

Electronic Supplementary material

Chemical profiling of organic contaminants in rural surface waters combining target and non-target LC-HRMS/MS analysis

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Text S1. Validation of the target method

The proposed method was validated using surface water samples. Linearity, matrix effects (ME), method quantification limits (MQLs), precision (expressed as intra-day and inter-day precision), and trueness (recovery) were evaluated.

Linear range was evaluated in matrix-matched calibration curves spiked at seven concentration levels, ranging from 10 ng L^{-1} to $10 \text{ } \mu\text{g L}^{-1}$. Linearity was assumed when regression coefficients (R^2) were ≥ 0.99 . The evaluation of matrix effects (%) was carried out by comparing the slope of the calibration curves prepared in solvent and matrix extract. The MQLs were considered as the minimum concentration of analyte with a signal-to-noise ratio (S/N) of 10 in terms of peak area. The precision of the method expressed in terms of repeatability (intra-day precision) and intermediate precision (inter-day precision) was evaluated by spiking samples' SPE extracts at $0.1 \text{ } \mu\text{g L}^{-1}$ ($n = 5$). The precision expressed as relative standard deviation (%RSD) of peak areas was considered satisfactory when %RSD was below 20%. Trueness was estimated by recovery studies of samples spiked at $0.1 \text{ } \mu\text{g L}^{-1}$ ($n = 5$) before the extraction protocol. Acceptable results were considered with recovery rates ranged between 70 – 120% with an $\text{RSD} \leq 20\%$. For compounds with recovery rates and/or precision outside these acceptable ranges, their concentrations in real samples should be considered as estimated values. The calculated recoveries have not been used in the calculation of the concentration of compounds in real samples.

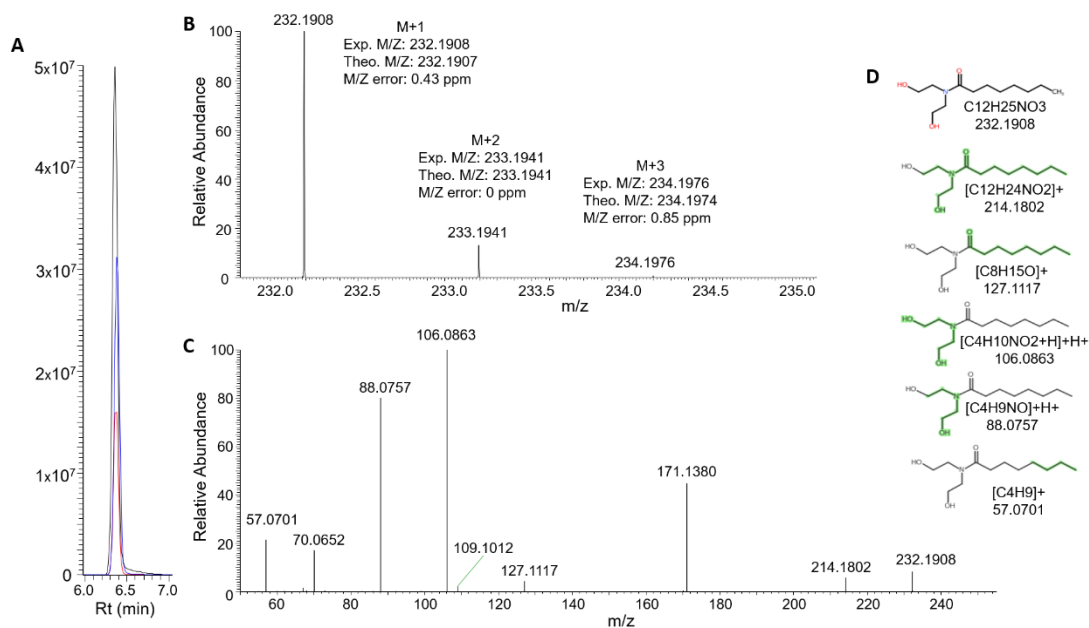


Figure S1. Tentative identification of N,N-bis(2-hydroxyethyl)octanamide. **A:** Extracted ion chromatograms of three samples of Campillo River (P7). Each color line corresponds to a sample. **B:** MS1 spectrum and isotopic pattern for M+1, M+2, and M+3 ions. **C:** MS2 spectrum of $[M+H]^+$ ion. **D:** Proposed fragmentation by MetFrag result.

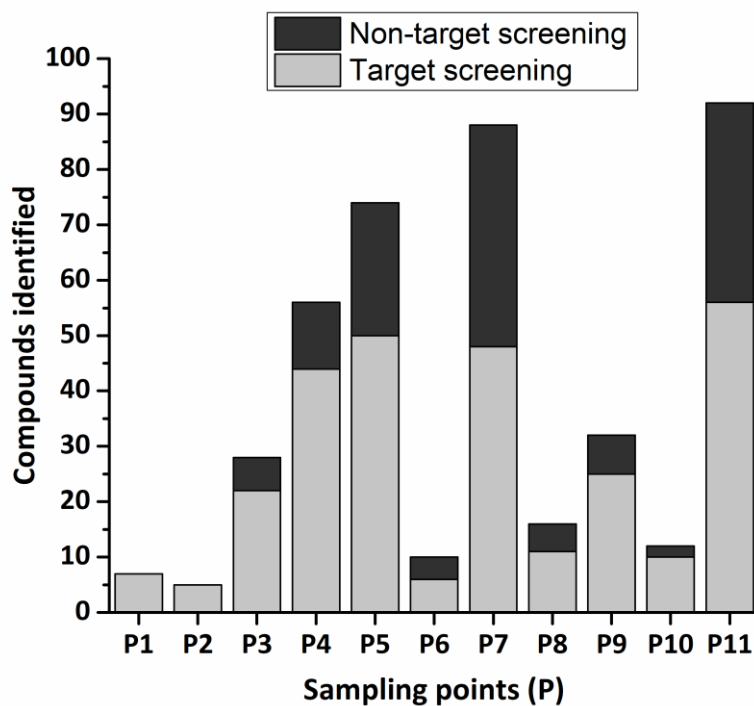


Figure S2. Total compounds identified by target and non-target screening approaches in each sampling site.

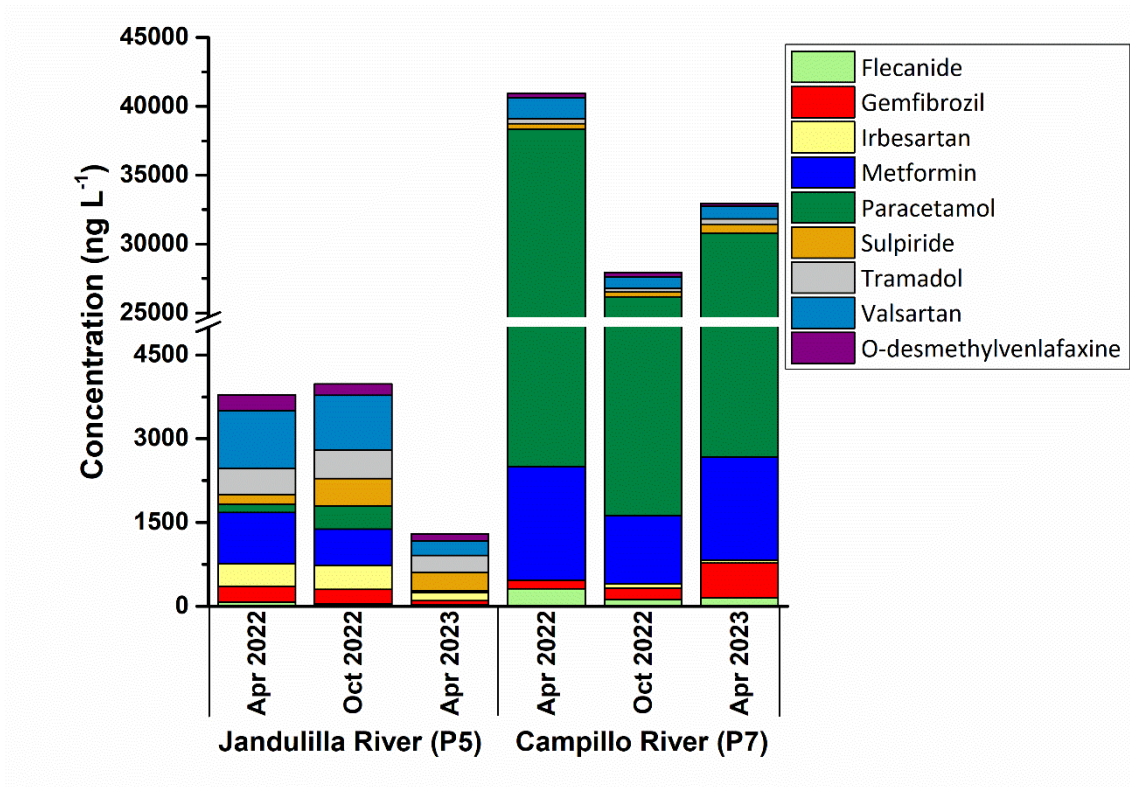


Figure S3. Comparison of the concentrations of pharmaceuticals determined in the Jandulilla River (P5, with WWTP – 6,000 inhabitants) and the Campillo River (P7, without WWTP – 1,700 inhabitants).

Table S1. List of compounds included in the target analysis.

Compound	Group
(-)-N-methylephedrine	Pharmaceutical
1-naphtalene-Acetamide	Pesticide
2,6-dimethylaniline	Industrial
2-ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine perchlorate	TP
4-androsten-3,17-dione	Pharmaceutical
9(10H)-acridone	TP
Acephate	Pesticide
Acetamiprid	Pesticide
Acridine	Pharmaceutical
Albendazole	Pharmaceutical
Albendazole sulfoxide	TP
Aldicarb	Pesticide
Ametryn	Pesticide
Aminocarb	Pesticide
Amitraz	Pesticide
Amitrol	Pesticide
Amphetamine	Drug of abuse
Anilophos	Pesticide
Antipyrine	Pharmaceutical
Asulam	Pesticide
Atenolol	Pharmaceutical
Atrazine	Pesticide
Atrazine desethyl	TP
Atrazine desisopropyl	TP
Atropine	Pharmaceutical
Azoxystrobin	Pesticide
Benalaxyl	Pesticide
Benfuracarb	Pesticide
Bensulfuron methyl	Pesticide
Benzidine	Industrial
Bitertanol	Pesticide
Boscalid	Pesticide
Bromacil	Pesticide
Bromuconazole Isomer 1	Pesticide
Bromuconazole Isomer 2	Pesticide
Bupirimate	Pesticide
Buprofezin	Pesticide
Bupropion	Pharmaceutical
Butocarboxim	Pesticide
Butoxy-carboxim	Pesticide
Buturon	Pesticide
Caffeine	Stimulant
Carbadox	Pharmaceutical

Compound	Group
Carbamazepine	Pharmaceutical
Carbamazepine 10,11-Epoxyde	TP
Carbendazim	Pesticide
Carboxine	Pesticide
Chlorbromuron	Pesticide
Chlordimeform	Pesticide
Chlorfenvinphos	Pesticide
Chloridazon (Pyrazon)	Pesticide
Chlorotoluron	Pesticide
Chloroxuron	Pesticide
Chlorpyrifos ethyl	Pesticide
Chlorpyrifos methyl	Pesticide
Chlorsulfuron	Pesticide
Cinosulfuron	Pesticide
Citalopram	Pharmaceutical
Clarithromycin	Pharmaceutical
Clenbuterol	Pharmaceutical
Clomazone	Pesticide
Clomiphene isomer 1	Pharmaceutical
Clomiphene isomer 2	Pharmaceutical
Clothianidin	Pesticide
Clotrimazole	Pharmaceutical
Cloxacillin	Pharmaceutical
Cocaine	Drug of abuse
Codeine	Pharmaceutical
Cotinine	TP
Coumaphos	Pesticide
Cyanazine	Pesticide
Cycloate	Pesticide
Cyproconazole	Pesticide
Cyprodinil	Pesticide
Cyromazine	Pesticide
Danofloxacin	Pharmaceutical
DEET	Pesticide
Demeclocycline	Pharmaceutical
Desmetryn	Pesticide
Diazepam	Pharmaceutical
Diazinon	Pesticide
Dichlorvos	Pesticide
Diclofenac	Pharmaceutical
Dicrotophos	Pesticide
Diethofencarb	Pesticide
Difenacoum	Pesticide
Difenoconazole	Pesticide
Difenoxuron	Pesticide

Compound	Group
Diflufenican	Pesticide
Dimethametryn	Pesticide
Dimethenamid	Pesticide
Dimethomorph E	Pesticide
Dimethomorph Z	Pesticide
Dimoxystrobin	Pesticide
Diniconazole	Pesticide
Diphenhydramine	Pharmaceutical
Diphenylamine	Industrial
Diuron	Pesticide
Edifenphos	Pesticide
Enoxacin	Pharmaceutical
Eprosartan mesylate	Pharmaceutical
Erythromycin	Pharmaceutical
Ethiofencarb sulfoxide	Pesticide
Ethion	Pesticide
Ethiprole	Pesticide
Ethoprophos	Pesticide
Ethoxyquin	Pesticide
Etrimphos	Pesticide
Famphur	Pesticide
Fenamiphos	Pesticide
Fenarimol	Pesticide
Fenazaquin	Pesticide
Fenhexamid	Pesticide
Fenobucarb	Pesticide
Fenoxycarb	Pesticide
Fenpropidine	Pesticide
Fenpropimorphe	Pesticide
Fensulfothion	Pesticide
Fenthion	Pesticide
Fenuron	Pesticide
Flecainide	Pharmaceutical
Fluazifop	Pesticide
Fluazifop-p-butyl	Pesticide
Fluconazole	Pharmaceutical
Flufenacet	Pesticide
Flufenamic acid	Pharmaceutical
Flumequine	Pharmaceutical
Fluometuron	Pesticide
Fluroxypyr	Pesticide
Flutolanil	Pesticide
Flutriafol	Pesticide
Fosthiazate	Pesticide
Fuberidazole	Pesticide

Compound	Group
Furmecyclox	Pesticide
Gabapentin	Pharmaceutical
Gemfibrozil	Pharmaceutical
Griseofulvin	Pharmaceutical
Haloxyfop	Pesticide
Heroin	Drug of abuse
Hexazinone	Pesticide
Hexythiazox	Pesticide
Imazalil	Pesticide
Imazamethabenz-methyl	Pesticide
Imazamox	Pesticide
Imazaquin	Pesticide
Indomethacin	Pharmaceutical
Ipconazole	Pesticide
Irbesartan	Pharmaceutical
Isocarbophos	Pesticide
Isoprocarb	Pesticide
Isoproturon	Pesticide
Isoxaben	Pesticide
Karbutilate	Pesticide
Ketamine	Drug of abuse
Ketoprofen	Pharmaceutical
Lamotrigine	Pharmaceutical
Lenacil	Pesticide
Leucomalachite green	Industrial
Levofloxacin	Pharmaceutical
Lidocaine	Pharmaceutical
Lincomycin	Pharmaceutical
Linuron	Pesticide
Malachite green	Industrial
MDA	Drug of abuse
MDEA	Drug of abuse
MDMA	Drug of abuse
Mebendazole	Pharmaceutical
Meclofenamic acid	Pharmaceutical
Mefenacet	Pesticide
Mefenamic acid	Pharmaceutical
Mepivacaine hydrochloride	Pharmaceutical
Metalaxyl	Pesticide
Metamitron	Pesticide
Metazachlor	Pesticide
Metformin	Pharmaceutical
Methabenzthiazuron	Pesticide
Methadone	Drug of abuse
Methamidophos	Pesticide

Compound	Group
Methamphetamine	Drug of abuse
Methidathion	Pesticide
Metobromuron	Pesticide
Metolachlor	Pesticide
Metoxuron	Pesticide
Metribuzin	Pesticide
Metronidazole	Pharmaceutical
Mevinphos	Pesticide
Miconazole	Pharmaceutical
Molinate	Pesticide
Monocrotophos	Pesticide
Monolinuron	Pesticide
Monuron	Pesticide
Morphine	Drug of abuse
Myclobutanil	Pesticide
Nadolol	Pharmaceutical
Naptalam	Pesticide
Neburon	Pesticide
Nicotine	Stimulant
Nifuroxazide	Pharmaceutical
Nitenpyram	Pesticide
Norflurazon	Pesticide
Norpseudophedrine (Cathine)	Drug of abuse
Nuarimol	Pesticide
O-desmethylvenlafaxine	Pharmaceutical
Ofurace	Pesticide
Omethoate	Pesticide
Oxadiazon	Pesticide
Oxadixyl	Pesticide
Oxfendazole	Pharmaceutical
Oxolinic acid	Pharmaceutical
Oxytetracycline	Pharmaceutical
Paclobutrazol	Pesticide
Paracetamol (Acetaminophen)	Pharmaceutical
Pebulat	Pesticide
Penconazole	Pesticide
Pencycuron	Pesticide
Phosalone	Pesticide
Picloram	Pesticide
Picolinafen	Pesticide
Pirimicarb	Pesticide
Pirimiphos methyl	Pesticide
Pretilachlor	Pesticide
Prochloraz	Pesticide
Promecarb	Pesticide

Compound	Group
Prometon	Pesticide
Prometryn	Pesticide
Propachlor	Pesticide
Propamocarb	Pesticide
Propanil	Pesticide
Propazine	Pesticide
Propiconazole	Pesticide
Propoxur	Pesticide
Propranolol	Pharmaceutical
Propyzamid	Pesticide
Proquinazid	Pesticide
Prosulfocarb	Pesticide
Prosulfuron	Pesticide
Pymetrozin	Pesticide
Pyraclostrobin	Pesticide
Pyranocoumarin	Pesticide
Pyrazophos	Pesticide
Pyridaben	Pesticide
Pyridaphenthion	Pesticide
Pyrimethanil	Pesticide
Pyriproxifen	Pesticide
Pyroquilon	Pesticide
Quinalphos	Pesticide
Quinmerac	Pesticide
Quinoclamine	Pesticide
Quinoxifen	Pesticide
Ranitidine	Pharmaceutical
Rotenone	Pesticide
Roxithromycin	Pharmaceutical
Simazine	Pesticide
Sotalol	Pharmaceutical
Spiroxamine	Pesticide
Sulcotrione	Pesticide
Sulfabenzamide	Pharmaceutical
Sulfacetamide	Pharmaceutical
Sulfachloropyridazine	Pharmaceutical
Sulfadiazine	Pharmaceutical
Sulfadimethoxyn	Pharmaceutical
Sulfadoxine	Pharmaceutical
Sulfaguandine	Pharmaceutical
Sulfamerazine	Pharmaceutical
Sulfamethazine	Pharmaceutical
Sulfamethoxazole	Pharmaceutical
Sulfamethoxypyridazine	Pharmaceutical
Sulfamonomethoxine	Pharmaceutical

Compound	Group
Sulfapyridine	Pharmaceutical
Sulfaquinoxaline	Pharmaceutical
Sulfathiazole	Pharmaceutical
Sulfisoxazol	Pharmaceutical
Sulfometuron methyl	Pesticide
Sulfotep	Pesticide
Sulpiride	Pharmaceutical
Tebuconazole	Pesticide
Tebufenpyrad	Pesticide
Tebuthiuron	Pesticide
Telmisartan	Pharmaceutical
Temephos	Pesticide
Tepraloxydim	Pesticide
Terbumeton	Pesticide
Terbutaline	Pharmaceutical
Terbuthylazine	Pesticide
Terbuthylazine desethyl	TP
Terbutryn	Pesticide
Testosterone	Pharmaceutical
Tetraconazole	Pesticide
Tetracycline	Pharmaceutical
Theobromine	TP
Theophylline	TP
Thiabendazole	Pesticide
Thiacloprid	Pesticide
Thiamethoxam	Pesticide
Thiocyclam (hydrogenoxalate)	Pesticide
Thiodicarb	Pesticide
Timolol	Pharmaceutical
Tramadol	Pharmaceutical
Triadimefon	Pesticide
Triadimenol	Pesticide
Triallat	Pesticide
Triasulfuron	Pesticide
Triazophos	Pesticide
Triazoxide	Pesticide
Tributyl phosphate	Industrial
Triclocarban	Pesticide
Trietazine	Pesticide
Triethyl phosphate	Industrial
Trifloxystrobin	Pesticide
Triflumizole	Pesticide
Triflumuron	Pesticide
Trimethoprim	Pharmaceutical
Trinexapac-ethyl	Pesticide

Compound	Group
Valsartan	Pharmaceutical
Venlafaxine	Pharmaceutical
Δ -9-THC	Drug of abuse

Table S2. Information of the monitored catchment points (P), main land use, upstream population, and presence/absence of upstream wastewater treatment plant (WWTP).

P	River name	Water course	Land use	Upstream population	Upstream WWTP
1	Headwaters Arbuniel	Headwaters	Natural areas / agriculture	-	no
2	Headwaters Mata-Bejid	Headwaters	Natural areas / agriculture	-	no
3	Arbuniel	Small stream	Agriculture / Urban	600	no
4	Cambil	Small stream	Agriculture / Urban	2100	yes
5	Jandulilla	Small stream	Agriculture / Urban	6000	yes
6	Rumblar	Small stream	Natural areas / agriculture	-	no
7	Campillo	Small stream	Agriculture / Urban	1700	no
8	Guadalbullón	Small stream	Agriculture / Urban	1300	no
9	Jaén	Small stream	Agriculture / Urban	6000	yes
10	Jándula	Small stream	Natural areas / agriculture	-	no
11	Guadalquivir	Main river	Agriculture / Urban / Industrial	2000	no

Table S3. HESI source parameters.

Spray voltage (kV)	3.5 / -2.5
Capillary temperature (°C)	300
Sheath gas (AU)	55
Auxiliary gas (AU)	15
S-lens RF level (AU)	60
Auxiliary gas heater temperature (°C)	350

Table S4. Settings of the Full MS/MS acquisition method.

MS1 resolution	70,000
Automatic Gain Control (AGC) target MS1	3×10^6
Maximum injection time MS1 (ms)	100
Scan range MS1 (m/z)	65 - 950
MS2 resolution	17,500
Automatic Gain Control (AGC) target MS/MS	2×10^5
Maximum injection time MS/MS (ms)	100
Loop count	5
TopN	5
Isolation window (m/z)	1
Normalized collision energy (NCE)	35

Table S5. Validation results of the SPE-UHPLC-HRMS/MS method. Method quantification limits (MQLs), matrix effect (ME), linearity expressed by the correlation coefficient (R^2), average recovery (%) and method repeatability (RSD, %), intraday and interday precision (RSD, %) at a concentration of 0.1 $\mu\text{g L}^{-1}$ ($n = 5$).

Compound	MQL (ng L ⁻¹)	ME (%)	Linearity (R^2)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
(-)-N-Methylephedrine	5	5.4	0.9993	70.8	7.1	2.4	10.8
1-Naphtalene-Acetamide	10	-24.3	0.9996	115.1	9.6	3.9	8.8
2,6-Dimethylaniline	5	-2.7	0.9966	22.3	4.8	3.3	9.1
2-Ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine perchlorate	5	-7.1	0.9985	44.0	10.4	2.8	3.4
4-Androsten-3,17-dione	10	-4.4	0.9936	97.5	4.7	6.7	8.0
9(10H)-Acridone	10	-11.5	0.9987	99.4	3.1	1.5	7.3
Acephate	10	-8.1	0.9978	10.7	15.6	5.6	13.6
Acetamidiprid	50	-21.2	0.9952	108.7	13.5	2.4	14.1
Acridine	1.7	-6.0	0.9994	83.1	3.5	2.9	15.3
Albendazole	5	-7.6	0.9975	70.4	4.1	2.5	17.2
Albendazole sulfoxide	10	-7.1	0.9995	118.3	8.5	3.2	1.6
Aldicarb	10	-21.3	0.9965	75.8	5.4	5.1	7.6
Ametryn	5	1.0	0.9972	94.3	4.9	2.3	7.7
Aminocarb	10	-2.6	0.9947	100.5	4.8	1.3	10.8
Amitraz	50	-30.7	0.9906	51.9	19.9	29.0	57.4
Amitrol	50	3.3	0.9917	0.0	-	9.3	16.0
Amphetamine	50	1.5	0.9997	52.2	7.6	4.8	26.5
Anilophos	5	1.9	0.9938	78.6	5.5	5.4	8.2
Antipyrine	0.1	4.2	1	92.6	8.5	2.7	6.3
Asulam	10	-13.0	0.9962	11.6	18.6	7.7	19.3
Atenolol	25	-1.4	0.9979	91.1	5.3	1.9	10.0

Compound	MQL (ng L ⁻¹)	ME (%)	Linearity (R^2)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Atrazine	5	-8.3	0.9951	96.6	2.3	2.1	6.7
Atrazine desethyl	50	-6.1	0.9994	97.6	5.8	3.4	3.6
Atrazine desisopropyl	5	-12.4	0.9986	94.0	11.3	4.0	2.1
Atropine	5	-3.9	0.9953	112.2	7.3	3.4	16.8
Azoxystrobin	10	-5.2	0.9948	118.5	7.7	5.7	6.1
Benalaxyl	10	4.8	0.9963	75.6	6.3	6.0	7.7
Benfuracarb	50	20.4	0.9938	68.6	12.2	14.2	9.5
Bensulfuron methyl	50	3.7	0.9951	115.8	7.6	4.5	10.0
Benzidine	10	-14.8	0.9975	48.3	4.0	2.6	35.1
Bitertanol	100	2.9	0.9967	93.8	12.9	7.4	7.1
Boscalid	50	-10.3	0.9959	99.2	3.1	4.9	6.8
Bromacil	50	-18.8	0.9984	108.6	14.2	6.9	8.5
Bromuconazole Isomer 1	50	-4.1	0.9974	104.3	5.2	6.8	8.8
Bromuconazole Isomer 2	50	-7.2	0.9914	111.9	11.6	5.1	8.3
Bupirimate	10	1.1	0.9997	62.4	5.4	4.8	7.8
Buprofezin	5	-4.9	0.9943	62.7	4.0	2.4	4.6
Bupropion	5	-47.7	0.9997	54.6	13.0	2.5	14.4
Butocarboxim	10	-21.3	0.9965	67.4	5.5	5.1	13.2
Butoxycarboxim	10	-2.2	0.9992	88.8	12.0	8.7	11.7
Buturon	10	-0.7	0.9946	100.9	4.5	7.7	9.8
Caffeine	30	-17.8	0.9987	100.2	6.9	4.0	16.0
Carbadox	100	-28.2	0.9988	106.1	16.5	9.1	9.9
Carbamazepine	5	-16.1	0.9946	105.8	7.9	2.9	7.6
Carbamazepine 10,11-Epoxyde	44.9	-10.8	0.9984	95.8	3.2	3.3	9.2
Carbendazim	1	-7.0	0.9987	100.9	5.9	3.4	15.4
Carboxine	50	-8.5	0.9916	74.2	13.6	4.6	9.4

Compound	MQL (ng L⁻¹)	ME (%)	Linearity (<i>R</i>²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Chlorbromuron	10	-7.6	0.997	107.9	3.6	6.9	7.9
Chlordimeform	10	-8.4	0.9478	70.6	13.4	8.9	6.1
Chlorfenvinphos	10	-0.8	0.9929	80.6	13.2	3.1	5.7
Chloridazon (Pyrazon)	5	-26.2	0.9955	118.4	11.6	4.5	16.4
Chlorotoluron	2.5	-19.3	0.999	104.2	7.3	1.3	12.8
Chloroxuron	5	0.2	0.9953	108.1	12.6	7.0	4.8
Chlorpyrifos ethyl	50	-17.3	0.9957	105.2	11.9	10.6	18.4
Chlorpyrifos methyl	50	-0.5	0.9974	94.0	7.4	8.2	15.0
Chlorsulfuron	5	-16.4	0.9947	112.6	14.1	5.2	7.5
Cinosulfuron	10	-12.6	0.9969	119.0	11.0	4.0	5.3
Citalopram	2.9	-5.2	0.9964	97.7	7.4	4.5	11.6
Clarithromycin	45.9	-9.8	0.9925	71.2	9.0	6.2	11.4
Clenbuterol	5	-6.0	0.9993	95.9	12.1	3.3	7.4
Clomazone	5	-5.2	0.9954	81.5	9.7	4.1	7.9
Clomiphene isomer 1	100	44.0	0.976	81.1	9.5	4.7	18.0
Clomiphene isomer 2	100	55.0	0.975	90.7	11.5	12.0	25.1
Clothianidin	50	-35.0	0.9969	110.3	16.6	7.9	13.5
Clotrimazole	10	-13.3	0.9959	105.8	4.0	4.9	4.9
Cloxacillin	100	-9.2	0.9999	17.4	56.2	11.4	16.0
Cocaine	100	60.9	0.9681	126.8	7.2	5.4	30.5
Codeine	5	3.1	0.9959	95.2	1.3	1.8	10.9
Cotinine	7.1	-11.5	0.9951	89.3	1.9	5.1	8.8
Coumaphos	10	0.2	0.9905	74.8	8.0	5.4	7.5
Cyanazine	10	-15.2	0.9965	108.4	6.1	6.0	15.5
Cycloate	5	0.2	0.9951	45.8	17.9	3.7	10.8
Cyproconazole	10	0.0	0.9957	99.4	5.3	4.7	7.6

Compound	MQL (ng L⁻¹)	ME (%)	Linearity (R²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Cyprodinil	5	-0.9	0.9951	96.7	4.9	2.4	3.5
Cyromazine	50	-2.8	0.9972	92.5	5.0	4.8	12.1
Danofloxacin	10	-12.8	0.9971	72.2	8.0	9.1	5.8
DEET	2.2	0.4	0.9934	81.4	10.1	3.1	2.9
Demeclocycline	100	-39.1	0.9979	0.0	-	-	17.6
Desmetryn	5	-4.4	0.9981	98.8	9.1	5.6	7.2
Diazepam	1.6	-0.6	0.9999	99.0	1.4	3.1	12.0
Diazinon	5	3.5	0.9957	80.4	9.4	2.6	7.1
Dichlorvos	10	-12.5	0.9987	30.1	16.3	3.6	12.5
Diclofenac	10	2.7	0.9937	110.7	10.9	2.9	8.7
Dicrotophos	5	-2.2	0.9978	111.9	16.7	7.3	9.7
Diethofencarb	50	-13.1	0.9997	115.2	11.3	5.5	17.0
Difenacoum	50	-6.2	0.9914	76.8	12.7	7.8	4.1
Difenoconazole	50	-7.6	0.9955	74.8	7.8	2.4	8.4
Difenoxyuron	10	-5.1	0.9912	109.8	6.1	5.2	7.0
Diflufenican	10	-13.6	0.9971	82.5	4.8	3.9	16.7
Dimethametryn	5	3.0	0.994	100.7	6.1	5.0	4.6
Dimethenamid	5	-1.0	0.994	100.8	9.4	6.3	6.0
Dimethomorph E	50	-10.1	0.9987	118.8	2.8	2.8	3.8
Dimethomorph Z	50	-5.8	0.9906	115.1	2.0	5.4	5.8
Dimoxystrobin	50	-1.9	0.9999	112.0	4.1	6.6	10.5
Diniconazole	5	-1.1	0.996	73.4	5.2	4.6	6.6
Diphenhydramine	10	-12.7	0.9951	83.6	13.9	4.5	5.4
Diphenylamine	5	5.5	0.9916	82.7	9.1	6.2	8.5
Diuron	5	-9.2	0.9952	101.4	7.9	3.2	9.3
Edifenphos	50	16.9	0.9473	175.3	21.7	12.9	48.2

Compound	MQL (ng L⁻¹)	ME (%)	Linearity (<i>R</i>²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Enoxacin	50	-13.3	0.9999	52.6	6.4	4.5	5.3
Eprosartan mesylate	6.1	-27.9	0.9985	84.4	9.6	4.5	6.5
Erythromycin	10	-12.2	0.9954	130.7	10.0	3.7	9.8
Ethiofencarb sulfoxide	10	2.2	0.9964	71.3	5.1	6.0	11.3
Ethion	50	-16.0	0.9976	65.1	14.6	8.7	5.8
Ethiprole	5	-7.6	0.9992	103.8	9.1	6.5	13.0
Ethoprophos	5	-2.7	0.9983	80.8	7.5	2.9	5.4
Ethoxyquin	50	-29.9	0.9962	0.0	-	8.5	18.8
Etrimphos	10	-2.3	0.9996	88.3	7.5	4.5	7.1
Famphur	10	-16.9	0.9983	111.9	4.9	3.0	16.2
Fenamiphos	5	0.5	0.9995	108.7	4.6	3.6	9.8
Fenarimol	5	-8.8	0.996	118.0	4.6	4.2	1.4
Fenazaquin	5	-42.0	0.99	77.9	15.7	5.4	12.7
Fenhexamid	5	-9.2	0.9989	112.6	10.1	3.7	5.5
Fenobucarb	50	4.1	0.9997	108.0	9.7	2.0	7.6
Fenoxycarb	50	-4.9	0.9977	118.0	7.8	5.7	5.7
Fenpropidine	5	-10.9	0.9956	93.5	10.3	2.1	12.2
Fenpropimorphe	5	-17.2	0.9902	80.0	10.4	7.2	6.8
Fensulfothion	5	-7.5	0.9993	108.7	7.4	3.3	3.2
Fenthion	10	-6.9	0.9992	84.1	4.4	6.5	8.4
Fenuron	50	-12.2	0.9999	102.5	3.5	2.9	16.4
Flecainide	2.1	-19.3	0.9971	108.0	4.5	3.4	4.6
Fluazifop	50	-49.0	0.9795	184.2	7.1	7.6	19.5
Fluazifop-p-butyl	10	4.7	0.9947	83.1	7.4	6.5	19.5
Fluconazole	8.5	-21.1	0.9978	100.6	2.1	5.8	11.1
Flufenacet	50	-4.1	0.999	118.9	4.0	3.5	4.0

Compound	MQL (ng L⁻¹)	ME (%)	Linearity (<i>R</i>²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Flufenamic acid	10	-3.5	0.9998	116.7	5.7	3.1	6.3
Flumequine	10	-14.1	0.9988	90.4	7.8	4.9	6.4
Fluometuron	50	-7.0	0.9983	113.7	4.5	4.0	11.5
Fluroxypyr	100	-18.6	0.9956	117.6	7.9	10.6	8.9
Flutolanil	5	-8.6	0.9999	107.0	4.5	2.8	5.9
Flutriafol	1	-12.0	0.9987	114.5	6.1	3.5	4.0
Fosthiazate	5	-4.2	0.9976	105.3	9.4	3.0	11.5
Fuberidazole	5	-10.4	0.9994	110.6	2.6	2.3	10.2
Furmecyclox	10	-2.3	0.9997	81.5	5.5	4.1	1.6
Gabapentin	2	-6.3	0.9998	14.3	5.5	3.4	14.5
Gemfibrozil	23.2	-8.2	0.9999	108.6	7.1	1.7	10.4
Griseofulvin	5	-10.7	0.9987	115.6	7.7	3.3	6.8
Haloxyfop	50	-8.3	1	112.9	6.9	3.1	14.3
Heroin	100	10.7	0.8971	132.9	14.6	11.0	12.5
Hexazinone	5	-12.0	0.9947	116.6	5.2	3.8	14.0
Hexythiazox	10	-14.3	0.9965	89.4	9.7	13.0	7.0
Imazalil	50	-16.2	0.997	111.2	8.4	4.3	10.6
Imazamethabenz-methyl	10	-3.4	0.9996	113.4	4.2	4.6	4.7
Imazamox	5	-5.6	0.9997	76.2	8.6	3.1	8.6
Imazaquin	5	-7.4	0.9967	113.3	4.2	3.0	3.5
Indomethacine	50	9.1	0.9935	112.4	14.1	5.1	17.2
Ipconazole	10	-5.9	0.9975	111.6	4.4	4.8	7.1
Irbesartan	19.3	-11.5	0.9991	96.8	1.7	2.9	18.6
Isocarboxiphos	10	97.3	0.9829	102.5	15.0	9.6	32.2
Isoprocab	100	-11.2	0.9999	96.0	14.0	3.2	19.6
Isoproturon	2.9	-2.7	0.9991	111.6	4.4	2.9	8.7

Compound	MQL (ng L⁻¹)	ME (%)	Linearity (<i>R</i>²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Isoxaben	5	-7.3	0.997	111.4	7.3	6.1	5.2
Karbutilate	50	-5.6	0.997	102.0	7.8	5.0	18.6
Ketamine	10	-10.8	0.9975	93.4	1.8	4.2	13.0
Ketoprofen	37.1	-1.1	0.9999	112.4	4.6	3.3	7.9
Lamotrigine	5	-37.0	0.999	99.0	1.5	2.3	10.3
Lenacil	100	-7.6	0.9994	103.0	11.5	14.1	8.4
Leucomalachite green	50	-33.0	0.9968	0.0	-	6.0	13.9
Levofloxacin	41.5	-4.9	0.9988	108.1	4.9	4.3	15.2
Lidocaine	2.1	-7.5	0.9962	95.1	3.8	1.3	12.9
Lincomycin	50	-13.2	0.999	109.4	5.9	10.0	17.0
Linuron	50	-11.8	0.9989	113.2	7.9	4.8	7.8
Malachite green	10	-6.6	0.9967	108.8	9.5	3.4	11.3
MDA	100	0.2	0.9995	62.5	17.7	10.9	12.1
MDEA	10	-6.5	0.9984	91.0	1.4	3.9	16.1
MDMA	50	-4.5	0.9993	86.3	2.1	3.8	11.6
Mebendazole	50	-6.8	0.9962	111.4	5.0	3.2	7.2
Meclofenamic acid	50	0.0	0.9991	94.7	6.8	5.7	5.1
Mefenacet	5	-2.7	0.9999	117.7	7.3	4.1	5.7
Mefenamic acid	5	-2.7	0.9994	94.6	9.8	4.7	3.8
Mepivacaine hydrochloride	10	-7.2	0.9982	93.2	4.0	1.9	18.1
Metalaxyl	10	-9.9	0.9993	108.2	6.8	6.5	9.3
Metamitron	5	-17.1	0.9998	115.6	7.0	2.4	9.2
Metazachlor	50	-8.5	0.9977	112.8	9.9	9.9	1.0
Metformin	10	10.5	0.9993	12.7	7.5	3.3	14.3
Methabenzthiazuron	1	-12.2	0.9992	110.9	7.2	3.1	10.0
Methadone	10	-9.3	0.9956	100.0	5.6	3.3	2.3

Compound	MQL (ng L ⁻¹)	ME (%)	Linearity (R^2)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Methamidophos	50	-1.1	0.9993	0.0	-	1.8	14.1
Methamphetamine	10	3.0	0.999	58.1	11.5	1.8	13.4
Methidathion	10	-17.1	0.998	102.2	3.7	4.2	7.2
Metobromuron	10	-14.4	0.9984	103.0	4.6	4.4	17.2
Metolachlor	10	-1.7	0.9992	105.4	8.3	2.8	1.4
Metoxuron	5	-13.1	0.9997	117.1	5.7	4.0	19.8
Metribuzin	3.6	-10.9	0.998	108.0	4.6	4.4	13.1
Metronidazole	5	-8.3	0.9997	113.3	6.1	3.5	8.9
Mevinphos	50	-11.0	0.9998	88.9	4.9	6.4	15.9
Miconazole	50	-25.6	0.9938	83.0	14.9	10.7	15.2
Molinate	5	1.3	0.9989	32.7	16.6	2.7	4.1
Monocrotophos	10	-13.2	0.9998	88.2	9.3	8.6	14.4
Monolinuron	5	-17.8	0.9998	91.9	2.9	1.6	14.4
Monuron	5	-14.2	0.9988	93.6	4.4	2.9	15.3
Morphine	5	-9.6	0.9994	79.7	4.6	5.6	8.7
Myclobutanil	5	-1.8	0.9986	102.0	4.8	2.6	5.0
Nadolol	50	-9.8	0.9995	105.8	4.6	3.2	10.9
Naptalam	50	-6.1	0.9978	92.4	10.4	5.1	18.2
Neburon	5	3.8	0.9957	107.6	3.1	2.0	13.2
Nicotine	33.7	-24.0	0.9991	110.9	14.3	2.3	16.7
Nifuroxazide	5	-24.1	0.9989	82.1	3.6	1.7	5.8
Nitenpyram	50	-6.9	0.9978	97.6	7.1	7.6	12.3
Norflurazon	5	-12.5	0.9996	92.1	3.8	3.7	6.4
Norpseudophedrine (Cathine)	11.3	4.5	0.9985	69.3	18.9	3.0	18.1
Nuarimol	10	-3.2	0.9991	101.4	2.0	3.7	10.5
O-desmethylvenlafaxine	5	27.1	1	98.7	3.7	3.3	13.6

Compound	MQL (ng L ⁻¹)	ME (%)	Linearity (<i>R</i> ²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Ofurace	50	-11.5	0.999	107.5	3.0	6.2	13.9
Omethoate	50	13.6	0.9989	106.5	12.9	5.9	10.5
Oxadiazon	50	-9.0	0.9984	85.1	6.6	17.5	16.2
Oxadixyl	50	-16.3	0.9942	93.0	6.4	7.5	19.4
Oxfendazole	5	-21.6	0.9988	90.7	6.7	2.4	5.0
Oxolinic acid	50	-16.6	0.9975	93.7	6.7	6.3	4.5
Oxytetracycline	50	-37.5	0.9976	0.0	-	8.5	12.6
Paclbutrazol	10	1.4	0.9963	102.7	5.5	3.6	12.6
Paracetamol (Acetaminophen)	10	-3.6	0.9998	97.0	5.1	2.6	5.6
Pebulat	5	0.7	0.9994	24.8	11.6	2.8	18.2
Penconazole	5	-1.6	0.9973	101.8	4.4	2.7	12.1
Pencycuron	5	-0.5	0.9986	100.5	6.9	2.9	13.8
Phosalone	50	0.3	0.9993	56.5	9.8	6.7	16.9
Picloram	10	-12.8	0.9995	14.5	22.9	5.0	13.4
Picolinafen	50	-17.7	0.9957	75.1	9.7	9.0	6.3
Pirimicarb	5	-4.8	0.9994	87.6	2.4	5.3	9.6
Pirimiphos methyl	5	-11.3	0.9994	117.7	6.5	2.0	14.8
Pretilachlor	50	-48.7	0.9988	112.7	5.7	8.5	14.1
Prochloraz	10	-6.5	0.9939	97.0	8.4	7.3	13.3
Promecarb	100	5.8	0.9989	110.7	5.6	8.5	14.1
Prometon	1	-6.7	0.9995	89.4	4.5	0.9	3.8
Prometryn	2.2	6.5	0.9982	98.0	2.8	1.8	7.1
Propachlor	5	-6.5	0.9973	70.9	7.5	4.3	7.3
Propamocarb	5	11.5	0.9985	68.1	8.9	3.0	14.8
Propanil	10	-2.1	0.9997	99.3	7.9	3.1	6.5
Propazine	5	5.1	0.9996	94.3	6.1	3.3	6.6

Compound	MQL (ng L⁻¹)	ME (%)	Linearity (<i>R</i>²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Propiconazole	10	-6.3	0.9979	112.8	3.9	6.3	16.4
Propoxur	10	-8.3	0.9993	119.7	14.7	12.6	17.7
Propranolol	3.5	-11.7	0.9955	102.5	2.8	6.4	3.4
Propyzamid	50	0.1	0.9987	97.0	6.8	5.3	4.8
Proquinazid	5	-14.1	0.9977	60.0	3.7	5.0	11.3
Prosulfocarb	10	-12.5	0.997	113.1	5.2	3.0	11.1
Prosulfuron	50	-14.1	0.9968	93.5	6.5	6.7	17.5
Pymetrozin	10	-2.0	0.9995	97.4	3.1	0.7	7.9
Pyraclostrobin	50	-1.4	0.9968	90.8	3.2	2.0	14.1
Pyranocoumarin	5	0.5	0.9979	142.9	4.7	6.3	5.5
Pyrazophos	5	2.0	0.9973	80.4	8.3	3.9	16.3
Pyridaben	50	-27.7	0.9984	126.4	10.6	14.5	4.5
Pyridaphenthion	10	-7.7	0.9999	112.1	4.4	2.4	12.0
Pyrimethanil	5	-6.5	0.9987	83.6	0.7	1.4	1.8
Pyriproxifen	10	9.3	0.9979	0.0	-	6.3	4.6
Pyroquilon	5	-16.4	0.9992	106.0	6.3	3.8	17.3
Quinalphos	5	1.9	0.9989	110.1	4.7	1.8	12.7
Quinmerac	5	-13.2	0.9988	62.4	7.5	2.4	3.4
Quinoclamine	10	-18.3	0.9974	93.6	8.7	4.4	9.9
Quinoxifen	10	-6.1	0.9989	110.3	6.7	7.0	15.7
Ranitidine	10	3.2	0.9989	80.9	6.9	5.5	16.1
Rotenone	100	-35.9	0.9975	129.8	9.7	12.8	26.8
Roxithromycin	100	-16.5	0.9982	102.5	15.7	15.4	4.1
Simazine	3.1	-11.4	0.9995	95.8	6.8	3.7	2.4
Sotalol	5	-7.0	0.9998	100.4	2.4	6.7	6.9
Spiroxamine	10	-13.9	0.9967	93.6	5.0	5.1	11.4

Compound	MQL (ng L ⁻¹)	ME (%)	Linearity (<i>R</i> ²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Sulcotrione	100	-16.3	0.9993	82.6	7.4	3.6	13.0
Sulfabenzamide	50	-32.3	0.9954	112.5	15.2	4.8	15.8
Sulfacetamide	50	-3.7	0.9973	0.0	-	2.0	13.3
Sulfachloropyridazine	5	-25.7	0.9992	84.0	2.7	5.1	5.6
Sulfadiazine	10	-7.8	0.9999	86.8	2.7	7.1	15.3
Sulfadimethoxyn	5	-9.7	0.9964	102.2	4.5	1.7	6.1
Sulfadoxine	5	-13.0	0.9995	110.1	4.4	4.9	5.0
Sulfaguanidine	5	-17.3	0.9988	64.4	7.3	2.4	4.3
Sulfamerazine	5	-20.7	0.9968	95.7	4.6	1.9	14.0
Sulfamethazine	5	-14.7	0.9985	97.3	6.0	3.1	2.6
Sulfamethoxazole	5	-27.1	0.9977	97.5	4.3	3.6	11.3
Sulfamethoxypyridazine	5	-16.4	0.9991	105.5	3.5	4.2	11.6
Sulfamonomethoxine	10	-27.2	0.9973	91.3	5.1	2.7	6.8
Sulfapyridine	16.1	-11.4	0.9974	105.8	4.9	2.9	16.1
Sulfaquinoxaline	10	-28.5	0.9974	85.0	5.9	4.0	3.4
Sulfathiazole	5	-14.6	0.9989	86.5	6.6	3.6	13.4
Sulfisoxazol	10	-19.8	0.9996	92.7	5.0	3.9	9.7
Sulfometuron methyl	10	-14.9	0.9983	106.8	5.6	5.6	2.3
Sulfotep	5	-7.5	0.9996	63.7	9.2	4.7	19.9
Sulpiride	5	-20.8	0.999	103.5	3.8	3.3	16.5
Tebuconazole	4.9	-1.6	0.9971	110.4	3.6	4.8	12.8
Tebufenpyrad	50	-10.0	0.9989	87.8	2.8	10.3	9.7
Tebuthiuron	5	-6.9	0.9984	95.5	3.8	2.6	1.8
Telmisartan	5	-13.7	0.9861	96.7	2.2	2.0	17.9
Temephos	50	-8.0	0.996	20.6	12.1	8.3	19.0
Tepraloxydim	50	-3.5	0.9994	114.6	6.9	6.6	6.7

Compound	MQL (ng L⁻¹)	ME (%)	Linearity (<i>R</i>²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Terbumeton	5	-6.7	0.9995	89.4	4.5	0.9	3.8
Terbutaline	50	-7.4	0.9998	93.5	7.3	2.3	14.8
Terbutylazine	6.5	-0.9	0.9991	95.5	2.8	2.9	9.6
Terbutylazine desethyl	50	-4.5	0.9994	95.8	6.6	3.8	15.9
Terbutryn	1.8	-5.8	0.9982	97.7	2.8	1.9	5.6
Testosterone	10	-8.1	0.9986	99.7	4.7	3.2	8.9
Tetraconazole	5	-6.4	0.9989	99.4	1.9	3.2	12.8
Tetracycline	50	-31.5	0.9963	0.0	-	10.2	18.1
Theobromine	100	-1.9	0.9983	98.1	5.7	4.4	16.0
Theophylline	5	-10.5	0.9991	97.7	5.6	5.8	12.3
Thiabendazole	10	-12.9	0.9984	97.1	3.3	2.6	14.4
Thiacloprid	10	-19.4	0.9998	111.6	9.5	5.7	3.6
Thiamethoxam	50	-36.3	0.9997	115.5	10.8	4.2	7.0
Thiocyclam (hydrogenoxalate)	10	-1.5	0.9998	30.3	18.0	2.7	10.3
Thiodicarb	50	302.2	0.9986	104.6	20.0	12.6	33.3
Timolol	10	-10.5	0.9991	101.4	4.8	4.6	10.2
Tramadol	2.9	-28.9	0.9955	98.8	6.0	3.7	11.6
Triadimefon	5	-6.0	0.9985	112.8	6.9	2.8	4.7
Triadimenol	50	-25.6	0.9961	109.4	12.6	8.4	12.2
Triallat	50	-10.7	0.9938	85.9	14.4	5.7	5.0
Triasulfuron	5	-24.5	0.9998	107.4	3.2	3.1	12.7
Triazophos	5	-5.2	0.9964	118.5	3.6	4.1	9.8
Triazoxide	5	-6.2	0.9975	113.0	5.3	5.2	4.0
Tributyl phosphate	10	2.3	1	90.5	8.1	5.0	10.3
Triclocarban	50	-14.8	0.9966	129.2	11.4	5.4	11.1
Trietazine	5	-2.3	0.9998	89.6	3.1	2.8	10.3

Compound	MQL (ng L⁻¹)	ME (%)	Linearity (<i>R</i>²)	Recovery (%)	RSD (%)	Intraday precision (RSD, %)	Interday precision (RSD, %)
Triethyl phosphate	10	-2.8	0.996	99.4	6.7	2.6	3.8
Trifloxystrobin	50	20.3	0.998	98.2	10.1	14.0	14.5
Triflumizole	50	22.4	0.9305	54.2	17.7	18.7	33.5
Triflumuron	50	-6.4	0.9981	120.5	3.9	5.6	10.6
Trimethoprim	5	-14.1	0.9975	113.7	4.5	5.4	16.1
Trinexapac-ethyl	50	-16.9	0.9971	96.9	5.7	8.7	17.0
Valsartan	50	0.4	0.999	98.0	6.1	3.3	14.9
Venlafaxine	2.6	-11.8	0.998	105.6	2.6	4.1	3.1
Δ-9-THC	100	2.9	0.9946	81.4	8.6	9.8	16.2

Table S6. Overview of workflow steps and settings for data preprocessing with MS-DIAL.

Data collection	
MS1 tolerance	0.002 Da
MS2 tolerance	0.05 Da
Execute Rt corrections	False
Maximum charged number	2
Consider Cl and Br	True
Peak detection	
Minimum peak height	50000 amplitude
Mass slice width	0.05 Da
Smoothing method	Linear weighted moving average
Smoothing level	4 scan
Minimum peak width	8 scan
Spectrum deconvolution	
Sigma window value	0.5
MS/MS abundance cut off	0 amplitude
Exclude after precursor ion	True
Keep the isotopic ions until	5 Da
Keep the isotopic ions w/o MS2Dec	True
Identification	
MSP file	MoNA LC-MS/MS library
Accurate mass tol (MS1)	0.002 Da
Accurate mass tol (MS2)	0.05 Da
Rt tolerance	0 min
Spectrum amplitude cutoff (absolute)	0
Spectrum amplitude cutoff (relative)	0%
Dot product score	600
Weighted dot product score	600
Reverse dot product score	800
Matched spectrum percentage	80%
Minimum number of matched spectrum	4
Use Rt for scoring	False
Use Rt for filtering	False
Adduct ion	
Positive mode	$[M+H]^+$; $[M+NH_4]^+$; $[M+Na]^+$; $[M+2H]^{2+}$
Negative mode	$[M-H]^-$; $[M+Cl]^-$; $[M+FA-H]^-$; $[M-2H]^{2-}$
Alignment parameters	
Rt tolerance	0.2 min
MS1 tolerance	0.002 Da
Rt factor	0.5
MS1 factor	0.5
Peak count filter	0%
N% detected in at least one group	0%
Remove features based on blank information	True
Sample average / blank average	10 fold change

Keep reference matched metabolite features	True
Keep suggested (w/o MS2) metabolite features	False
Keep removable features and assign the tag	True
Gap filling by compulsion	True

Table S7. List of compounds determined by target analysis and concentration results. Detection frequency (DF, %), median concentrations, range of concentrations, and compound class.

Compound	DF (%) (n=36)	Median C (ng L ⁻¹)	Range (ng L ⁻¹)	Class
2,6-Dimethylaniline ^a	3	5.6	5.6	Chemical intermediate
4-Androsten-3,17-dione	3	264	264	Hormone
Acetamiprid	6	214	142 - 285	Insecticide
Acridine	14	4.3	1.8 - 11.5	Antibiotic
Albendazol-sulfoxide	3	51.4	51.4	Pharmaceutical TP
Antipyrine (phenazone)	50	14.8	1.2 - 741	Analgesic / anti-inflammatory
Atenolol	28	147	24.7 - 886	Beta-blocker
Atrazine	8	46.8	14.7 - 53.4	Herbicide
Atrazine desisopropyl	6	53.2	7.9 - 98.5	Pesticide TP
Azoxystrobin	3	310	310	Fungicide
Caffeine	97	269	30.2 - 8090	Stimulant
Carbamazepine	22	39.5	10.9 - 532	Anticonvulsant
Carbamazepine 10,11-Epoxyde	8	48.2	44.9 - 48.5	Pharmaceutical TP
Carbendazim	22	164	1.1 - 1055	Fungicide
Chlorotoluron	28	63.1	2.5 - 772	Herbicide
Citalopram	22	7.9	2.9 - 31.1	Antidepressant
Clarithromycin	6	251	45.9 - 457	Antibiotic
Cocaine	6	467	102 - 833	Drug of abuse
Codeine	25	62.2	9.5 - 119	Analgesic
Cotinine	64	63.2	7.1 - 1302	Nicotine TP
DEET	33	14.2	2.3 - 962	Insecticide
Diazepam	8	8.4	1.6 - 21.3	Anxiolytic
Diclofenac	14	1864	142 - 2281	Anti-inflammatory
Diuron	22	58.2	10.2 - 372	Herbicide
Eprosartan	22	114	6.2 - 480	Antihypertensive
Fenuron	8	178	172 - 387	Herbicide
Flecainide	47	24.9	2.1 - 317	Antiarrhythmic
Fluconazole	25	35.9	8.6 - 85.9	Antifungal
Flufenamic acid	14	105	47.7 - 225	Analgesic
Fluometuron	3	175	175	Insecticide
Gabapentin ^a	39	17.7	2.1 - 95.2	Anticonvulsant
Gemfibrozil	33	91.0	23.2 - 625	Lipid regulator
Hexazinone	6	20.4	9.8 - 32.0	Herbicide
Irbesartan	42	150	19.4 - 428	Antihypertensive
Isoproturon	14	34.5	3.0 - 55.6	Herbicide
Ketamine	6	31.6	23.1 - 40.0	Drug of abuse
Ketoprofen	11	158	37.1 - 379	Anti-inflammatory
Lamotrigine	50	36.9	8.6 - 198	Anticonvulsant
Levofloxacin	3	41.6	41.6	Antibiotic
Lidocaine	39	13.6	2.1 - 2994	Anesthetic

Compound	DF (%) (n=36)	Median C (ng L⁻¹)	Range (ng L⁻¹)	Class
MDEA	8	58.8	41.6 - 108	Drug of abuse
Mefenamic acid	3	100	100	Anti-inflammatory
Mepivacaine hydrochloride	8	37.9	36.5 - 117	Anesthetic
Metformin ^a	61	111	10.3 - 2031	Antidiabetic
Metribuzin	8	12.5	3.7 - 32.0	Herbicide
Metronidazole	3	13.3	13.3	Antibiotic
Morphine	3	38.4	38.4	Drug of abuse
Myclobutanil	6	21.4	21.1 - 21.7	Fungicide
Nicotine	25	118	33.7 - 2060	Stimulant
Norpseudophedrine (Cathine)	25	47.2	11.3 - 1542	Drug of abuse
<i>O</i> -desmethylvenlafaxine	64	82.5	5.4 - 337	Pharmaceutical TP
Oxolinic acid	3	247	247	Antibiotic
Paclitaxel	6	16.8	13.3 - 20.3	Fungicide
Paracetamol (Acetaminophen)	42	299	21.3 - 3856	Analgesic / anti-inflammatory
Penconazole	3	8.3	8.3	Fungicide
Prometryn	17	4.7	2.2 - 12.1	Herbicide
Propoxur	3	11.2	11.2	Insecticide
Propranolol	11	4.4	3.6 - 5.5	Beta-blocker
Pymetrozin	3	67.2	67.2	Insecticide
Pyrimethanil	8	6.7	6.2 - 17.3	Fungicide
Simazine	22	11.9	3.1 - 96.0	Herbicide
Sulfamethoxazole	22	64.4	20.2 - 117	Antibiotic
Sulfapyridine	8	20.2	16.2 - 21.6	Antibiotic
Sulpiride	39	359	85.0 - 1040	Antipsychotic
Tebuconazole	19	17.1	4.9 - 49.3	Fungicide
Telmisartan	22	150	74.8 - 381	Antihypertensive
Terbutylazine	8	9.8	6.6 - 22.8	Herbicide
Terbutryn	22	7.3	1.8 - 11.7	Herbicide
Tetraconazole	3	116	117	Fungicide
Theobromine	56	2108	112 - 29050	Caffeine TP
Theophylline	67	60.4	5.1 - 2316	Caffeine TP
Thiabendazole	8	260	246 - 302	Fungicide
Tramadol	67	102	2.9 - 1493	Analgesic / anti-inflammatory
Tributyl phosphate	100	86.8	16.2 - 3572	Plasticizer / flame retardant
Triethyl phosphate	44	151	19.7 - 3004	Plasticizer / flame retardant
Trimethoprim	42	28.8	8.9 - 89.3	Antibiotic
Valsartan	42	424	59.4 - 1501	Antihypertensive
Venlafaxine	53	14.0	2.6 - 297	Antidepressant

^a Compounds with a recovery rate below 20%. Concentration values should be considered as estimated.