

SUPPLEMENTARY INFORMATION

Table 3: Analytes included in the post-target and the non-target with theoretical library screening in **positive ESI mode** grouped by compounds family.

**A) List of Pesticides included.**

1-Naphtalene acetamide	Cyanofenphos oxygen	Flamprop methyl	Pencycuron
1-Naphthaleneacetic acid	Cycloate	Flazasulfuron	Pendimethalin
2,4,5-T	cycloheximide	Florasulam	Penxoxazole
2,4,5-T Isopropyl ester	Cyfluthrin	Fluacrypyrim	Phenmedipham
2,4-D	Cymoxanil	Fluazifop acid	Phenoxyacetic acid
2,4-D Butyl ester	Cyprodinil	Fluazifop-P-butyl	Phenyl mercuric acetate
2,4-D isopropyl ester	Cyproconazole	Flucythrinate	Phorate
2,4-D methyl ester	Cyromazine	Fludioxonil	Phorate oxygen analogue
2-aminobenzimidazol	Dacthal	Flufenacet	Phorate sulfoxide
2-hydroxy-simazine	Daminozide	Flufenoxuron	Phorate-sulfone
2-hydroxy-terbuthylazine	Dazomet	Fluometuron	Phosalone
2-Naphtoxyacetic acid	DDVP (dichlorvos)	Fluquinconazole	Phosfon
2-phenoxypropionic acid	Deethyl ametryn	Fluridone	Phosmet
3,4,5-trimethacarb	Deethyl cyanazine	Fluroxypyr	Phosphamidon
3,4-Dichloraniline	Deethyl cyanazine acid	Flurtamone	Phoxim
5-hydroxy-imidacloprid	Deethyl cyanazine amide	Flusilazole	Picolinafen
5-OH-clethodim-sulfon	Deethyl terbuthylazine	Flutriafol	Pirimicarb
6-chloro-4-hydroxy-3-phenyl-pyridazin	Deethyl-2-hydroxy-terbuthylazine	Folpet	Pirimiphos ethyl
8-hydroxyquinoline	Deethylatrazine	Fonofos	Pirimiphos-methyl
Absidic acid	Deethyldeisopropyl-2-hydroxyatrazine	Forchlorfenuron	Primisulfuron-methyl
ACC	Deethylhydroxyatrazine	Fosmet	Prochloraz
Acephate	Deethylsymetrine	Fosthiazate	Prochloraz
Acetamiprid	Deethylterbumeton	Fuberidazole	Procymidone
Acetate	Deethylterbutryn	Furathiocarb	Profenofos
Acetochlor	Deisopropyl-2-hydroxy-atrazine	Gibberellic acid	Promecarb
Acibenzolar-S-methyl	Deisopropylatrazine	Haloxypop	Prometon
Aclonifen	Deisopropylprometryne	Haloxypop-ethoxyethyl	Prometryne
Acrinathrin	Deltamethrin	Haloxypop-ethoxyethylester	Propachlor

Alachlor	Demethon-S-methyl	Haloxyfop-etotyl	Propamocarb
Alanycarb	Demethon-S-methyl sulfon	Haloxyfop-methyl	Propanil
Albendazole	Demethon-S-methyl sulfoxide	Heptenophos	Propargite
Aldicarb	Demethyl fluometuron	Hexaconazole	Propethamphos
Aldicarb sulfoxide	Demethyl isoproturon	Hexazinone	Propham
Aldicarb sulphone	Demethyl monuron	Hexythiazox	Propiconazole
Ametryne	Desmedipham	Hormodin	Propoxur
Amidosulfuron	Desmethylpyrimicarb	Hydroxy atrazine	Propyzamide
Aminocarb	Diafenthuron	Imazalil	Prosulfuron
Amitraz	Dialifos	Imazameth	Prosulfuron
Anilazine	Diallate	Imazamethabenz-methyl	Prothiophos
Anilofos	Diazinon	Imidacloprid	Pymetrozine
ANTU	Dibenzylamine	Indoxacarb	Pyrazophos
Atrazine	Dichlofluanid	Iprodione	Pyridaben
Avermectin B1a	Dichlone	Iprodione desisopropyl (metabolite)	Pyridaphenthion
Avermectin B1b	Dichlorprop	Iprovalicarb	Pyridate
Azamethiphos	Diclobutrazol	Isazofos	Pyrifenox isomer Z/E 1
Azinphos-ethyl	Diclofop-methyl	Isofenphos	Pyrifenox isomer Z/E 2
Azinphos-methyl	Dicloran	Isoproturon	Pyrimethanil
Azoxystrobin	Dicrotophos	Isoxaflutole	Pyriproxyfen
Benalaxyl	Dicryl	Isoxathion	Quinalphos
Bendiocarb	Dieldrin	Kresoxim-methyl	Quinmerac
Benfuracarb	Diethofencarb	Linuron	Quinoclamine
Bensulfuron-methyl	Difenoconazole	Lufenuron	Quinoxyfen
Bensulide	Difenoxuron	Malaoxon	Quizalofop-ethyl
Bensultap	Diflubenzuron	Malathion	Reserpine
Bentazone	Di flufenican	MCPA	Rimsulfuron
Benzoximate	Disulfoton	MCPA methylester	Rotenone
Bifenazate	Dimefuron	Mecarbam	Silvex
Bifenox	Dimethachlor	Mepanipyrim	Simazine
Bifenthrin	Dimethoate	Merphos	Simetryn
Bitertanol	Dimethomorph estereoisomer 1	Mesotrione	Spinosyn A
Bromacil	Dimethomorph estereoisomer 2	Metalaxyl	Spinosyn D
Bromoxynil	Dimethylvinphos	Metamitron	Spiroxamine

Bromuconazole	Diniconazole	Metazachlor	Strychnine
Bupirimate	Dinocap	Metconazole	Sulfallate
Buprofezin	Diphacinone	Methabenzthiazuron	Sulfosulfuron
Butocarboxym	Diphenylamine	Methamidophos	Sulfotep
Butoxycarboxim-sulfoxid (FC)	Diquat dibromide monohydrate	Methfuroxam	Sulprofos
Butoxycarboxym	Diuron	Methidathion	Tebuconazole
Buturon	Dixanthogen	Methiocarb	Tebufenozide
Cambendazole	Dodemorph	Methiocarb sulfone	Tebufenpyrad
Captan	Dodine	Methiocarb sulfoxide	Tebuthiuron
Carbaryl	Edifenphos	Methomyl	Teflubenzuron
Carbendazim	Endrin	Methoxyfenozide	Terbacil
Carbetamide	EPN	Metobromuron	Terbufos
Carbofuran	Epoxiconazole	Metolachlor	Terbufos sulfone
Carbofuran-3-OH	EPTC	Metosulam	Terbufos sulfoxide
Carbosulfan	Ethephon	Metoxuron	Terbumeton
Carboxin	Ethiofencarb	Metribuzin	Terbuthylazine
Chlorbromuron	Ethiofencarb sulfone	Metsulfuron-methyl	Terbutryn
Chlorfenapyr	Ethiofencarb sulfoxide	Mevinphos 1	Tetrachlorvinphos
Chlorfenvinphos	Ethiofencarbsulfon	Mevinphos 2	Tetraconazole
Chlorfenvinphos-Met	Ethion	Molinate	Thiabendazole
Chlorfluazuron	Ethiprole	Monocrotophos	Thiacloprid
Chloridazon	Ethoxyquin	Monolinuron	Thiamethoxam
Chlorophenoxyacetic acid	Ethofenprox	Monuron	Thifensulfuron-methyl
Chloropicrin	Ethofumesate	Myclobutanil	Thiobencarb
Chlorotoluron	Ethoprophos	Naled	Thiodicarb
Chloroxuron	Etoxazole	Napropamide	Thiofanox
Chlorpropham	Etrimfos	Neburon	Thiofanox-sulfone
Chlorsulfuron	Famoxadone	Nicosulfuron	Thiofanox-sulfoxide
Chromafenozide	Fenamiphos	Nicotine	Thiophanate-ethyl
Cinosulfuron	Fenarimol	N-m-Tolylphthalamic acid	Thiophanate-methyl
Clethodim	Fenazaquin	Nuarimol	Thiram
Clethodim-imin-sulfon	Fenbendazole	Ofurace	Tolclofos-methyl
Clethodim-imin-sulfoxide	Fenbuconazole	Omethoate	Tolylfluanid
Clethodim-sulfon	Fenfuram	Oxamide	Triadimefon
Clethodim-sulfoxid	Fenhexamid	Oxadixyl	Triadimenol

Clodinafop-propargyl	Fenoxaprop	Oxamyl	Triasulfuron
Clofentezine	Fenoxaprop-ethyl	Oxycarboxin	Triazophos
Clomazone	Fenoxycarb	Oxydemeton-methyl	Tribenuron-methyl
Clopyralid	Fenpiclonil	Oxyfluorfen	Trichlorfon
Cloquintocet-mexyl	Fenpropathrin	Oxygen	Tricyclazole
Clorpyrifos	Fenpropidin	Paclobutrazol	Trietazine
Clorpyrifos-methyl	Fenpropimorph	Paraoxon	Trifloxystrobin
Clothianidin	Fenpyroximate	Paraoxon-methyl	Triflumizole
Coroxon	Fensulfothion	Paraquat dichloride	Triflumuron
Coumaphos	Fensulfothion-sulfone	Parathion	Trifluralin
Cyanazine	Fenthion	Parathion-methyl	Trisulfuron-methyl
Cyanazine acid	Fenuron	Parathion-ethyl	Triticonazole
Cyanazine amide	Flamprop	Pebulate	Vamidothion
Cyanofenphos	Flamprop isopropyl	Penconazole	Vinclozolin

**B) List of Pharmaceuticals included.**

Aceclofenac	Cimaterol	Hydroxymethylclenbuterol	Papaverine
Acetobutolol	Cimbuterol	Ibuprofen	Paracetamol/Acetaminophen
Acetazolamide	Cimetidine	Ibuprofen (Met 1) Carboxyibuprofen	Paroxetine
Acetylsalicylic acid/Aspirine	Ciproheptadina	Ibuprofen (Met 1) Hydroxyibuprofen	Pavabid
Adrafinil	Citalopram	Ifosfamide	Pentoxifylline
Albuterol	Clenbuterol	Indomethacin	Phenazone/Antipyrine
Aldosterone	Clencyclohexerol	Iopamidol	Phenylbutazone
Alendronic acid	Clenhepterol	Iopromide	Phenylbutazone (Met 1) Oxyphenbutazone
Alprazolam	Clenhexerol	Irbesartan	hydroxylated Phenylbutazone (Met 2)
Amfepramone	Clenisopenterol	Isoprenaline	Phenylthiouracil
Amiloride	Clenpenterol	Isoxsuprine	Pindolol
Aminoglutethimide	Clenproperol	Ketoprofen	Pirbuterol
Amiphenazole	Clobetasol propionate	Lansoprazole	Pravastatin
Anastrozole	Clobetasone butryate	Latanoprost	Prednisolone
Bendroflumethiazide	Clofibrate	Loratadine	Prednisone
Benzylpiperazine	Clofibric acid	Lorazepam	Procaterol
Bumetanide	Clopidogrel	Lorazepam glucuronide	Propranolol
Bupropion	Codeine	Mabuterol	Propylthiouracil
Canrenone	Cortisol/Hydrocortisone	Mahexerol	Propyphenazone
Carphedon	Cortisone	Mapenterol	Quinapril
Carteolol	Cyclophosphamide	Mefenamic acid	Ractopamine
Cathine	Desoxycortisone	Meloxicam	Raloxifene
Celiprolol	Dexamethasone	Mercaptobenzimidazol	Ramipril
Amfetaminil	Diatrizoate	Mestranol	Ranitidine
Chlorothiazide	Diazepam	Metamizole (Met 1) 4-Aminoantipyrine	Reproterol
Chlorphentermine	Diclofenac	Metamizole/Dypirone	Risedronic acid
Chlorthalidone	Diltiazem	Metaprotenerol	Risperidone
Amidotrizoic acid	Dimethylaminophenazone	Methotrexate	Salbutamol
Amitriptyline	Donepezil	Methylprednisolone	Salicylic acid
Amlodipine	Doxazosine	Methylprednisone	Salmeterol
Astemizol	Enalapril	Methylthiouracil	Sertralina
Atenolol	Etofibrate	Metoprolol	Simvastatin

Atorvastatin	Famotidine	Metrapolol	Sotalol
Bamethane	Fenofibric acid/Fenofibrate	Mevastatin	Sulfapyridine
Beclomethasone	Fenoprofen	Mizolastine	Tamsulosin
Benzafibrate	Fenoterol	Montelukast	Tapazol
Benzylthiouracil	Fentanilo	N-(2-Hydroxyethyl)lorazepam	Temazepam
Betaxolol	Florfenicol	Naproxen	Terbutaline
Bethamethasone	Fludrocortisone	Nicotine	Thiouracil
Bezafibrate	Fludrocortisone acetate	Nifedipine	Timolol
Bisoprolol	Flumethasone	N-isopropyl-clenbuterol	Tiotropio bromuro
Brombuterol	Flunixin	Nitroglicerine	Tolfenamic acid
Broom-clenbuterol	Fluocinolone acetonide	N-methyl-mapenterol	Torasemide
Broom-clenproperol	Fluorometholone	Nordiazepam	Tramadol
Broom-mapenterol	Fluoxetine	Noscapine	Triamcinolone
Budesonide	Furosemide	Olanzapine	Triamcinolone acetonide
Buprenorphine	Furosemide glucuronide	Omeprazole	Tulobuterol
Captopril	Gabapentina	Oxazepam	Valsartan
Carbamazepine	Gemfibrozil	Oxprenolol	Venlafaxine
Carbamezapine	Hydrochlorothiazide	Palaudine/(n-hydroxypapaverine)	Warfarin
Carbuterol	Hydrocodone	Pancuronium	Zafirlukast
Carprofen	Hydroxy-clenbuterol	Pancuronium Bromide	Zilpaterol
Chloramphenicol	Hydroxy-clenhepterol	Pantoprazol	
AHD	Dicloxacillin	Midecamycin	Spiramycin II
Albendazole	Difloxacin	Minocycline	Spiramycin III
Amikacin	Dimetridazole	Monesin	Streptomycin
Amoxicillin	Doxycycline	Moxifloxacin	Sulfacetamide
AMOZ	Doxytetracycline	Nafcilline	Sulfachlorpyrazine
Ampicilline	emamectin B1a	Nalidixic acid	Sulfachlorpyridazine
AOZ	emamectin B1a benzoate	Narasin	Sulfadiazine
Azaperol	emamectin B1b	Naxilinic acid	Sulfadimethoxine
Azaperone	emamectin B1b benzoate	Nitrofurantoin	Sulfadimidine
Azepromazine	Enoxacin	Nitrofurazone	Sulfadoxine
Azithromycin (+2)	Enrofloxacin	Norfloxacin	Sulfaguanidine
Carozolole	Erythromycin (-H2O)	Ofloxacin	Sulfamerazine
Cefaclor	Erythromycin A	Oleandomycin	Sulfamethazine
Cefazoline	Erythromycin B	Cyclamycin	Sulfamethizole

Cefoperazone	Erythromycin C	Oxacillin	Sulfamethoxazole
Cefotaxime	Ethopabate	Oxfendazole	Sulfamethoxy pyridazine
Cefoxatime	Febantel	Oxibendazole	Sulfamonometoxine
Ceftazidime (2+)	Fenbendazole	Oxonilic acid	Sulfanilamide
Ceftizoxime	Fleroxacin	Oxytetracycline	Sulfapyridine
Ceftriaxone	Flubendazole	Pefloxacin	Sulfaquinoxaline
Cephadroxile	Flumequine	Penicillin	Sulfasalazine
Cephalexin	Furaltadone	Penicillin G	Sulfathiazole
Cephapirin	Furazolidone	Penicillin V	Sulfisoxazole
Cephradine	Gatifloxacin	Penicillines generic fragment	Sulfonamides generic fragment
Chlorpromazine	Gemifloxacin	Pipedimico	Temafloxacin
Chlortetracyclin	Gentamicin	Piperacillin	Tetracycline
Cinoxacin	Grepafloxacin	Pirlimycin	Tiamulin
Ciprofloxacin	Griseofulvin	Piromidic acid	Tilmicosin
Ciprofloxacin (Met 1)	Halofuginone	Propionylpromazine	Tinidazole
Ciprofloxacin (Met 2)	HMMNI	Rifampicin	Tobramycin
Ciprofloxacin (Met 3)	Josamycin	Robenidine	Triclabendazole
Ciprofloxacin (Met 4)	Lasalocid	Ronidazole	Trimethoprim
Ciprofloxacin (Met 5)	Leucomalachite green	Rosoxacin	Trovafoxacin
Clarythromycin	Levamisole	Roxythromycin	Tylosin A
Clindamycin	Lincomycin	Rufloxacin	Tylosin B
Clopidol	Lomefloxacin	Salinomycin	Tylosin C
Cloxacillin	Maduramicin	Sarafloxacin	Tylosin D
Danofloxacin	Malachite green	SEM	Xylazine
Diaveridine	Marbofloxacin	Sparfloxacin	
Diclazuril	Metronidazole	Spiramycin I	

**C) List of Illicit drugs included.**

10-Hydroxymorphine	Cocaine	LSD	Nor LSD / nor-iso-LSD
11-hydroxy-THC	Codeine	MDA	Norbenzoylecgonine
11-nor-9-carboxy- $\Delta$ 9-THC	Codeine epoxide	MDEA	Norcocaethylene
14-Hydroxycodine	Codeine-6-glucuronide	MDMA	Norcocaine
2-oxo-3-hydroxyLSD	Cotinine	Methadone	Norcodeine
3-Acetylmorphine	Diacetylmorphine	Methamphetamine	Normorphine
3'-Hydroxycocaine	Ecgonidine	Methylecgonidine	Normorphine-6-glucuronide
3-Hydroxyflunitrazepam	Ecgonine	Methylecgonine	Nortropacocaine
4-hydroxybutanoate	Ecgonine methyl ester	m-Hydroxybenzoylecgonine	Paramorphine
6-Acetylmorphine (6-AM)	EDDP	Morphine	Paraxanthine
7-aminoflunitrazepam	Ephedrine	Morphine-3 $\beta$ -glucuronide	PCP
7-aminonorflunitrazepam	Ethylecgonine	Morphine-6 $\beta$ -glucuronide	Pseudomorphine
Acetylcodeine	Ethylen cocaine	Morphine-7,8-oxide	Pseudomorphine (C17 alkaoid)
Amphetamine	Fentanyl	Morphine-gsh	Psicolin
Benzoylecgonine	Flunitrazepam	N-Benzoylnormethylecgonine	Speed
Caffeine	GHB	N-Demthylflunitrazepam	THC
Cinnamoylcocaine	Heroin	N-Hydroxynorcocaine	THC-glucuronide
Cocaethylene	Ketamine	Nicotine	



**D) List of Hormones included.**

1,4,6-androstatrien-17-ol-3-one	Androstanolone	Ethinylestradiol	Nandrolone
1,4-androstadiene-3,17-dione	Bolandiol	Ethisterone	Nandrolone
16B-hydroxyfurazabol	Bolasterone	Ethylestrenol	Norclostebol
16B-hydroxystanozolol	Boldenone	Ethynodiol	Norclostebol
17alpha-Trenbolone	Boldenone metabolite	Ethynloestradiol	Norethandrolone
17B-oestradiol	Broparoeostrole	Fluoxymesterone	Norethisterone
17-hydroxy-progesterone	Calusterone	Formebolone	Norethynodrel
17-oestradiol	Chlormadinone	Formebolone metabolite	Norprogesterone
17-Methyl-1.testosterone	Chlormadinone acetate	Gestonorone-caproate	Norvinisterone
19-hydroxyandrostenedione	Clostebol	Gestrinone	Oestriol
19-Nortestosterone	Cyclofenil	Hexestrol	Oestrone
1-testosterone	Cyproteron	Lynestrol	Oxandrolone
3'-hydroxy-progesterone	Danazol	Medrogestone	Oxymesterone
3'-hydroxystanozolol	Dehydrochloromethyl testosterone	Medroxyprogesterone	Oxymetholone
4,6-androstadien-17-ol-3-one	Delmadinone acetate	Medroxyprogesterone acetate	Progesterone
4,9-androstadien-17-methyl-17-ol-3-one	DHT	Megestrol acetate	Quinbolone
4,9-androstadien-17-ol-3-one	Dienestrol	Melengestrol	Quinestrol
4B-hydroxy-progesterone	Diethylstilbestrol	Melengestrol acetate	Stanozolol
4-Cl-17a-methyl-androsta-1,4-diene-6b,17b-diol-3-one	Dimethisterone	Mestanolone	Stenbolone
4-hydroxystanozolol	DI-norgestrel	Mesterolone	Taleranol
4-hydroxytestosterone	Drostanolone	Mestranol	Tamoxifen
6alpha-hydroxy-androst-4-ene-3,17-dione	Dydrogesterone	Methandienone	Testosterone
6b-hydroxymetandienone	Epimestrol	Metenolone	THG
6b-hydroxytestosterone	Epi-nortestosterone	Methandrol	Trenbolone
6-hydroxy-4-Cl-dehydromethyltestosterone	Epi-testosterone	Methenolone	Vinyltestosterone
6-hydroxyandrostenedione	Epi-trenbolone	Methylestrenolone	Zearalenone
Algestone acetophenide	Estradiol	Methyltestosterone	Zearanol
Allylestrenol	Estriol	Methyltrenolone	Zearalenol
Allyltrenbolone	Estrone	Mibolerone	

**E) List of Mycotoxins included.**

15-Acetoxy-scirpenol	Beta-Zearalenol	Ergosine	Moniliformin Sodium
15-Acetyldeoxynivalenol	Chaetoglobosin A	Ergotamine	Monoacetoxy-scirpenol
3-Acetyldeoxynivalenol	Chanoclavine	Festuclavine	Mycophenolic acid
3alpha-Acetyldiacetoxy-scirpenol	Chetomin	Fumitremorgin C	Neosolaniol
5-Methoxysterigmatocystin	Citrinin	Fumonisin A1	Nivalenol
Aflatoxicol I	Cytochalasin E	Fumonisin A2	Norsolorinic acid
Aflatoxin B1	Deepoxy-deoxynivalenol	Fumonisin B1	Ochratoxin Alpha
Aflatoxin B2	Deoxynivalenol	Fumonisin B2	Ochratoxin B
Aflatoxin B2 alpha	Deoxynivalenol-3-glucoside	Fumonisin B3	Parasiticol
Aflatoxin G1	Diacetoxy-scirpenol	Fumonisin B4	Paxilline
Aflatoxin G2	Dihydroergosine	Fusarenon-X	Penitrem A
Aflatoxin M1	Dihydroergotamine	Gibberallic acid	Roridin A
Aflatoxin M2	Dihydrolysergol	Gliotoxin	Scirpentriol
Agroclavine	Dihydroxy-sterigmatocystin	Griseofulvin	Sterigmatocystin
Alpha-ergocryptine	Elymoclavine	HT-2 Toxin	Sulochrin
Alpha-Zearalenol	Emodin	Hydrolyzed zearalenone	T-2 Toxin
Altenuene	Enniatin A	Lysergol	T-2 Triol
Alternariol	Enniatin B	Meleagrin	Tentoxin
alternariol methyl ether	Ergine	Methis-ergide	Verrucaric acid
Austocystin A	Ergocornine	Methoxysterigmatocystin	Verrucarol
Avenacein Y	Ergocristine	Mevinolin	Verruculogen
Averufin	Ergometrine	Moniliformin	Zearalenone
Beauvericin	Ergometrinine	Moniliformin Potassium	Zearalenone-4-glucoside

**F) List of Surfactants included.**

C11-DEA	C12-AEO9	C14-AEO8	C16-AEO9
C12-AEO10	C13-DEA	C14-AEO9	C18-AEO10
C12-AEO11	C14-AEO10	C15-DEA	C18-AEO3
C12-AEO12	C14-AEO11	C16-AEO10	C18-AEO4
C12-AEO13	C14-AEO12	C16-AEO11	C18-AEO5
C12-AEO14	C14-AEO13	C16-AEO12	C18-AEO6
C12-AEO3	C14-AEO14	C16-AEO4	C18-AEO7
C12-AEO4	C14-AEO4	C16-AEO5	C18-AEO8
C12-AEO5	C14-AEO5	C16-AEO6	C18-AEO9
C12-AEO6	C14-AEO6	C16-AEO7	C7-DEA
C12-AEO7	C14-AEO7	C16-AEO8	C9-DEA

**G) List of Dyes included.**

Brilliant green	Sudan Black B	Sudan Orange G
Butter yellow	Sudan I	Sudan Para-red
Crystal Violet	Sudan II	Sudan Red 7B
Leucocrystal violet	Sudan III	Sudan Red B
Rhodamine B	Sudan IV	Sudan Red G

**H) List of UV filters included.**

4-MBC	BP-3	OC
BM-DBM	IAMC	OD-PABA

**I) List of Phenols included.**

2,4-dimethylphenol	4-chloro-3-methylphenol	Catechol	o-Cresol
Chlorophenol	4-chlorophenol	Dinoseb	p-Cresol
3-methyl-4-nitrophenol	Bisphenol A	m-Cresol	Phenol

SUPPLEMENTARY INFORMATION

Table 4: Analytes included in the post-target and the non-target with theoretical library screening in **negative ESI mode** grouped by compounds family.

**A) List of Pesticides included.**

2,4-D	Chlorsulfuron F1	Fluroxypyr F2*	Primisulfuron methyl
2,4-DB	Dicamba	Haloxypop	Propanil
6-chloronicotinic acid	Dichlorprop	Hexaflumuron	Teflubenzuron
Absidic acid	Fenazaquin	Ioxynil	Terbacil
Acifluorfen	Fenpropathrin	MCPA	Toxaphene
Bentazone	Fludioxonyl	Mecoprop	Triflumuron
Bromacil	Fludiozonil	Mestrione	
Bromoxynil	Fluroxypyr	Oxyfluorfen	
Chlorsulfuron	Fluroxypyr F1	Pentachlorophenol	

**B) List of Pharmaceuticals included.**

Acetazolamide	Fenoprofen	Cefuroxime
Acetylsalicylic acid/Aspirine	Furosemide	Chloramphenicol
Adrafinil	Ibuprofen	Diclazuril
Bendroflumethiazide	Ketoprofen	Enrofloxacin
Bezafibrate	Mefenamic acid	Flumequine
Clofibric acid	Naproxen	Nalidixic acid
Diclofenac	Nimesulide	Nicarbazine
diclofenac sodium salt	Piroxicam	Nitrofurantoina
Diflusal	Pravastatin	Oxonilic acid
Digoxin	Salicylic acid	Sulfamethoxazole
Enalapril	Sulfasalazine	
Enalaprilat	Valsartan	

**C) List of Illicit drugs included.**

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4-hydroxybutanoate
11-nor-9-carboxy- $\Delta^9$ -THC
GHB

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**D) List of Hormones included.**

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Boldenone	Progesterone	Trenbolone
Estrone	Testosterone	Zearalenol
Nandrolone		

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**E) List of Mycotoxins included.**

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Citrinin	Mycophenolic acid
Gibberallic acid	Patulin

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**F) List of Surfactants included.**

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C10-LAS	C12-LAS	C14-AE1S	NPEO2-SO4
C11-LAS	C13-AE1S	C14-AE2S	NPEO3-SO4
C12-AE1S	C13-AE2S	C14-AE3S	NPEO4-SO4
C12-AE2S	C13-AE3S	C14-AE4S	NPEO5-SO4
C12-AE3S	C13-AE4S	C14-AE5S	NPEO6-SO4
C12-AE4S	C13-AE5S	C14-AS	NPEO7-SO4
C12-AE5S	C13-AE6S	C16-AS	OP1EC
C12-AE6S	C13-AS	DHSS	
C12-AS	C13-LAS	NP1EC	

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**G) List of Dyes included.**

Acid blue 1	Brilliant blue FCF	Metanil Yellow	Quinoline yellow
Acid green 9	Chrysoine	Naphtol yellow S	Red 10B
Acid red 52	Eosine	New coccine	Red 2G
Acid violet	Erythrosine	Orange I/II/RN	Rose bengal
Allura Red AC	Fast green FCF	Patent blue V	Sunset Yellow
Amaranth	Fast Red E	Phloxine B	Tartrazine
Amido black 10B	Fast Yellow AB	Ponceau 3R	Uranine
Azorubine	Green S	Ponceau 4R	Yellow 2G
Benzyl violet 4B	Indigotine	Ponceau 6R	
Brilliant black PN	Martius yellow	Ponceau SX	

**H) List of UV filters included.**

Benzophenone-1 (BP-1)	PDT	2,2'-dihydroxy-4-methoxy benzophenone
Benzophenone-2 (BP-2)	4-hydroxybenzophenone (HBP)	2,3,4-Trihydroxybenzophenone (THB)
Benzophenone-3 (BP-3)	4-hydroxybenzophenone (HBP)	Terephthalylidene dicamphor sulfonic acid
Benzophenone-4 (BP-4)	2-hydroxy-4-methoxy benzophenone	Ethylhexyl salicylate (EHS)
PBSA	2,4-dihydroxy benzophenone (DHB)	

**I) List of Phenols included.**

2,3,4,5-tetrachlorophenol	2,4-dichlorophenol	3,4-dichlorophenol	4-octylphenol
2,3,4,6-tetrachlorophenol	2,4-dimethylphenol	3,5-dichlorophenol	Bisphenol A
2,3,4-trichlorophenol	2,4-dinitrophenol	3,5-dinitrophenol	Catechol
2,3,5,6-tetrachlorophenol	2,5-dichlorophenol	3-chlorophenol	Dinoseb
2,3,5-trichlorophenol	2,6-dichlorophenol	3-methyl-4-nitrophenol	m-Cresol
2,3,6-trichlorophenol	2,6-dinitro-2-methylphenol	4,6-dinitro-4-methylphenol	o-Cresol
2,3-dichlorophenol	2-chlorophenol	4-nonylphenol	p-Cresol
2,4,5-trichlorophenol	2-nitrophenol	4-chloro-3-methylphenol	Pentachlorophenol
2,4,6-trichlorophenol	p-nitrophenol	4-chlorophenol	Phenol
2,4,6-trichlorophenol	3,4,5-trichlorophenol	4-nitrophenol	