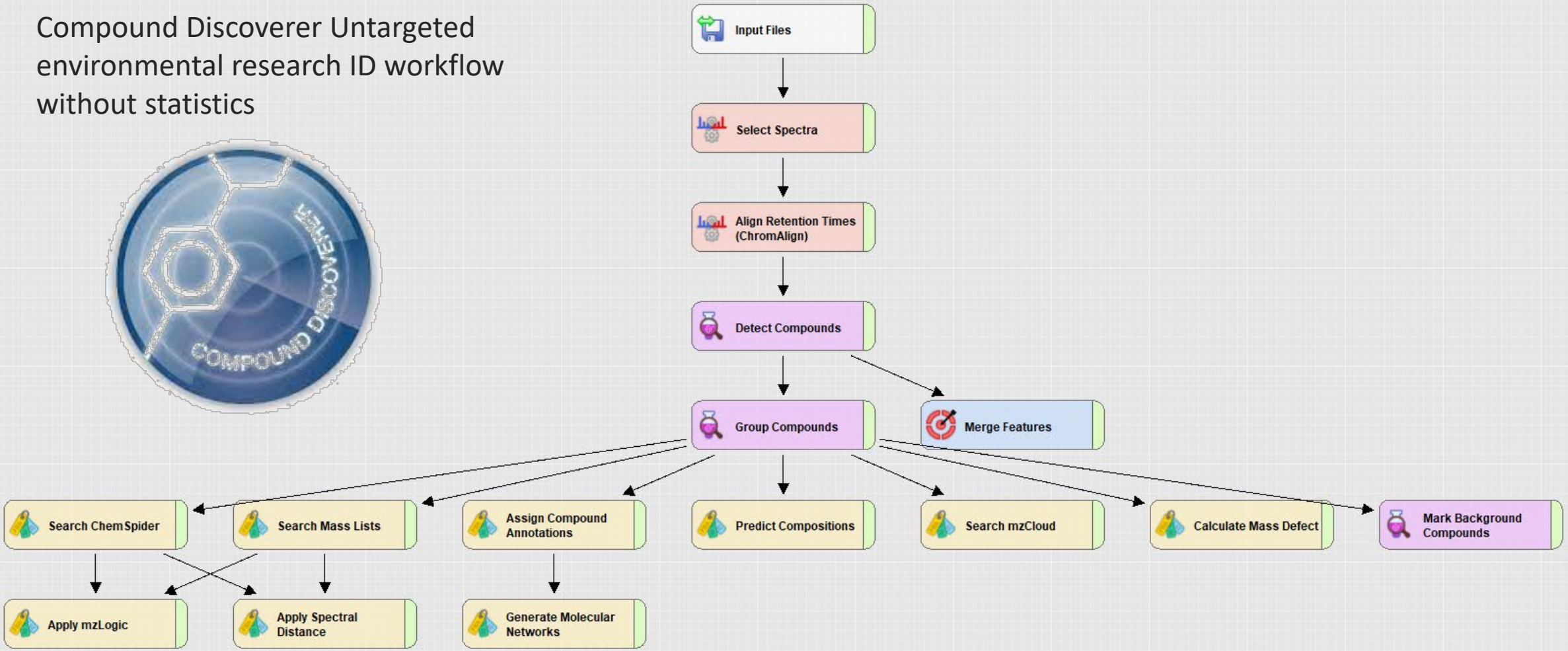
Calibration Curve

Caffeine
Y = 2.891e6X; R^2: 0.8925; Origin: Force; W: 1/X; Area



9:28 PM
10/1/2023

Compound Discoverer Untargeted environmental research ID workflow without statistics

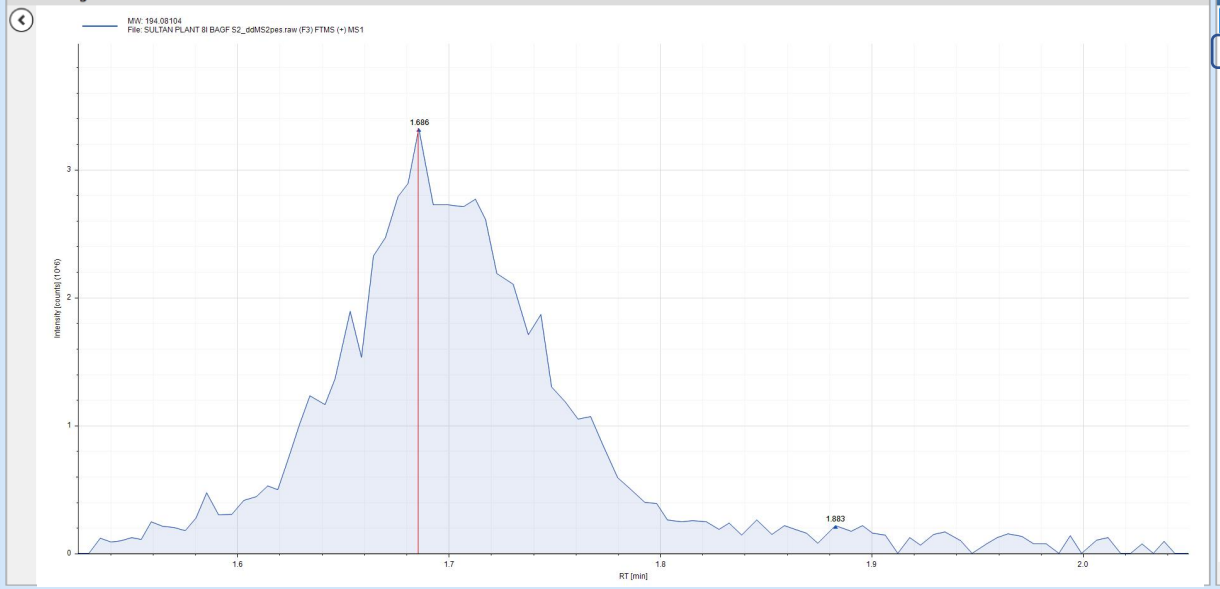


Compound Discoverer 3.3.1.111

File Reporting Lists & Libraries View Window Help

Start Page | Lists & Libraries | Job Queue | Yolanda9 | Yolanda9-(2) | Yolanda | Yolat11 | Yolat11-(2) | Yolat11-(3)

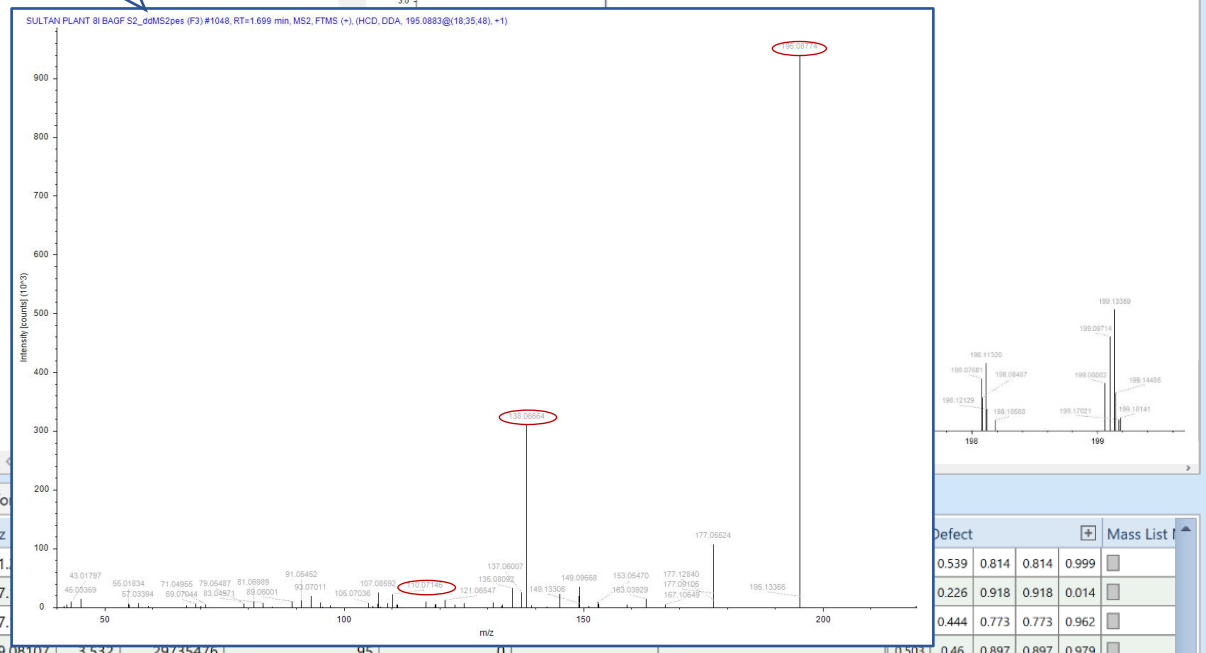
Chromatograms



Mass Spectrum

F3 #1039, RT=1.686 min, MS1, FTMS (+)

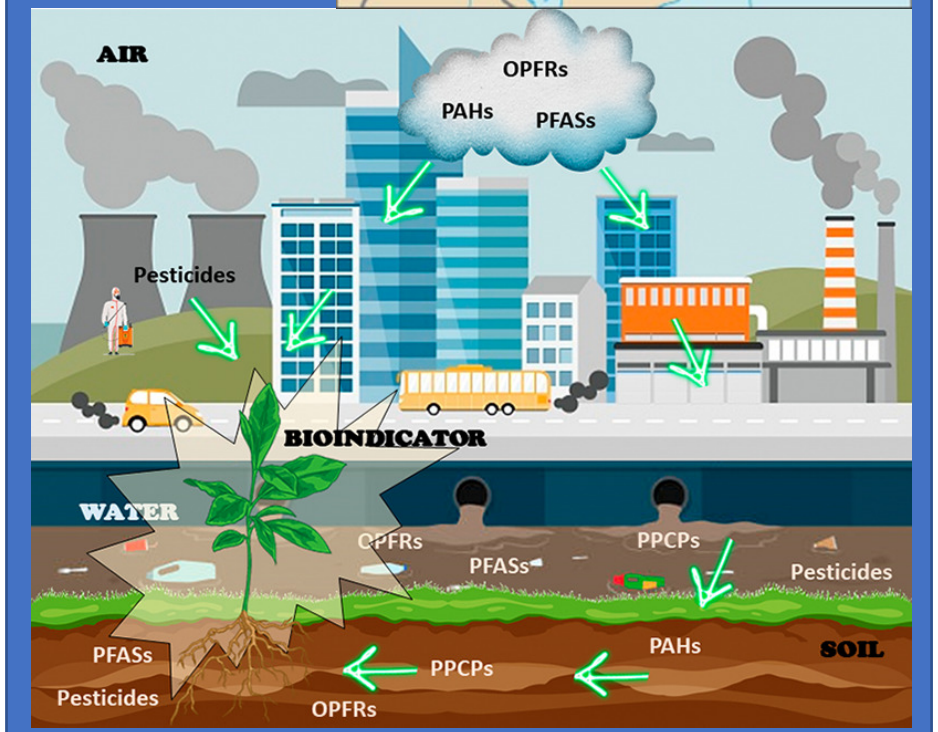
F3 #1048, RT=1.699 min, MS2, FTMS (+), (H



Compounds | Compounds per File | Merged Features | Features per File | mzCloud Results | ChemSpider Results | Mass List Search Results | Input Files | Study Info

	Tags	Checked	Name	Formula	Annot. Source	Annot. ΔMass [ppm]	Calc. MW	m/z							Defect				Mass List
1459			Citroflex 4	C18 H32 O7		3.80	360.21617	361.							0.539	0.814	0.814	0.999	
1460			Queen Bee Acid	C10 H18 O3		3.46	186.12624	187.							0.226	0.918	0.918	0.014	
1461			PSB-SB1202	C23 H26 O4		-2.05	366.18236	367.							0.444	0.773	0.773	0.962	
1462			2-Naphthylmethanol	C11 H10 O		3.98	158.07379	159.08107	3.532	29735476	95	0			0.503	0.46	0.897	0.897	0.979	
1463			Butylparaben	C11 H14 O3		3.42	194.09496	195.10223	2.220	52474910	710	0			0.166	0.114	0.878	0.878	0.978	
1464			MOCPAC	C27 H31 N3 O6		4.17	493.22334	494.23062	5.168	26269577	8	0			0.322	0.188	0.673	0.673	0.927	
1465			Carvone	C10 H14 O		3.34	150.10497	151.11224	3.648	33650671	531	2	96.2	76.9	0.613	0.573	0.937	0.937	0.015	
1466			p-cymenene	C10 H12		5.00	132.09456	133.10184	12.557	11289493	103	0			0.782	0.746	0.947	0.947	0.015	
1467				C12 H15 F S		-1.25	210.08759	211.09486	3.530	28056070	15	0			1	0.943	0.853	0.853	0.961	
1468			[2-(hydroxymethyl)-5,5,8a-trimethyl-1,4,4a,5,6,7,8,8a-oc	C15 H26 O2		92299.59	260.17842	261.18570	6.651	45452722	123	2	84.4	52.6	0.593	0.522	0.888	0.888	0.022	
1469			NP-011223	C10 H18 O3		3.21	186.12619	187.13347	10.003	20405908	489	2	68.1	47.7	0.277	0.226	0.918	0.918	0.014	
1470			Caffeine	C8 H10 N4 O2		3.43	194.08104	195.08832	1.685	22066714	109	3	95.7	85.1	0.153	0.1	0.864	0.864	0.964	
1471				C17 H35 F O3		-0.18	306.25697	307.26428	6.455	27082290	117	0			0.214	0.131	0.915	0.915	0.073	

Show Related Tables

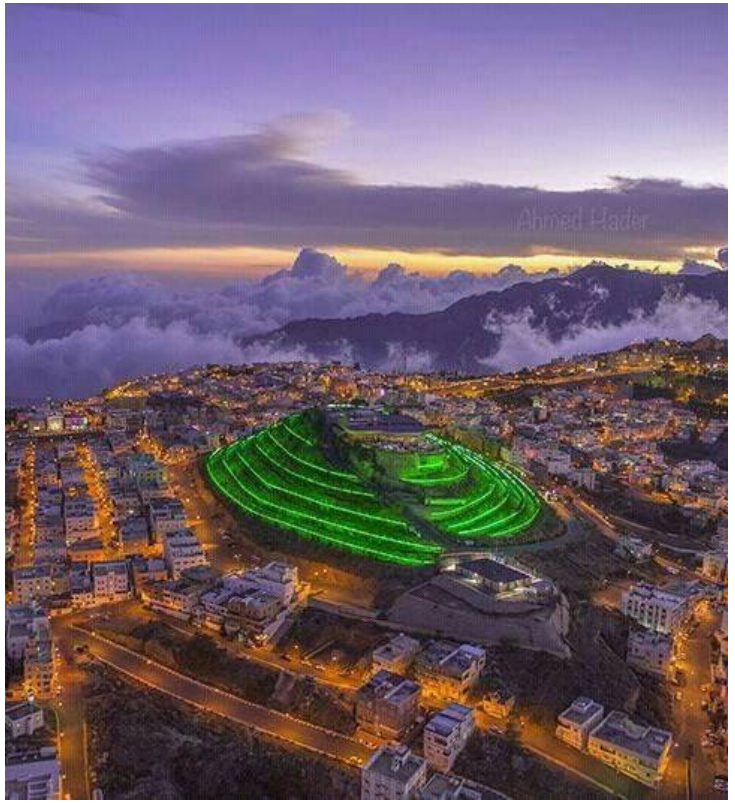


Riyadh city (24°39'N 46°43'E)

- Population of ca. **7.4 million people** (2021)
- **Most populated city** in Saudi Arabia
- **Country's center**
- About *600 m above the Sea level*
- Sourround by a **large industrial city**
- Deserted climate
- Arid and dry conditions (humidity from 0 to 10.3 %)

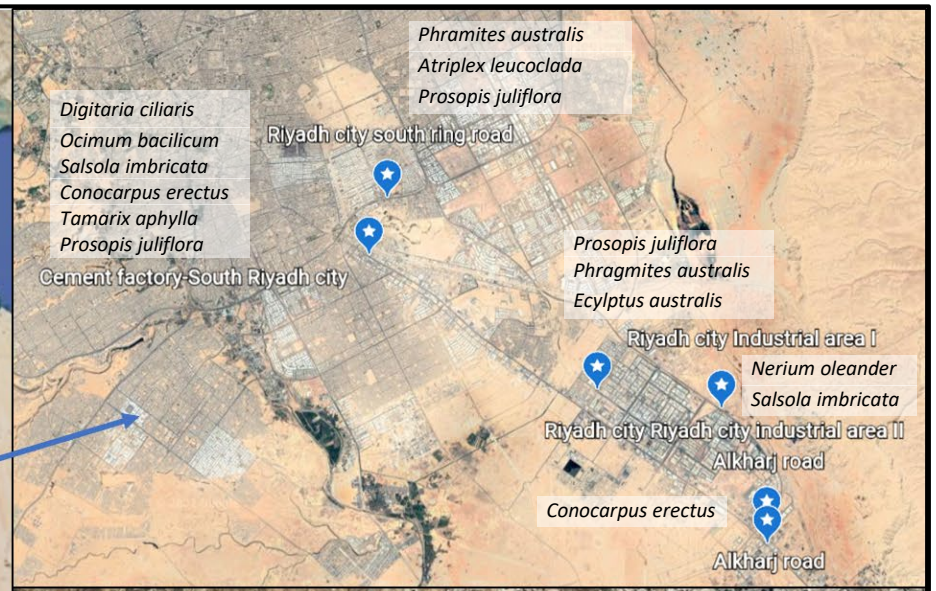
Abha (18°13'1"N 42°30'19"E)

- Population of **1.1 million people** (2021)
- **6th largest population** in Saudi Arabia
- **Country's South-West**
- Hilly area at *2270 m above the Sea level*
- Surround by the **Asir National Park**
- Continental semi-arid climate
- cooler and wetter climate



Experimental

Sampling



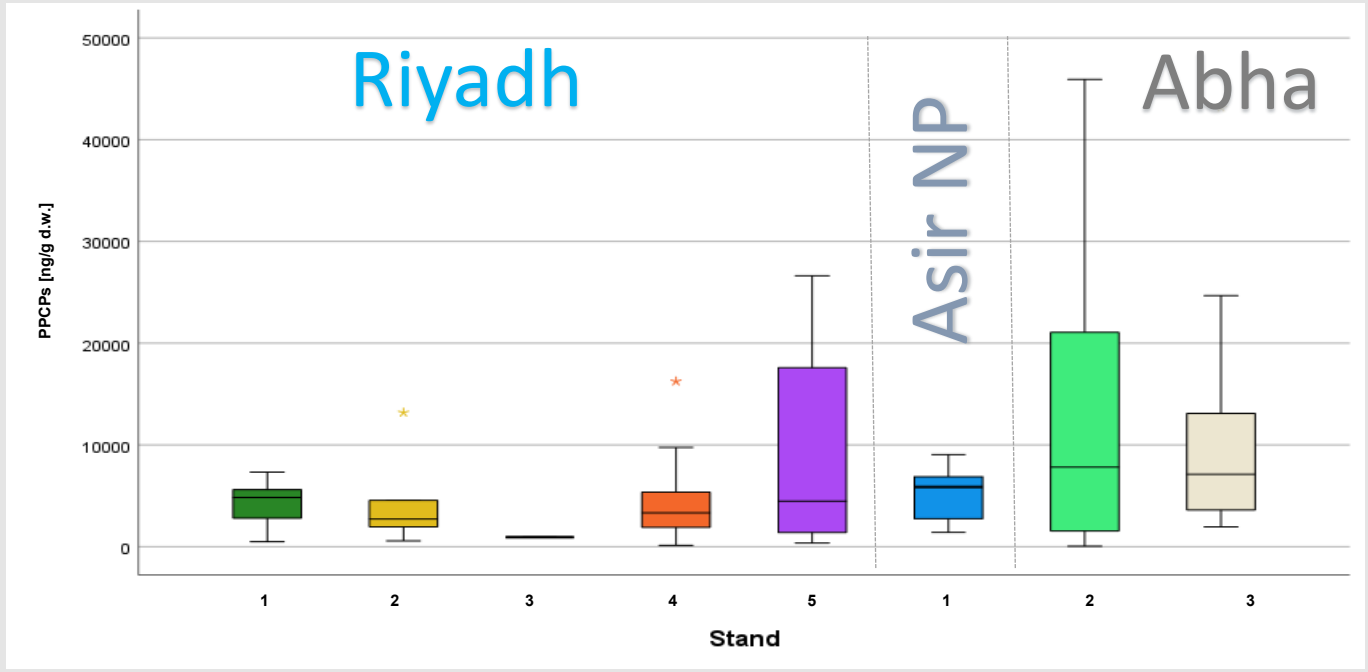
ICRAPHE

The most notable similarity, in terms of plant species, is that *Conocarpus erectus* is present in all five stands in Riyadh, while *Dondonea viscosa* is found in the Abha stands and in the Asir National Park stand

PPCPs	Riyadh (n=37)				Abha city (n=28)				Ashir Natural Park (n=5)			
	Concentration (ng/g d.w.)			Frequency (# Ocurrences)	Concentration (ng/g d.w.)			Frequency (# Ocurrences)	Concentration (ng/g d.w.)			Frequency (# Ocurrences)
	Min	Max	Average		Min	Max	Average		Min	Max	Average	
Salicylic acid	<LOD	**6605**	670	35	<LOD	**9954**	2030.3	22	302.1	**2204.8**	1147.9	7
Thiamphenicol	<LOD	**109**	4	6	<LOD	**0**	0	0	—	—	—	—
Furosemide	<LOD	**655**	3	11	<LOD	**168.7**	21.8	6	<LOD	**90.1**	26.6	3
Chloramphenicol	<LOD	**20**	0.5	1	<LOD	**0**	0	0	—	—	—	—
Methylparaben	1.3	**1271**	109	37	<LOD	**953.8**	110.8	19	14.4	**147.4**	73.9	7
Ethylparaben	<LOD	**21**	4	15	<LOD	**8.1**	1.1	6	<LOD	**3**	0.4	1
Naproxen	<LOD	**3**	0.1	1	—	—	—	—	—	—	—	—
Benzafibrate	<LOD	**6**	0.2	1	<LOD	**42.9**	6.5	7	—	—	—	—
Propyparaben	<LOD	**5**	0.5	6	<LOD	**6.5**	1.2	8	<LOD	**7.1**	2.7	4
Warfarin	<LOD	**3**	0.1	1	<LOD	**13.6**	0.6	2	—	—	—	—
BPA	<LOD	**1609**	95	6	<LOD	**201**	9.3	7	<LOD	**5.2**	0.7	1
Diclofenac	<LOD	**687**	92	17	<LOD	**287.7**	20.9	6	<LOD	**129.7**	20.6	3
Indomethacin	—	—	—	—	<LOD	**3.3**	0.1	1	—	—	—	—
Ibuprofen	<LOD	**1214**	60	9	—	—	—	—	—	—	—	—
Metformin	<LOD	**30**	4	13	—	—	—	—	—	—	—	—
Atenolol	<LOD	**1010**	142	9	<LOD	**2069.1**	235.9	8	—	—	—	—
Codeine	<LOD	**27**	0.6	1	<LOD	**13**	0.5	1	—	—	—	—
Ofloxacin	<LOD	**387**	11	1	—	—	—	—	—	—	—	—
Paracetamol	<LOD	**14**	3	12	<LOD	**25.6**	1.8	3	—	—	—	—
Tramadol	<LOD	**234**	18	5	<LOD	**2.9**	0.1	1	—	—	—	—
Caffeine	<LOD	**42**	8	32	<LOD	**4128.2**	192.4	11	—	—	—	—
Etoricoxib	<LOD	**8**	0.2	1	—	—	—	—	—	—	—	—
Enelapril	<LOD	**204**	6	1	—	—	—	—	—	—	—	—
Lorazepam	<LOD	**195**	5	1	—	—	—	—	—	—	—	—
Simvastatin	<LOD	**544**	15	1	<LOD	**279.2**	10	1	—	—	—	—
ΣPPCPs	22	**2363**	572	37	<LOD	**5496**	591.2	25	19.6	**189.6**	98.4	7

Concentration and frequency of each PPCP

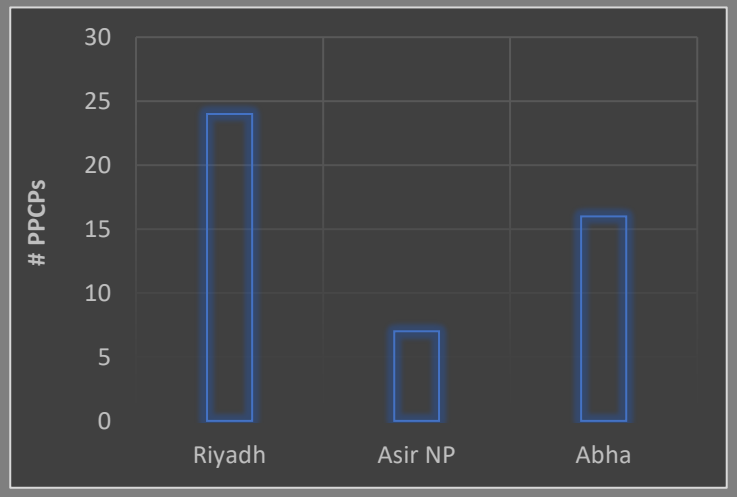
ICRAPHE

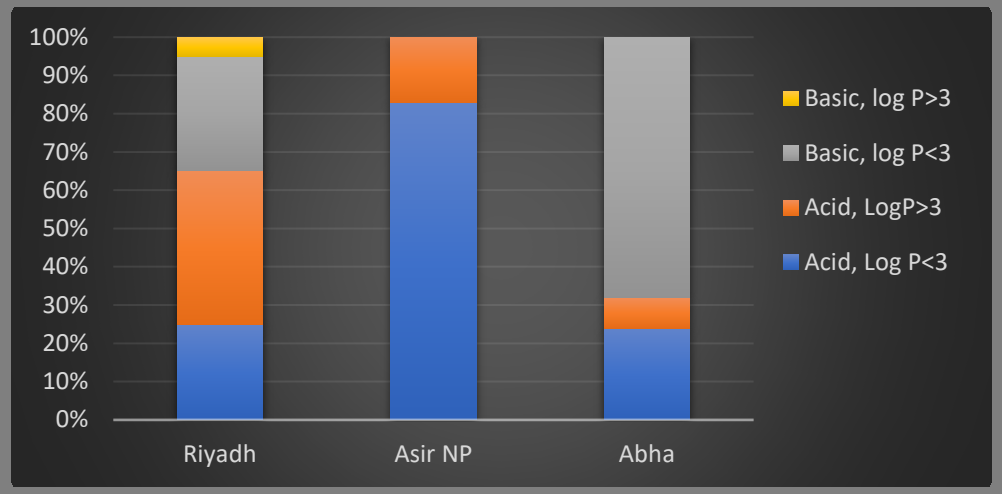


Statisticals:

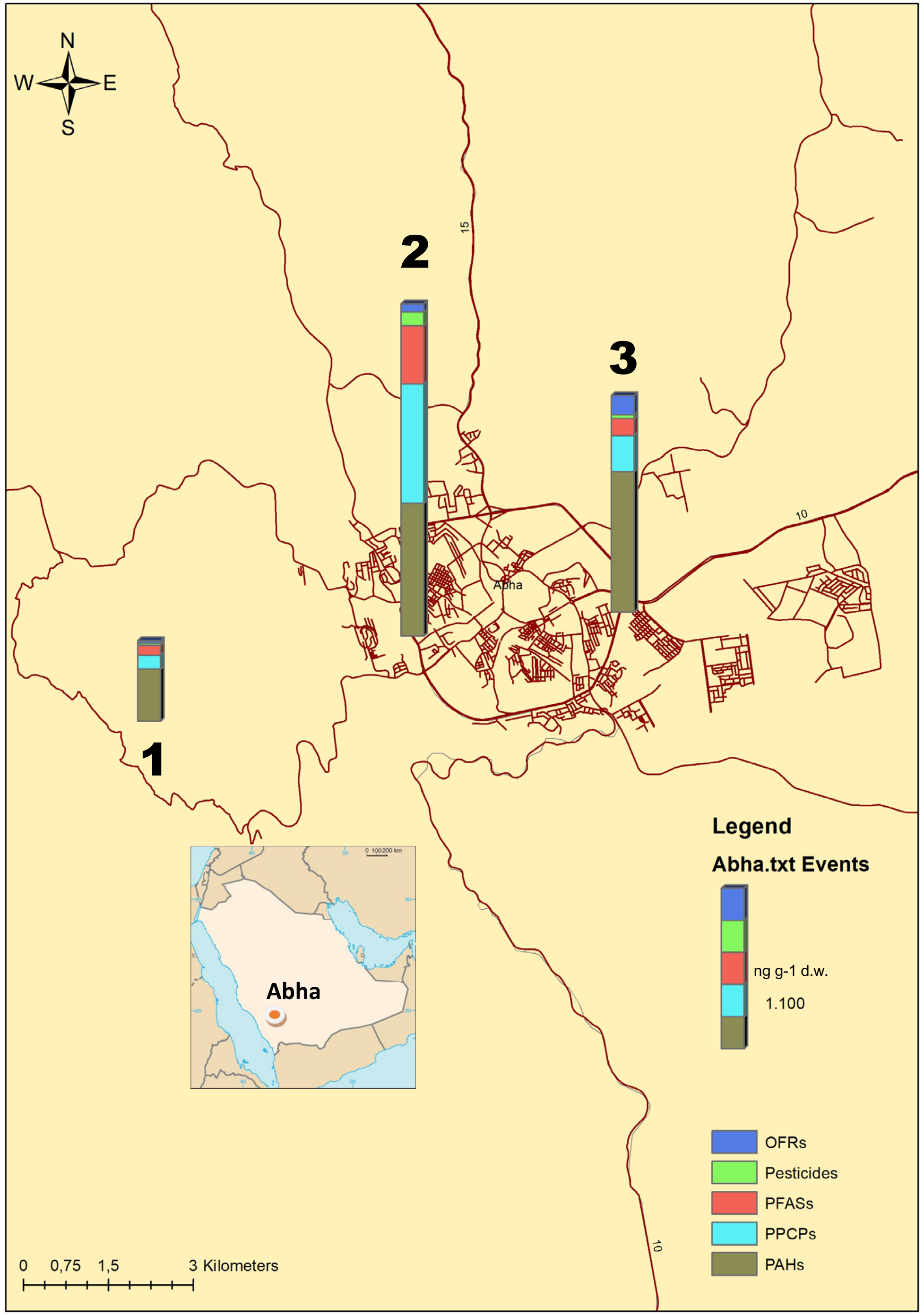
- **Concentrations** were compared to **location** and to sampling stand.
- **Kolmogorov-Smirnov** ($n > 50$) or **Shapiro–Wilk** ($n < 50$) tests were used **for normality** and **Levene**'s test for **homogeneity of variances**.
- **Differences in concentrations** were established through Mann–Whitney U (M–W) or Kruskal–Wallis (K–W) tests, considering places, sampling stands (1 to 8)

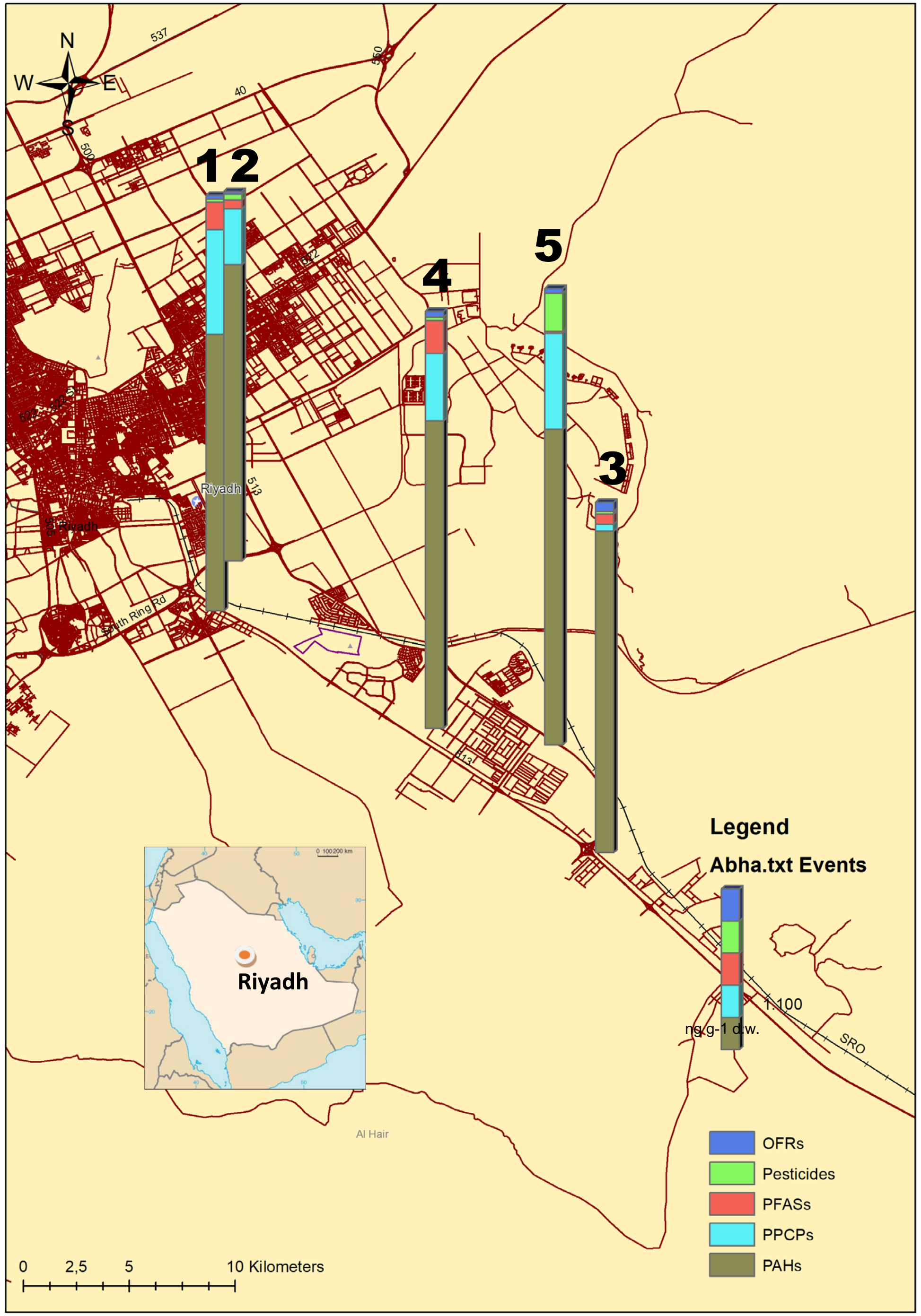
NO STATISTICAL SIGNIFICANT DIFFERENCES



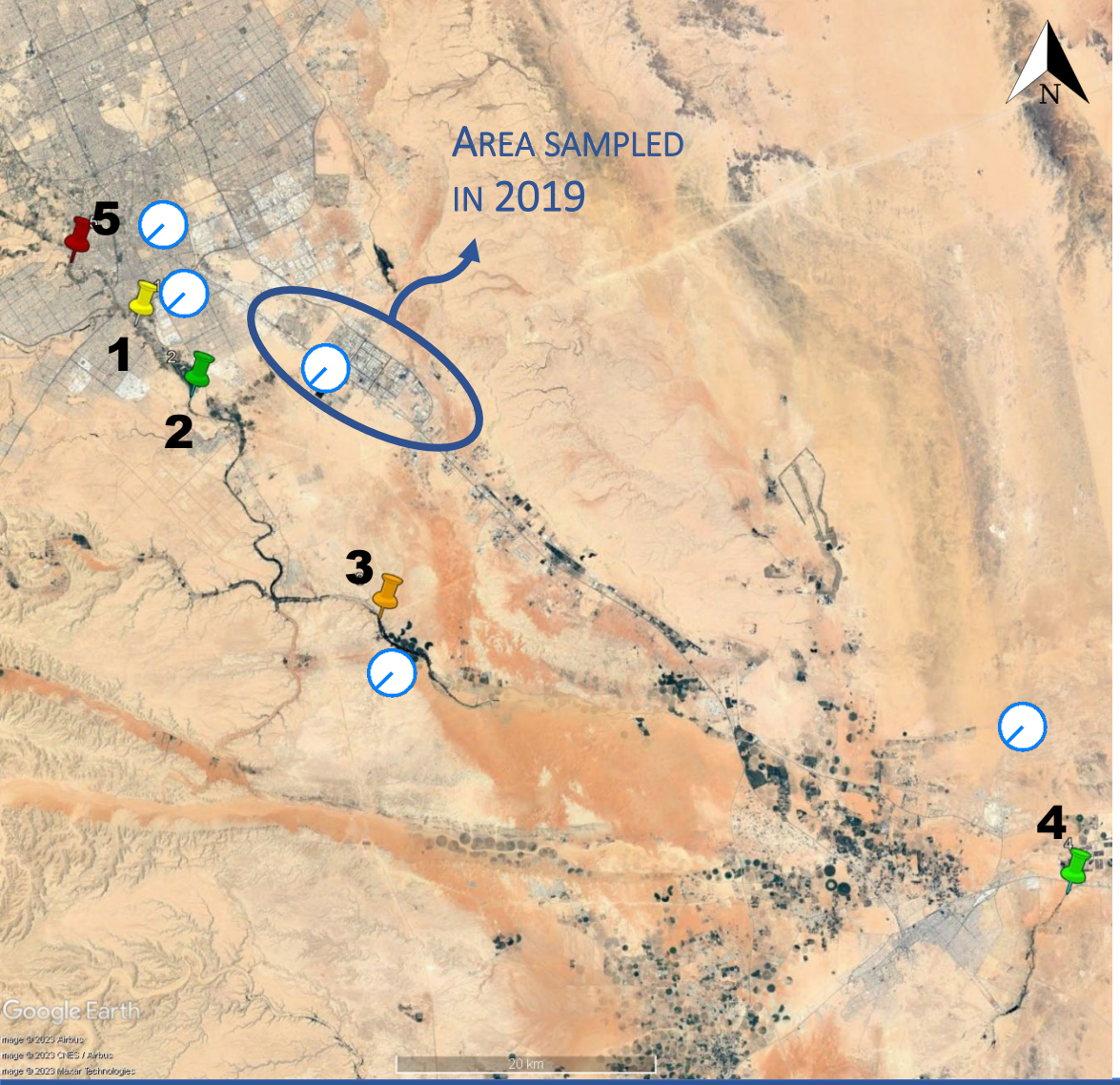


ICRAPHE


N
W
E
S
2
3
1
15
10
Abha
Legend
Abha.txt Events
ng g-1 d.w.
1.100
Abha
OFRs
Pesticides
PFASs
PPCPs
PAHs
0 0,75 1,5 3 Kilometers


N
W
E
S
1 2
4
5
3
Riyadh
Legend
Abha.txt Events
1.100
ng g-1 d.w.
Riyadh
Al Hair
SRO
OFRs
Pesticides
PFASs
PPCPs
PAHs
0 2,5 5 10 Kilometers

- PPCPs was found to be the second-highest group of contaminants in wild and ruderal plants.
- The ΣPPCPs concentration in the wild plants ranged from <LODs to 5496.0 ng g^{-1} d.w. with an average of 63 ng g^{-1} d.w.
- The highest values are due to salicylic acid that reached averages >2000 ng g^{-1} d.w. This can be a natural product from plants produced specifically due to hydric stress.
- In addition to this, 23 PPCPs were detected in Riyadh, 17 in Abha and 7 in the stand at the Asir National Park.
- Abha had the highest average concentration of ΣPPCPs (excluding salicylic acid) (25 ng g^{-1} d.w.), followed by Riyadh (18 ng g^{-1} d.w.), while Asir National Park had the lowest concentration (4 ng g^{-1} d.w.).
- These differences between ΣPPCPs concentration were not statistically significant.
- Comparison of *C. erectus* in Riyadh stands shows the presence in stand 4 of high concentrations of diclofenac and ibuprofen not present in the other stands. This could be related to the irrigation with treated wastewater.
- The absorption of PPCPs by plants is ruled by their acid/basic character and most of the detected PPCPs in this study have also log P < 3. It is noteworthy that in Abha only acid PPCPs were detected mostly of logP<3 but also of log P>3.



- Wastewater effluent (KFSHRC WWTP)
- Water before the point of effluent release
- Water after the point of effluent release
- Soil
- Plant

5

- Wastewater effluent (Manfouha WWTP)
- Water before the point of effluent release
- Water after the point of effluent release
- Soil
- Plant

1

- Wastewater effluent (STP WWTP) sería punto 3 y no 2
- Water before the point of effluent release
- Water after the point of effluent release
- Soil
- Plant

2

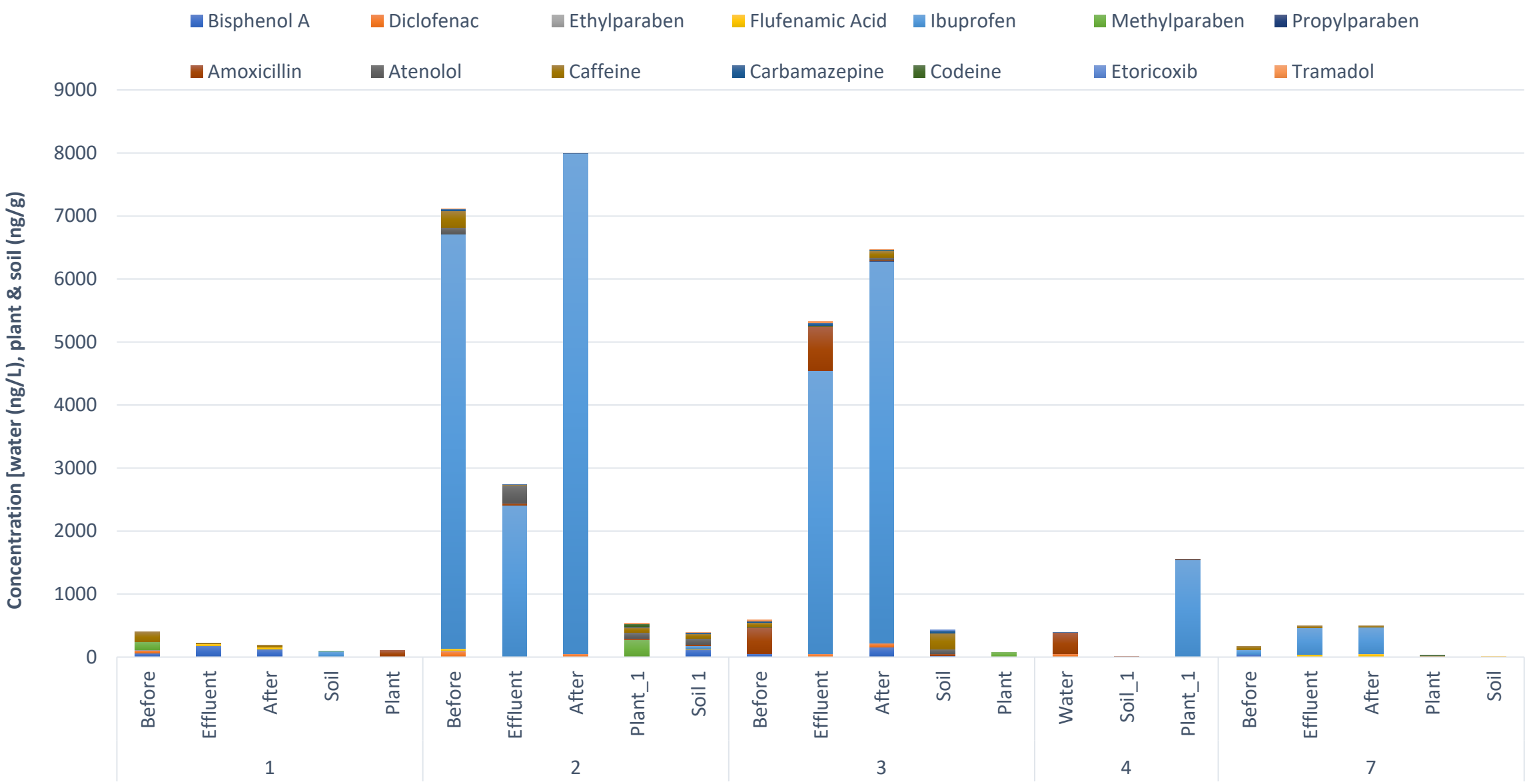
- **Water**
- **Soil**
- **Plant**

3

- Wastewater effluent
- Water before the point of effluent release
- Water after the point of effluent release
- Soil

4

STUDY AREA SAMPLED IN 2022


Bisphenol A
Diclofenac
Ethylparaben
Flufenamic Acid
Ibuprofen
Methylparaben
Propylparaben
Amoxicillin
Atenolol
Caffeine
Carbamazepine
Codeine
Etoricoxib
Tramadol
Concentration [water (ng/L), plant & soil (ng/g)
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
Before
Effluent
After
Soil
Plant
Before
Effluent
After
Plant_1
Soil 1
Before
Effluent
After
Soil
Plant
Water
Soil_1
Plant_1
Before
Effluent
After
Plant
Soil
1
2
3
4
7

Compound Discoverer 3.3.1.111

File Reporting Lists & Libraries View Window Help

Start Page | Lists & Libraries | Job Queue | Yolanda9 | Yolanda9-(2) | Yolanda | Yolat11 | Yolat11-(2) | Yolat11-(3)

Chromatograms

MW: 341.07106 ::File: SULTAN PLANT 8I BAGF S2_ddMS2pes.raw (F3) FTMS (+) MS1

9.257

Mass Spectrum

F3 #6884, RT=9.166 min, MS1, FTMS (+)
F3 #6890, RT=9.176 min, MS2, FTMS (+), (HCD,
F3 #6949, RT=9.244 min, MS1, FTMS (+)
F3 #6955, RT=9.255 min, MS2, FTMS (+), (HCD,
F3 #6954, RT=9.252 min, MS1, FTMS (+)
F3 #6960, RT=9.259 min, MS2, FTMS (+), (HCD,

RAWFILE(top): SULTAN PLANT 8I BAGF S2_ddMS2pes (F3) #9276, RT=12.420 min, MS2, FTMS (+), (HCD, DDA, 342.0783@(18;35;48), +1)
REFERENCE(bottom): mzCloud library, Propiconazole, C15 H17 Cl2 N3 O2, MS2, FTMS, (HCD, 342.0771@(20;30;50))

SULTAN PLANT 8I BAGF S2_ddMS2pes (F3) #6890, RT=9.176 min, MS2, FTMS (+), (HCD, DDA, 342.0783@(18;35;48), +1)

Compounds | Compounds per File | Merged Features

Tags	Checked	Name																Mass List Match
		Trinexapac-ethyl								337825								
		Ethyl Paraben								732751								
		3-Indoleacetic Acid								349249								
		Atrazine-D5	C8 H9 Cl D5 N5		3.45	220.12592	221.13319	9.525	6322248	78	0			0.939	0.879	0.88	0.88	0.993	
		Propiconazole	C15 H17 Cl2 N3 O2		3.75	341.07106	342.07834	9.257	853296278	14	2	99.2	97.5	0.682	0.589	0.69	0.69	0.866	
		Piperonyl-butoxide	C19 H30 O5		3.11	338.21037	339.21765	8.109	17331357	47	0			0.85	0.758	0.833	0.833	0.007	
		Dopamine	C8 H11 N O2		3.61	153.07953	154.08681	4.906	8263078	394	0			0.558	0.517	0.909	0.909	0.987	
		AZT	C10 H13 N5 O4		3.56	267.09770	268.10498	1.197	20191872	2	0			0.444	0.371	0.799	0.799	0.937	
		Methandienone	C20 H28 O2		3.29	300.20992	301.21719	6.261	11697560	123	0			0.227	0.145	0.875	0.875	0.029	
		Dibutyl Phthalate	C16 H22 O4		3.52	278.15279	279.16006	12.574	20154160	242	0			0.389	0.313	0.842	0.842	0.985	
		Fenoxycarb	C17 H19 N O4		3.20	301.13237	302.13965	7.590	10473409	165	0			0.14	0.058	0.796	0.796	0.951	
		11-nor-9-Carboxy-Delta-9-THC	C21 H28 O4		-3.67	344.19750	345.20477	8.694	17504464	59	0			0.777	0.684	0.813	0.813	0.99	
		(6E)-10-Heptyl-5,8,9-trihydroxy-3,4,5,8,9,10-hexahydro	C16 H28 O5		73237.76	322.17919	323.18646	5.700	45118837	1	3	66.1	47.3	0.978	0.89	0.819	0.819	0.985	

Show Related Tables

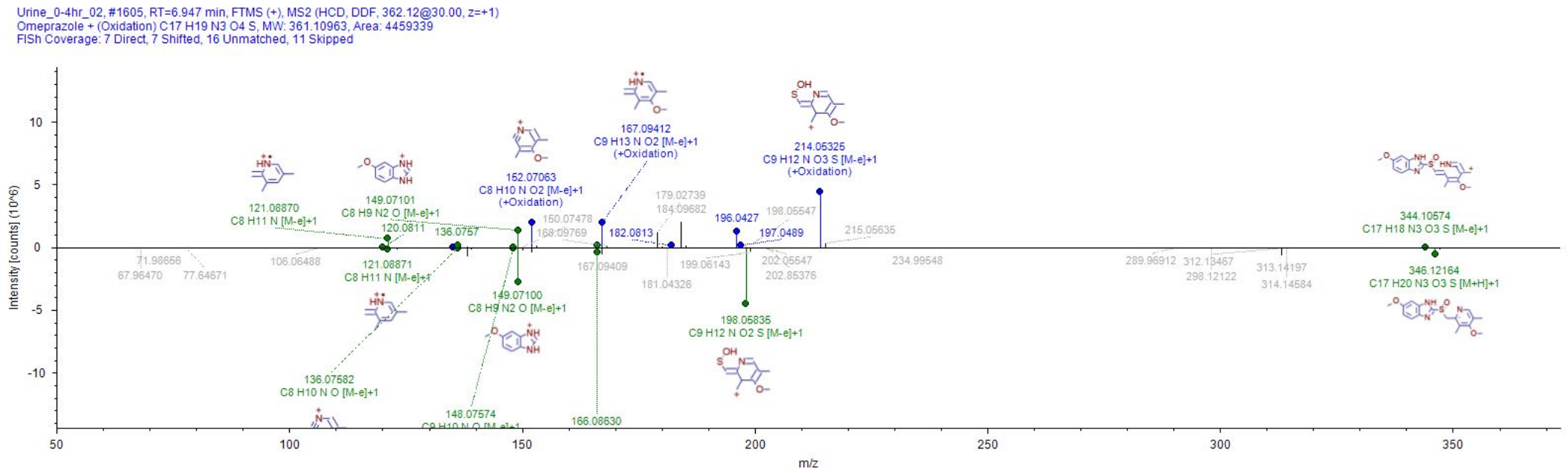
Compound Discoverer 2.0.0.303

File Reporting Libraries View Help

Start Page | Find Expected Mark Background with FISh Scoring

Mass Spectrum

#1537, RT=6.823 min, FTMS (+)
#1541, RT=6.835 min, FTMS (+), M
#1543, RT=6.837 min, ITMS (+)
#1544, RT=6.837 min, ITMS (+)
#1575, RT=6.892 min, FTMS (+)
#1595, RT=6.930 min, FTMS (+)
#1605, RT=6.947 min, FTMS (+), M
#1607, RT=6.948 min, ITMS (+)
#1608, RT=6.949 min, ITMS (+)



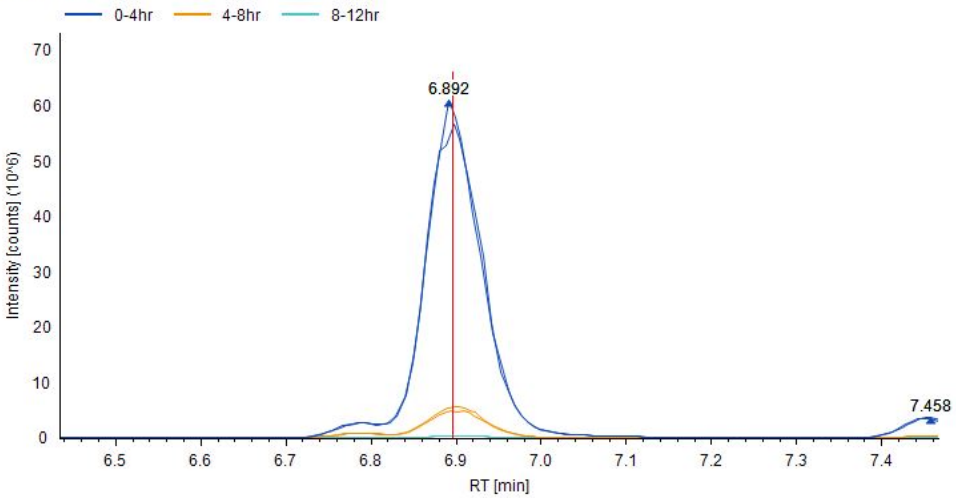
Merged Features | Expected Features | Custom Explanations | Specialized Traces

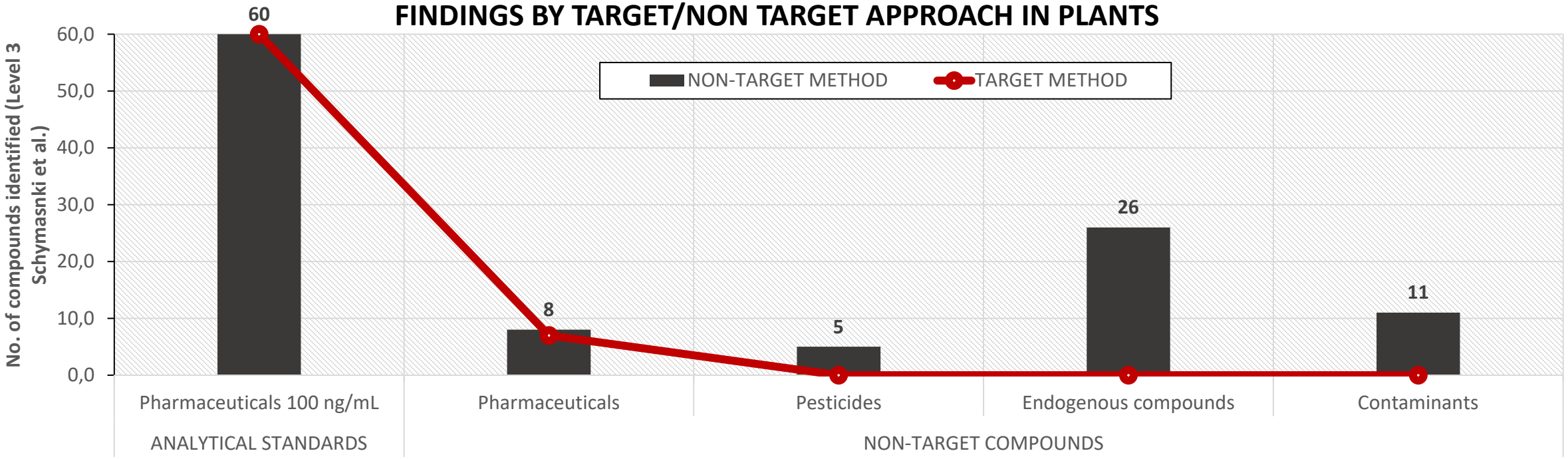
Expected Compounds | Expected Compounds per File | Expected Formulas

	Checked	Parent Compound	Formula	Molecular Weight	Dealkylated	Transformations
1	☑	Omeprazole	C17 H19 N3 O3 S	345.11471		
2	☑	Omeprazole	C17 H19 N3 O4 S	361.10963		Oxidation
3	☑	Omeprazole	C16 H17 N3 O2 S	315.10415	X	Dehydration, Reduction
4	☑	Omeprazole	C17 H17 N3 O4 S	359.09398		Desaturation, Oxidation
5	☑	Omeprazole	C16 H17 N3 O3 S	331.09906	X	
6	☑	Omeprazole	C17 H19 N3 O5 S	377.10454		Oxidation, Oxidation
7	☑	Omeprazole	C16 H17 N3 O2 S	315.10415	X	Dehydration, Reduction
8	☑	Omeprazole	C18 H18 N4 O3 S	370.10996	X	Dehydration, Glycine Conjugation
9	☑	Omeprazole	C17 H19 N3 O4 S	361.10963		Oxidation

Show Related Tables

Chromatograms

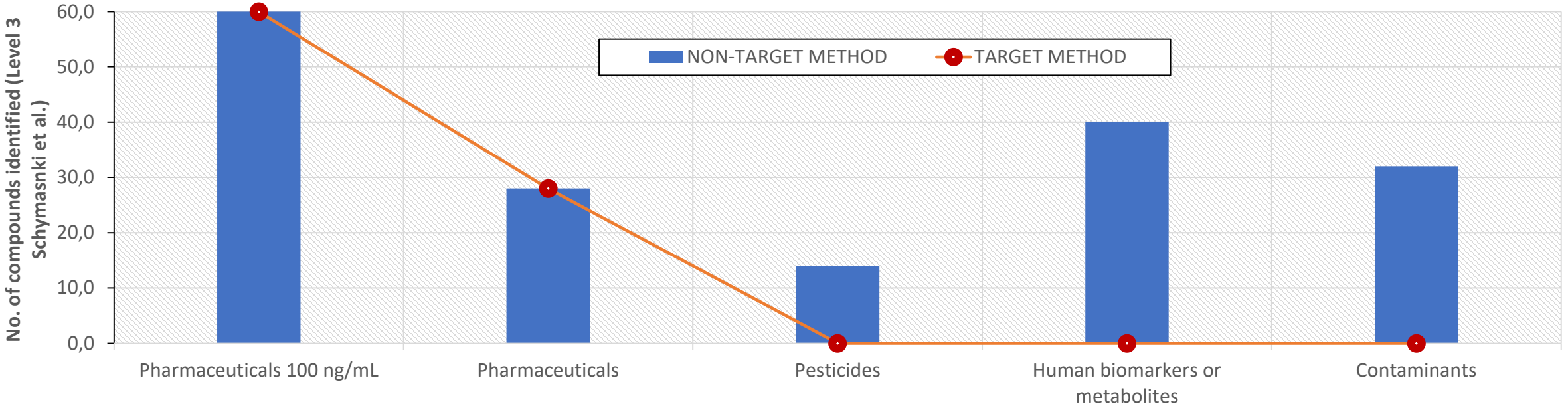




Some examples of non-target compounds identified using non-target ddMS2 of the 4 more intense ions per cycle

Pesticides	Pharmaceuticals	Endogenous compounds	Contaminants
Propyconazole	Benzenesulfonamide	Aa (Tryphtophan, Phenylalanine)	Stearamide
DEET		Oleamide	PEG (5,6,7,..10, etc.)
Cyhalofop acid		Galaxolido	Phthalates (Bis(2-ethylhexl); dimethyl)
Imazamox		Mothoxyquiruline	Citroflex 4
Buprofezim		Cafetol	Steroyl glycerol
		Trybuthyl citrate	Tris-(2-butoxyethyl)phosphete
		Sedenoline	Ethyl miristate

FINDINGS BY TARGET/NON TARGET APPROACH IN EFLUENTS



Some examples of non-target compounds identified using non-target ddMS2 of the 4 more intense ions per cycle

Pesticides	Pharmaceuticals	Endogenous compounds	Contaminants
Fungicides (propiconazole, dibenzoconazole, tebicpmazpñe)	Benzenesulfonamide	Aa (Tryphtophan, Phenylalanine)	Stearamide
DEET		Oleamide	PEG (5,6,7,..10, etc.)
Neonicotinoids (imidacloprid, acetamiprid)		Galaxolido	Phthalates (Bis(2-ethylhexl); dimethyl)
Triazines (atrazine, terbuthylazine and their met.)		Mothoxyquiruline	Citroflex 4
Organophosphorus (chlorpyrifos, chlorfenvinfos)		Cafetol	Steroyl glycerol
Carbamates (carbofuran, carbofuran 3-hydroxy)		Trybuthyl citrate	Tris-(2-butoxyethyl)phosphete
Other (hexitiazox, pyriproxyfen)		Sedenoline	Ethyl miristate

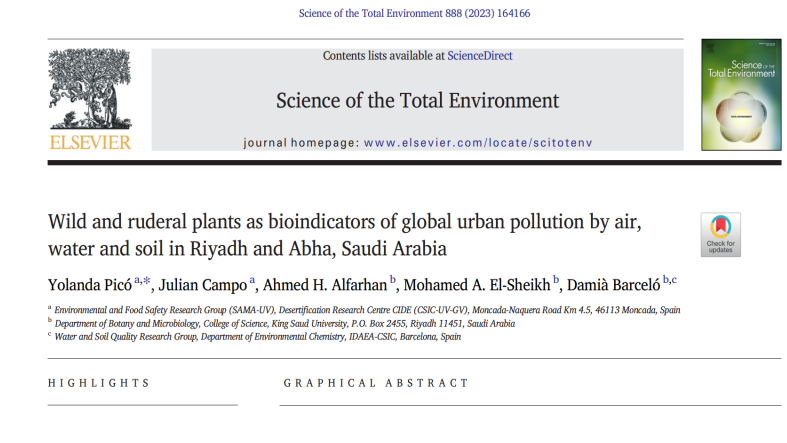
Conclusions

- High-resolution mass spectrometry (orbitrap) provides different non-target workflows with a high capacity for compound identification.
- Combination of targeted analysis using ddMS^2 when using as dependent data the inclusion of the compound in a database and of non-target analysis to also perform **dependent scan on most intense ions if no target as are found** allows to broaden the number of determinable compounds and to expand the quantification capabilities.
- The selection of intensity as a dependent parameter for ddMS^2 provides high-quality information about the major compounds in the sample. However, it fails to determine those that co-elute with compounds of higher intensity.
- The combination of both target and non-target analysis in the same injection provides an interesting profile of the compounds presents in the samples enlarging the identification of chemicals..

Acknowledgements

- Other coauthors of this study: Julian Campo, Ahmed H. Alfarhan, Mohamed A. El-Sheikh, Damià Barceló

- The financial support from the project number (RSP-2021/11) King Saud University, Riyadh, Saudi Arabia is acknowledged.



Science of the Total Environment 888 (2023) 164166

Contents lists available at ScienceDirect

Science of the Total Environment

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Wild and ruderal plants as bioindicators of global urban pollution by air, water and soil in Riyadh and Abha, Saudi Arabia

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HIGHLIGHTS

GRAPHICAL ABSTRACT

Many thanks for your attention!!!