

Article

Multi-Target Analysis and Suspect Screening of Xenobiotics in Milk by UHPLC-HRMS/MS

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Table S1. Information and physicochemical properties of the 245 target analytes.

Compound	Type of compound	Molecular formula	Exact mass (g/mol)	log P	pKa	RT (min)	Commercial vendor	Purity (%)	Solvent
[M-H]									
2,4-Dinitrophenol	Pharmaceutical/Antiseptic	C ₆ H ₄ N ₂ O ₅	184.012021	1.67	4.1	2.77	Sigma-Aldrich	99	MeOH
2,6-Di-tB-4-DMAMP	Industrial chemical/Antioxidant	C ₁₇ H ₂₉ NO	262.21764	-	11.2	10.23	Sigma-Aldrich	99	MeOH
Atorvastatin	Pharmaceutical/ Anti-cholesterol	C ₃₃ H ₃₅ FN ₂ O ₅	558.25300	4.3	5.4	10.33	Sigma-Aldrich	98	DMSO
Bentazone	Herbicide	C ₁₀ H ₁₂ N ₂ O ₃ S	240.05686	2.0	0.8	2.80	Sigma-Aldrich	99.9	AcN
Bicalutamide	Pharmaceutical/ Anticarcinogenic	C ₁₈ H ₁₄ F ₄ N ₂ O ₄ S	430.061041	2.5	12	11.10	Sigma-Aldrich	99	MeOH
BPA	Industrial chemical/Plastic component	C ₁₅ H ₁₆ O ₂	227.10775	3.3	9.6	9.30	Sigma-Aldrich	99	MeOH
Butylparaben	Industrial chemical/Antifungal	C ₁₁ H ₁₄ O ₃	193.08702	8.5	3.0	10.63	Sigma-Aldrich	99.9	MeOH
Clofibric acid	Pharmaceutical/ Lipid-regulating	C ₁₀ H ₁₁ ClO ₃	214.03967	3.4	2.9	4.80	MP bio-medicals	100	MeOH
Efavirenz	Pharmaceutical/ Antiretroviral	C ₁₄ H ₉ ClF ₃ N ₂ O ₂	315.027391	4.6	10.2	12.51	Sigma-Aldrich	99	MeOH
Estriol	Pharmaceutical/Estrogenic	C ₁₈ H ₂₄ O ₃	287.16527	2.4	10.5	5.99	Sigma-Aldrich	99	MeOH
Flufenoxuron	Insecticide	C ₂₁ H ₁₁ ClF ₆ N ₂ O ₃	488.03624	10.1	6.2	13.77	Sigma-Aldrich	98.1	AcN
Flutamide	Pharmaceutical/ Anticarcinogenic	C ₁₁ H ₁₁ F ₃ N ₂ O ₃	276.072177	3.3	13.1	11.85	Sigma-Aldrich	99	MeOH
Furosemide	Pharmaceutical/ Sulphonamide	C ₁₂ H ₁₀ ClN ₂ O ₅ S	330.00772	2.1	3.8	4.30	Sigma-Aldrich	99	MeOH
Hydrochlorothiazide	Pharmaceutical/ Thiazide	C ₇ H ₈ ClN ₃ O ₄ S ₂	296.96447	7.9; 9.2	-0.1	2.43	Sigma-Aldrich	> 95.0	MeOH
MBP	Industrial chemical/Plasticizer	C ₁₂ H ₁₄ O ₄	221.08193	2.4	-	3.98	Sigma-Aldrich	99	MeOH
Mecoprop	Herbicide	C ₁₀ H ₁₁ ClO ₃	214.03967	3.8	3.1	4.82	Sigma-Aldrich	99.6	MeOH
Monensin	Pharmaceutical/Antibiotic	C ₃₆ H ₆₂ O ₁₁	669.42194	5.4	6.6	15.14	Sigma-Aldrich	99	MeOH
Monobenzyl phthalate	Industrial chemical/Plasticizer	C ₁₅ H ₁₂ O ₄	255.06628	3	3.1	4.58	Sigma-Aldrich	99	MeOH
Nitrofurantoin	Pharmaceutical/ Antibiotic	C ₈ H ₆ N ₄ O ₅	238.03381	7.2	-0.5	3.32	Sigma-Aldrich	99.9	DMSO
Nonylphenol	Industrial chemical/Antioxidant	C ₁₅ H ₂₄ O	219.17544	5.8	10.3	13.84	Sigma-Aldrich	99	MeOH
PFBS	Industrial chemicals/ PFASs	C ₄ H ₉ O ₃ S	299.95026	-3.3	5.4	6.46	Sigma-Aldrich	98	MeOH
PFOA	Industrial chemicals/ PFASs	C ₈ HF ₁₅ O ₂	413.97369	-4.2	5.1	9.20	Sigma-Aldrich	99	MeOH
PFOS	Industrial chemicals/ PFASs	C ₈ HF ₁₇ O ₃ S	499.93750	-3.3	2.6	11.47	Sigma-Aldrich	97	MeOH
PFOSA	Industrial chemicals/ PFASs	C ₈ H ₂ F ₁₇ NO ₂ S	498.95349	3.4	4.8	13.16	Dr. Ehrestofer	99.5	MeOH
Pravastatin	Pharmaceutical/ Antilipemic	C ₂₃ H ₃₅ NaO ₇	424.24609	-	4.2	5.75	Sigma-Aldrich	100	MeOH
Propanil	Herbicide	C ₉ H ₉ Cl ₂ NO	217.006119	2.3	19.1	10.50	Sigma-Aldrich	99	MeOH
Propofol	Pharmaceutical/Anaesthetic	C ₁₂ H ₁₈ O	177.12849	3.8	11.1	12.90	Sigma-Aldrich	99	MeOH
Valsartan	Pharmaceutical/ Antihypertensive	C ₂₄ H ₂₉ N ₅ O ₃	436.23432	5.3	4.4; 8.3	5.85	Boehringer	99	MeOH
[M+H] ⁺									

2-HBT	Industrial chemicals/Corrosion inhibitor	C ₇ H ₅ NOS	152.01646	2.5	6.4	5.70	Sigma-Aldrich	99.9	MeOH
4,4-BDMABP	Industrial chemical/Photosensitizer	C ₁₇ H ₂₀ N ₂ O	269.16484	3.8	11.4	12.16	Sigma-Aldrich	99	MeOH
4-Hydroxytamoxifen	Metabolite/ Tamoxifen	C ₂₆ H ₂₉ NO ₂	388.22711	6.8	8.7	8.46	Sigma-Aldrich	100	MeOH
4-MBP	Industrial chemical/Coating agent	C ₁₄ H ₁₂ O	197.09609	-	7.35	12.53	Sigma-Aldrich	99	MeOH
4-PBZ	Industrial chemical/Coating agent	C ₁₉ H ₁₄ O	259.11174	-	-	13.50	Sigma-Aldrich	99	MeOH
Acetaminophen	Pharmaceutical/ Anti-inflammatory	C ₈ H ₉ NO ₂	152.07061	0.9	9.5	1.75	Fluka	99.9	MeOH
Acetamiprid	Herbicide	C ₁₀ H ₁₁ CIN ₄	223.07450	0.8	0.7	5.10	Sigma-Aldrich	100	MeOH
Acetochlor	Herbicide	C ₁₄ H ₂₀ ClNO ₂	270.12553	4.1	-	12.49	Sigma-Aldrich	95.2	MeOH
Acyclovir	Pharmaceutical/ Antiviral agent	C ₈ H ₁₁ N ₅ O ₃	226.09347	-1.6	2.3; 9.3	1.06	Sigma-Aldrich	100	DMSO
Alachlor	Herbicide	C ₁₄ H ₂₀ ClNO ₂	270.12553	3.5	-	12.49	Sigma-Aldrich	99.8	MeOH
Albendazole	Pharmaceutical/ Anthelmintic	C ₁₂ H ₁₅ N ₃ O ₂ S	266.09577	2.9	6.9	6.80	Sigma-Aldrich	100	DMSO
Amantadine	Pharmaceutical/ Antiviral, antiparkinsonian and antihyperalgesic	C ₁₀ H ₁₈ CIN	152.14338	2.4	10.7	1.68	Sigma-Aldrich	100	MeOH
Ambroxol	Pharmaceutical/ Anti mucolytic	C ₁₃ H ₁₈ Br ₂ N ₂ O	376.98586	2.7	0.7; 9.0; 15.3	3.70	Sigma-Aldrich	100	MeOH
Ametryn	Herbicide	C ₉ H ₁₇ N ₅ S	228.12774	2.6	0.5; 6.7; 14.6	6.90	Sigma-Aldrich	98.6	MeOH
Amiodarone	Pharmaceutical/ Anti-arrhythmic, Vasodilatory	C ₂₅ H ₃₀ ClI ₂ N ₃ O ₃	646.03096	7.6	8.5	11.53	Sigma-Aldrich	98	MeOH
Amitriptyline	Pharmaceutical/ Antidepressant	C ₂₀ H ₂₃ N	278.19033	4.8	9.8	6.48	Sigma-Aldrich	100	MeOH
Anastrozole	Pharmaceutical/ Anticarcinogenic	C ₁₇ H ₁₉ N ₅	294.17132	3.0	2.0	8.20	Sigma-Aldrich	98	AcN:H ₂ O (20:80)
Atenolol	Pharmaceutical/ β-blocker antihypertensive	C ₁₄ H ₂₂ N ₂ O ₃	267.17032	0.2	9.6	0.97	Sigma-Aldrich	> 95.0	MeOH
Atrazine	Herbicide	C ₈ H ₁₄ CIN ₅	216.10105	2.2	4.2	8.90	Fluka	99	MeOH
Azelastine	Pharmaceutical/ Antihistaminic	C ₂₂ H ₂₅ Cl ₂ N ₃ O	382.16807	4.0	8.9	6.79	Sigma-Aldrich	98	MeOH
Azithromycin	Pharmaceutical/ Antibiotic	C ₃₈ H ₇₂ N ₂ O ₁₂	749.51580	2.4	12.4	3.97	Sigma-Aldrich	95	MeOH
Azoxystrobin	Fungicide	C ₂₂ H ₁₇ N ₃ O ₅	404.12410	4.2	1.9	11.88	Sigma-Aldrich	99.3	MeOH
BBP	Industrial chemical/Plasticizer	C ₁₉ H ₂₀ O ₄	313.14344	4.7	-	13.48	Sigma-Aldrich	99	MeOH
BEHA	Industrial chemical/Plasticizer	C ₂₂ H ₄₂ O ₄	371.31559	8.1	-	15.93	Sigma-Aldrich	99	MeOH
BEHP	Industrial chemical/Plasticizer	C ₂₄ H ₃₈ O ₄	391.28429	7.6	3.1	15.87	Sigma-Aldrich	99	MeOH
Bendiocarb	Insecticide	C ₁₁ H ₁₃ NO ₄	224.09173	1.6	14.8	8.10	Sigma-Aldrich	99.9	MeOH
Benzethonium	Pharmaceutical/ Bactericide	C ₂₇ H ₄₂ ClNO ₂	412.32101	-0.5	-	11.85	Sigma-Aldrich	99	MeOH
Benzophenone	Industrial chemical/UV filter	C ₁₃ H ₁₀ O	183.08044	3.2	11.3	11.75	Sigma-Aldrich	99	MeOH
Benzothiazole	Food additive	C ₇ H ₅ NS	136.02155	2.1	2.3	6.50	Sigma-Aldrich	97	MeOH
Bezafibrate	Pharmaceutical/ Lipid-regulating	C ₁₉ H ₂₀ ClNO ₄	362.11536	4.0	3.8	10.47	MP bio-medicals	98	MeOH
Bisoprolol	Pharmaceutical/ β-blocker antihypertensive	C ₁₈ H ₃₁ NO ₄	283.11761	1.9	9.3	8.18	Sigma-Aldrich	95.0	MeOH

BMGP	Industrial chemical/Plasticizer	C ₁₄ H ₁₈ O ₆	282.11034	1.11	-	-	Sigma-Aldrich	99	MeOH
Boscalid	Fungicide	C ₁₈ H ₁₂ Cl ₂ N ₂ O	343.03994	4.9	14.3	12.02	Sigma-Aldrich	99.9	MeOH
Bosentan	Pharmaceutical/ Hypertensive	C ₂₇ H ₂₉ N ₅ O ₆ S	552.19113	4.9	5.8	12.04	Sigma-Aldrich	98	MeOH
Bupropion	Pharmaceutical/ Antidepressant	C ₁₃ H ₁₉ Cl ₂ N ₂ O	240.11497	3.3	8.2, 18.3	4.10	Sigma-Aldrich	100	MeOH
Caffeine	Lifestyle products/ Stimulant	C ₈ H ₁₀ N ₄ O ₂	195.08765	-1.2	-0.6	2.50	Sigma-Aldrich	98	MeOH
Caprolactam	Industrial product	C ₆ H ₁₁ NO	114.09134	-0.2	8.2	2.35	Sigma-Aldrich	99	MeOH
Captopril	Enzymatic inhibitor	C ₉ H ₁₅ NO ₃ S	218.08454	0.3	3.7, 9.8	4.00	Sigma-Aldrich	> 95.0	MeOH
Carbamazepine	Pharmaceutical/ Antidepressant	C ₁₅ H ₁₂ N ₂ O	237.10224	2.8	16.0	7.80	Sigma-Aldrich	100	MeOH
Carbaryl	-	C ₁₂ H ₁₁ NO ₂	202.08626	2.5	14.8	8.63	Sigma-Aldrich	99.9	MeOH
Carbendazim	Fungicide	C ₉ H ₉ N ₃ O ₂	192.07675	1.8	9.7	1.50	Sigma-Aldrich	99.5	DMSO
Celecoxib	Pharmaceutical/ Anti-inflammatory	C ₁₇ H ₁₄ F ₃ N ₃ O ₂ S	382.08316	-	11.1	12.50	Sigma-Aldrich	99	MeOH
Cetirizine	Pharmaceutical/ Antihistaminic	C ₂₁ H ₂₅ ClN ₂ O ₃	389.16265	-	2.7; 3.6; 7.6	7.40	Sigma-Aldrich	99	MeOH
Chloridazon	Herbicide	C ₁₀ H ₈ ClN ₃ O ₂	222.04287	1.1	3.4	4.55	Sigma-Aldrich	99.8	MeOH
Chloroxuron	Herbicide	C ₁₅ H ₁₅ ClN ₂ O ₂	291.08948	3.4	14.0	11.58	Sigma-Aldrich	98.8	MeOH
Chlortoluron	Herbicide	C ₁₀ H ₁₃ ClN ₂ O	213.07892	2.4	13.5	8.60	Sigma-Aldrich	99.5	MeOH
Ciprofloxacin	Pharmaceutical/Fluoroquinolone	C ₁₇ H ₁₈ FN ₃ O ₃	332.14050	-0.8	5.7; 8.7	2.40	Fluka	99.9	MeOH
Clarithromycin	Pharmaceutical/ Antibiotic	C ₃₈ H ₆₉ NO ₁₃	748.48417	3.2	12.5	7.92	Sigma-Aldrich	100	DMSO
Clomazone	Herbicide	C ₁₂ H ₁₄ ClNO ₂	240.07858	2.9	3.9	10.40	Sigma-Aldrich	98.3	MeOH
Clomipramine	Pharmaceutical/ Antidepressant	C ₁₉ H ₂₃ ClN ₂	315.16225	4.9	9.2	7.82	Sigma-Aldrich	98	MeOH
Clonidine	Pharmaceutical/ Hypertensive	C ₉ H ₉ Cl ₂ N ₃	230.02463	2.5	8.2	1.47	Sigma-Aldrich	99	MeOH
Clopidogrel	Pharmaceutical/ Anticoagulant	C ₁₆ H ₁₆ ClNO ₂ S	322.06630	3.8	5.3	11.86	Sigma-Aldrich	100	MeOH
Clozapine	Pharmaceutical/ Antipsychotic	C ₁₈ H ₁₉ ClN ₄	327.13710	3.4	3.9; 7.4	4.54	Sigma-Aldrich	100	MeOH
Cortisone	Pharmaceutical/ corticoid	C ₂₁ H ₂₈ O ₅	361.20095	1.7	12.6	7.12	Sigma-Aldrich	98	MeOH
Cotinine	Metabolite/ Nicotine	C ₁₀ H ₁₂ N ₂ O ₃ S	177.10224	0.2	4.8	1.00	Sigma-Aldrich	98.5	MeOH
Crotamiton	Pharmaceutical/ Scabicide, Antipruritic	C ₁₃ H ₁₇ NO	204.13829	2.8	1.2	10.43	Sigma-Aldrich	97	EtOH
Cyclophosphamide	Pharmaceutical/ Anticarcinogenic	C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P	261.03210	0.1	13.4	5.40	Sigma-Aldrich	100	MeOH
Cyproterone	Hormone/ Progesterone derivate	C ₂₂ H ₂₇ ClO ₃	375.17215	3.1	9.7	11.75	Toronto Research Chemicals	100	MeOH
Danofloxacin	Pharmaceutical/Fluoroquinolone	C ₁₉ H ₂₀ FN ₃ O ₃	358.15615	0.1	5.6; 6.7	2.62	Sigma-Aldrich	99	MeOH
DBP	Industrial chemical/Plasticizer	C ₁₆ H ₂₂ O ₄	279.15909	4.5	3.8	13.59	Sigma-Aldrich	99	MeOH
DCHP	Industrial chemical/Plasticizer	C ₂₀ H ₂₆ O ₄	331.19039	4.14	7.3	14.32	Sigma-Aldrich	99	MeOH
DEAB	Industrial chemical/Photochemical	C ₂₁ H ₂₈ N ₂ O	325.22744	-	2.55	13.51	Sigma-Aldrich	99	MeOH

DEP	Industrial chemical/Plasticizer	C ₁₂ H ₁₄ O ₄	222.08921	2.42	3.1	9.28,10.72	Sigma-Aldrich	99	MeOH
Desloratadine	Metabolite/ Loratadine	C ₁₉ H ₁₉ ClN ₂	311.13095	4.5	-	3.53	Sigma-Aldrich	100	MeOH
DETX	Industrial product/Coating	C ₁₇ H ₁₆ OS	269.09946	-	-	14.30	Sigma-Aldrich	99	MeOH
Dexamethasone	Pharmaceutical/ Anti-inflammatory	C ₂₂ H ₂₉ FO ₅	393.20718	1.7	12.4	8.30	Sigma-Aldrich	98	MeOH
Diazepam	Pharmaceutical/Sedative	C ₁₆ H ₁₃ ClN ₂ O	285.07892	2.82	3.4	10.50	Sigma-Aldrich	> 95.0	MeOH
Dichlorvos	Pesticide	C ₄ H ₇ Cl ₂ O ₄ P	220.95318	1.4	9.1	7.28	Sigma-Aldrich	99	MeOH
Diethyl Toluamide	Insecticide	C ₁₂ H ₁₇ NO	192.13829	2.5	-1.0	9.35	Sigma-Aldrich	98.8	MeOH
Diflufenican	Herbicide	C ₁₉ H ₁₁ F ₅ N ₂ O ₂	395.08135	5.1	13.3	13.35	Sigma-Aldrich	98.3	AcN
Dimethachlor	Herbicide	C ₁₃ H ₁₈ ClNO ₂	256.10988	2.6	1.6	10.25	Sigma-Aldrich	99.8	AcN
Dimethoate	Insecticide	C ₅ H ₁₂ NO ₃ PS ₂	230.00690	0.3	15.9	4.82	Sigma-Aldrich	99.8	MeOH
Diphenhydramine	Pharmaceutical/ Antihistaminic	C ₁₇ H ₂₂ ClNO	256.16959	3.7	8.9	5.47	Sigma-Aldrich	100	MeOH
Diuron	Herbicide	C ₉ H ₁₀ Cl ₂ N ₂ O	233.02429	2.5	13.2	9.26	Fluka	98	MeOH
Domperidone	Pharmaceutical/ Antiemetic, Gastric prokinetic	C ₂₂ H ₂₄ ClN ₅ O ₂	426.16913	2.9	12.5	4.71	Sigma-Aldrich	98	DMSO
DOP	Industrial chemical/Plasticizer	C ₂₄ H ₃₈ O ₄	391.28429	8.1	7.3	15.87	Sigma-Aldrich	99	MeOH
Drospirenone	Pharmaceutical/ Hormonal	C ₂₄ H ₃₀ O ₃	367.22677	4.0	-	11.50	Sigma-Aldrich	100	MeOH
Duloxetine	Pharmaceutical/ Antidepressant	C ₁₈ H ₁₉ BOS	298.12601	4.2	9.7	6.45	Sigma-Aldrich	99.9	MeOH
EDAB	Industrial chemical/UV filter	C ₁₁ H ₁₅ NO ₂	194.11756	3.2	2.5	11.69	Sigma-Aldrich	99	MeOH
EDDP	Fungicide	C ₂₀ H ₂₄ ClNO ₄	278.19033	3.5	-	6.50	Sigma-Aldrich	100	MeOH
EHDAB	Industrial chemical/UV filter	C ₁₇ H ₂₇ NO ₂	278.21146	-	2.4	14.45	Sigma-Aldrich	99	MeOH
Enoxacin	Pharmaceutical/Fluoroquinolone	C ₁₅ H ₁₇ FN ₄ O ₃	321.13575	-0.2	5.5; 8.6	1.98	Sigma-Aldrich	99	MeOH
Enrofloxacin	Pharmaceutical/Fluoroquinolone	C ₁₉ H ₂₂ FN ₃ O ₃	360.17180	1.15	5.7; 6.7	2.82	Sigma-Aldrich	99	MeOH
Eprosartan	Pharmaceutical/ Hypertensive	C ₂₃ H ₂₄ N ₂ O ₇ S	425.15295	3.8	3.6; 6.7	5.00	Solvay Pharma	99	MeOH
Equilin	Pharmaceutical/Estrogenic	C ₁₈ H ₂₀ O ₂	269.15361	-	9.4	7.88	Sigma-Aldrich	99	MeOH
Erythromycin	Pharmaceutical/ Antibiotic	C ₃₇ H ₆₇ NO ₁₃	734.46852	3.1	12.5	6.39	Sigma-Aldrich	100	EtOH
Ethion	Pesticide	C ₉ H ₂₂ O ₄ P ₂ S ₄	384.99489	5.1	-	13.87	Sigma-Aldrich	97.6	MeOH
Exemestane	Pharmaceutical/ Anticarcinogenic	C ₂₀ H ₂₄ O ₂	297.18491	3.0	19.6	11.23	Sigma-Aldrich	100	MeOH
Fenoxycarb	Insecticide	C ₁₇ H ₁₉ NO ₄	302.13868	4.3	13.9	12.50	Sigma-Aldrich	100	AcN
Fenpropidin	Fungicide	C ₁₉ H ₃₁ N	274.25293	5.5	10.1	8.00	Sigma-Aldrich	97.3	Acetone
Fenpropimorph	Fungicide	C ₂₀ H ₃₃ NO	304.26349	5.2	6.7	8.23	Sigma-Aldrich	96	Acetone
Fenthion	Insecticide	C ₁₀ H ₁₅ O ₃ PS ₂	279.02730	4.1	-	13.00	Sigma-Aldrich	98.6	AcN
Finasteride	Pharmaceutical/Hair restorer	C ₂₃ H ₃₆ N ₂ O ₂	373.28495	3.0	14.5	11.13	Sigma-Aldrich	99.8	MeOH

Fluconazole	Pharmaceutical/ Antifungal	C ₁₃ H ₁₂ F ₂ N ₆ O	307.11134	0.6	12.7	3.91	Sigma-Aldrich	100	MeOH
Flumequine	Pharmaceutical/ Antibiotic	C ₁₄ H ₁₂ FNO ₃	262.08740	1.6	6.5	7.97	Sigma-Aldrich	99.1	AcN
Flusilazole	Fungicide	C ₁₆ H ₁₅ F ₂ N ₃ S _i	316.10761	3.7	2.5	12.12	Sigma-Aldrich	100	Acetone
Fluvoxamine	Pharmaceutical/ Antidepressant	C ₁₅ H ₂₁ F ₃ N ₂ O ₂	319.16279	3.2	8.9	7.00	Sigma-Aldrich	100	MeOH
Gabapentin	Pharmaceutical/Antiepileptic	C ₉ H ₁₇ NO ₂	172.13321	-1.1	3.7; 10.7	1.39	Sigma-Aldrich	100	MeOH
Genistein	Phytoestrogen	C ₁₅ H ₁₀ O ₅	271.06010	3.1	6.6; 8.0; 9.0	7.48	Extrasynthese	98	MeOH
Genistin	Phytoestrogen	C ₂₁ H ₂₀ O ₁₀	433.11292	0.8	7.3; 9.0; 12.5	4.21	Extrasynthese	99.9	MeOH
Glibenclamide	Pharmaceutical/Antidiabetic	C ₂₃ H ₂₈ ClN ₃ O ₅ S	494.15110	4.7	5.3	12.10	Sigma-Aldrich	> 95.0	MeOH
Glimepiride	Pharmaceutical/Antidiabetic	C ₂₃ H ₃₄ N ₄ O ₅ S	491.23227	3.9	4.3	12.48	Sigma-Aldrich	100	DMSO
Glycitin	Phytoestrogen	C ₂₂ H ₂₂ O ₁₀	447.12857	1.3	9.0; 12.2	3.43	Extrasynthese	99	MeOH
Hexazinone	Herbicide	C ₁₂ H ₂₀ N ₄ O ₂	253.16590	1.9	2.2	6.82	Sigma-Aldrich	100	MeOH
Hydrocortisone	Pharmaceutical/ corticoid	C ₂₁ H ₃₀ O ₅	363.21660	1.6	12.6	7.09	Sigma-Aldrich	98	MeOH
Hydroxychloroquine	Pharmaceutical/ Chemotherapeutic, Antibiotic	C ₁₈ H ₂₈ ClN ₃ O ₅ S	336.18372	?	9.7	0.98	Sigma-Aldrich	98	AcN:H ₂ O (60:40)
Ifosfamide	Pharmaceutical/ Anticarcinogenic	C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P	261.03210	0.9	13.2	5.42	Sigma-Aldrich	98	MeOH
Imatinib	Pharmaceutical/ Anticarcinogenic	C ₂₉ H ₃₁ N ₇ O	494.26629	3.5	12.5	4.02	Sigma-Aldrich	100	MeOH
Imazalil	Fungicide	C ₁₄ H ₁₄ Cl ₂ N ₂ O	297.05560	3.8	6.5	6.54	Sigma-Aldrich	99.3	Acetone
Imidacloprid	Insecticide	C ₉ H ₁₀ ClN ₅ O ₂	256.05958	0.8	1.5; 11.1	4.56	Sigma-Aldrich	99	MeOH
Iminostilbene	Pharmaceutical/ Antidepressant	C ₁₄ H ₁₁ N	194.09643	4	1.7	12.31	Sigma-Aldrich	100	MeOH
Imipramine	Pharmaceutical/ Antidepressant	C ₁₉ H ₂₄ N ₂	281.20123	4.3	9.2	6.80	Sigma-Aldrich	99	MeOH
Indometacin	Pharmaceutical/Anti-inflammatory	C ₁₉ H ₁₆ ClNO ₄	358.08406	4.3	4.5	12.14	Sigma-Aldrich	100	MeOH
Irbersartan	Pharmaceutical/ Hypertensive	C ₂₅ H ₂₈ N ₆ O	429.23974	5.5	4.1; 8.3	8.50	Sanofi	99	MeOH
Isoproturon	Herbicide	C ₁₂ H ₁₈ N ₂ O	207.14919	2.6	13.8	9.40	Fluka	99	MeOH
ITX	Industrial product/Packaging	C ₁₆ H ₁₄ OS	255.08381	5.6	-	13.88	Sigma-Aldrich	99	MeOH
Ketoconazole	Pharmaceutical/ Antifungal	C ₂₆ H ₂₈ Cl ₂ N ₄ O ₄	531.15604	4.3	4.0; 6.8	7.01	Sigma-Aldrich	99	MeOH
Ketoprofen	Pharmaceutical/ Anti-inflammatory	C ₁₆ H ₁₄ O ₃	255.10157	3.6	3.9	9.96	MP bio-medicals	99	MeOH
Lenacil	Herbicide	C ₁₃ H ₁₈ N ₂ O ₂	235.14410	1.7	10.7	7.92	Sigma-Aldrich	99.9	MeOH
Levofloxacin	Pharmaceutical/Fluoroquinolone	C ₁₈ H ₂₀ FN ₃ O ₄	362.15106	-	5.4; 6.2	2.16	Sigma-Aldrich	99	MeOH
Lidocaine	Pharmaceutical/ Anaesthetic	C ₁₄ H ₂₂ N ₂ O	235.18049	2.4	7.9	2.39	Sigma-Aldrich	99.0	MeOH
Linuron	Herbicide	C ₉ H ₁₀ Cl ₂ N ₂ O ₂	249.01921	3.2	11.9	11.16	Sigma-Aldrich	99.7	AcN
Lomefloxacin	Pharmaceutical/Fluoroquinolone	C ₁₇ H ₁₉ F ₂ N ₃ O ₃	352.14672	-	5.6; 8.7	2.61	Sigma-Aldrich	99	MeOH
Lorazepam	Pharmaceutical/ Anxiolytic	C ₁₅ H ₁₀ Cl ₂ N ₂ O ₂	321.01921	2.4	13.0	8.66	Sigma-Aldrich	95	MeOH

Losartan	Pharmaceutical/ Hypertensive	C ₂₂ H ₂₃ ClN ₆ O	423.16946	5.1	3.8; 8.3	9.06	Merck	98	MeOH
MBHB	Industrial chemical/Antioxidant	C ₁₆ H ₂₄ O ₃	265.17982	-	-	13.62	Sigma-Aldrich	99	MeOH
Mebendazole	Pharmaceutical/ Anthelmintic	C ₁₆ H ₁₃ N ₃ O ₃	296.10297	2.8	6.6	7.10	Sigma-Aldrich	100	DMSO
Mebeverine	Pharmaceutical/ Anticholinergic	C ₂₅ H ₃₆ ClNO ₅	430.25880	?	10.3	6.50	Sigma-Aldrich	100	MeOH
Meclocycline	Pharmaceutical/ Antibiotic	C ₂₉ H ₂₇ ClN ₂ O ₁₄ S	477.10592	?	8.2	5.25	Sigma-Aldrich	100	MeOH
Medroxyprogesterone	Pharmaceutical/ Anticarcinogenic	C ₂₂ H ₃₂ O ₃	345.24242	3.5	17.8	12.24	Sigma-Aldrich	98.6	MeOH
Mefenamic acid	Pharmaceutical/ Anti-inflammatory	C ₁₅ H ₁₅ NO ₂	242.11756	5.1	4.2	12.73	Sigma-Aldrich	98.5	DMSO
Memantine	Pharmaceutical/ Antiparkinsonian agent	C ₁₂ H ₂₂ ClN	180.17468	?	10.7	4.42	Sigma-Aldrich	98	MeOH
Metalaxyl	Fungicide	C ₁₅ H ₂₁ NO ₄	280.15433	1.7	14	9.40	Sigma-Aldrich	99.8	MeOH
Metamitron	Herbicide	C ₁₀ H ₁₀ N ₄ O	203.09274	0.8	1.5	4.10	Sigma-Aldrich	100	Acetone
Metazachlor	Herbicide	C ₁₄ H ₁₆ ClN ₃ O	278.10547	2.7	-	10.05	Sigma-Aldrich	99.4	MeOH
Metconazole	Fungicide	C ₁₇ H ₂₂ ClN ₃ O	320.15242	3.7	11.4	12.49	Sigma-Aldrich	98.9	AcN
Metformin	Pharmaceutical/ Antidiabetic	C ₄ H ₁₂ ClN ₅	130.10872	-2.6	12.4	0.92	Sigma-Aldrich	100	MeOH
Methiocarb	Pesticide	C ₁₁ H ₁₅ NO ₂ S	226.08963	2.9	14.8	10.98	Sigma-Aldrich	99.8	MeOH
Methotrexate	Pharmaceutical/ Anticarcinogenic	C ₂₀ H ₂₂ N ₈ O ₅	455.17859	-1.8	4.7	1.58	Sigma-Aldrich	100	H ₂ O + 10 µL NaOH
Methylparaben	Personal care product	C ₈ H ₈ O ₃	153.05462	1.7	8.5	5.30	Sigma-Aldrich	98	MeOH
Metolachlor	Herbicide	C ₁₅ H ₂₂ ClNO ₂	284.14118	3.1	16.8	12.46	Sigma-Aldrich	97.6	MeOH
Metoprolol	Pharmaceutical/ β-blocker antihypertensive	C ₁₅ H ₂₅ NO ₃	268.19072	?	14.1	3.17	Sigma-Aldrich	> 95.0	MeOH
Metribuzin	Herbicide	C ₈ H ₄ N ₄ OS	215.09611	1.7	1.0	7.40	Sigma-Aldrich	99	Acetone
Miconazole	Pharmaceutical/ Antibiotic	C ₁₈ H ₁₄ Cl ₄ N ₂ O	414.99330	5.3	6.8	9.81	Sigma-Aldrich	100	MeOH
Mirtazapine	Pharmaceutical/ Antidepressant	C ₁₇ H ₁₉ N ₃	266.16517	2.9	6.6	2.82	Sigma-Aldrich	99.9	MeOH
Montelukast	Pharmaceutical/ Antidepressant	C ₃₅ H ₃₅ ClNO ₃ Na	586.21772	?	4.6	13.87	Sigma-Aldrich	100	MeOH
Myclobutanil	Fungicide	C ₁₅ H ₁₇ ClN ₄	289.12145	2.9	2.3	11.63	Sigma-Aldrich	99.6	MeOH
Mycophenolic acid	Pharmaceutical/ Antibiotic	C ₁₇ H ₂₀ O ₆	321.13326	2.8	5.6	9.53	Sigma-Aldrich	98.5	MeOH
Naproxen	Pharmaceutical/ Anti-inflammatory	C ₁₄ H ₁₄ O ₃	231.10157	3.2	4.2	9.98	Sigma-Aldrich	100	MeOH
Norfloxacin	Pharmaceutical/ Fluoroquinolone	C ₁₆ H ₁₈ FN ₃ O ₃	320.14050	-0.9	5.7; 8.7	2.16	Fluka	99	MeOH
Norgestimate	Hormone	C ₂₃ H ₃₁ NO ₃	370.23767	4.1	11.5	13.12	Sigma-Aldrich	100	MeOH
Nortriptyline	Pharmaceutical/ Antidepressant	C ₁₈ H ₂₁ N	264.17468	4.4	10.5	6.90	Sigma-Aldrich	99	MeOH
Ofloxacin	Pharmaceutical/ Fluoroquinolone	C ₁₈ H ₂₀ FN ₃ O ₄	362.15106	-	5.4; 6.2	2.20	Sigma-Aldrich	99	MeOH
Omeprazole	Pharmaceutical/Anti gastrointestinal bleeding	C ₁₇ H ₁₉ N ₃ O ₃ S	346.12199	2.2	1.2; 7.4	4.50	Sigma-Aldrich	98.5	MeOH

Ondansetron	Pharmaceutical/ Antie-metic	C ₈ H ₂₀ ClN ₃ O ₂	294.16009	4.0	7.3; 15.4	3.30	Sigma-Al-drich	100	DMSO
Orlistat	Pharmaceutical/Lipase in-hibitor	C ₂₉ H ₅₃ NO ₅	496.39965	10.0	12.7	15.36	Sigma-Al-drich	98	MeOH
Oryzalin	Herbicide	C ₁₂ H ₁₈ N ₄ O ₆ S	347.10198	3.7	9.4	12.20	Sigma-Al-drich	99.1	MeOH
Oxazolam	Pharmaceutical/Anticon-vulsant	C ₁₈ H ₁₇ ClN ₂ O ₂	329.10513	3.0	12.7	4.42	Sigma-Al-drich	> 95.0	MeOH
Oxybutynin	Pharmaceutical/ Anticho-linergic	C ₂₂ H ₃₂ ClNO ₃	358.23767	4.3	8.4	7.60	Sigma-Al-drich	98	MeOH
Parathion	Pesticide	C ₁₀ H ₁₄ NO ₃ P S	292.04031	3.8	-	12.92	Sigma-Al-drich	99	MeOH
Paroxetine	Pharmaceutical/ Antide-pressant	C ₁₉ H ₂₁ ClFN O ₃	330.15000	2.5	9.9	6.00	Sigma-Al-drich	100	EtOH
Pefloxacin	Pharmaceutical/Fluoro-quinolone	C ₁₇ H ₂₀ FN ₃ O ₃	334.15615	0.3	5.7; 6.5	2.24	Sigma-Al-drich	99	MeOH
Pendimethalin	Herbicide	C ₁₃ H ₁₉ N ₃ O ₄	282.14483	5.2	10.9	13.90	Sigma-Al-drich	99	MeOH
Pentoxifylline	Pharmaceutical/ Antico-agulant	C ₁₃ H ₁₈ N ₄ O ₃	279.14517	0.3	19.6	4.42	Sigma-Al-drich	100	H ₂ O
Pindolol	Pharmaceutical/ Hyper-tensive	C ₁₄ H ₂₀ N ₂ O ₂	249.15975	1.8	9.3	1.52	Sigma-Al-drich	> 95.0	MeOH
Pipamperone	Pharmaceutical/ Antide-pressant	C ₂₁ H ₃₂ Cl ₂ F N ₃ O ₂	376.23948	2.2	13.0	1.60	Sigma-Al-drich	99.9	H ₂ O
Pirimicarb	Insecticide	C ₁₁ H ₁₈ N ₄ O ₂	239.15025	1.7	4.5	3.95	Sigma-Al-drich	98.7	MeOH
Pirimiphos-me-thyl	Insecticide	C ₁₁ H ₂₀ N ₃ O ₃ PS	306.10358	4.2	4.3	13.14	Sigma-Al-drich	98.5	MeOH
Prednisone	Pharmaceutical/ Anti-in-flammatory	C ₂₁ H ₂₆ O ₅	359.18530	1.5	12.6	6.96	Sigma-Al-drich	100	MeOH
Primidone	Pharmaceutical/ Antiepi-leptic	C ₁₂ H ₁₄ N ₂ O ₂	219.11280	0.9	11.5	3.86	Sigma-Al-drich	100	MeOH
Prochloraz	Pesticide	C ₁₅ H ₁₆ Cl ₃ N ₃ O ₂	376.03809	4.6	3.8	11.21	Sigma-Al-drich	98.6	MeOH
Progesterone	Hormone	C ₂₁ H ₃₀ O ₂	315.23186	4.2	-	12.79	Sigma-Al-drich	99	MeOH
Propachlor	Herbicide	C ₁₁ H ₁₄ ClNO ₂	212.08367	2.2	0.3	9.96	Sigma-Al-drich	99.8	MeOH
Propamocarb	Fungicide	C ₉ H ₂₀ N ₂ O ₂	189.15975	1.2	9.5	1.36	Sigma-Al-drich	98.5	MeOH
Propanil	Herbicide	C ₉ H ₉ Cl ₂ NO	218.01340	3.1	-	10.29	Sigma-Al-drich	99.7	MeOH
Propiconazole	Fungicide	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	342.07706	3.5	1.1	12.43	Sigma-Al-drich	99.1	MeOH
Propranolol	Pharmaceutical/ β-blocker antihypertensive	C ₁₂ H ₁₈ O	260.16451	3.8	11.1	4.95	Sigma-Al-drich	99.0	MeOH
Propyphenazone	Pharmaceutical/ Anti-in-flammatory	C ₁₄ H ₁₈ N ₂ O	231.14919	1.7	4.16	8.57	Sigma-Al-drich	100	MeOH
Propyzamide	Herbicide	C ₁₂ H ₁₁ Cl ₂ N O	256.02905	3.4	12.3	11.95	Sigma-Al-drich	99.8	MeOH
Prosulfocarb	Herbicide	C ₁₆ H ₂₁ NO ₂	252.14166	2.6	9.7; 14.1	13.56	MP bio-medicals	99	MeOH
Pyrantel	Pharmaceutical/Anti-par-asitic	C ₃₄ H ₃₀ N ₂ O ₆ S	207.09505	6.1	2.4	2.11	Sigma-Al-drich	99.9	DMSO
Pyrazophos	Fungicide	C ₁₄ H ₂₀ N ₃ O ₅ PS	374.09340	3.1	1.4	13.11	Sigma-Al-drich	99.8	MeOH
Quinmerac	Herbicide	C ₁₁ H ₈ ClNO ₂	222.03163	2.7	4.3	5.00	Sigma-Al-drich	99.9	MeOH
Quinoxifen	Fungicide	C ₁₅ H ₈ Cl ₂ FN O	308.00397	4.7	3.6	13.39	Sigma-Al-drich	99.9	MeOH
Raloxifene	Pharmaceutical/Estro-genic	C ₁₄ H ₂₁ NOS	474.17336	3.9	8.9	5.50	Sigma-Al-drich	100	MeOH

Ranitidine	Pharmaceutical/ Antihistaminic	C ₂₈ H ₂₈ ClNO ₄ S	315.14854	0.9	8.2	1.02	Sigma-Aldrich	100	MeOH
Risperidone	Pharmaceutical/ Antipsychotic	C ₁₃ H ₂₃ ClN ₄ O ₃ S	411.21908	0.3	8.8	3.80	Sigma-Aldrich	100	MeOH
Ropinirole	Pharmaceutical/Antiparkinsonian agent	C ₁₆ H ₂₅ ClN ₂ O	261.19614	1.1	9.5	1.95	Sigma-Aldrich	100	MeOH
Roxithromycin	Pharmaceutical/ Antibiotic	C ₄₁ H ₇₆ N ₂ O ₁₅	837.53185	3.1	125	8.14	Sigma-Aldrich	100	MeOH
Sertraline	Pharmaceutical/ Antidepressant	C ₁₇ H ₁₇ Cl ₂ N	306.08108	4.8	9.5	7.52	Sigma-Aldrich	98.0	MeOH
Simazine	Herbicide	C ₇ H ₁₂ ClN ₅	202.08540	1.8	4.2	7.05	Fluka	99	MeOH
Sotalol	Pharmaceutical/ β -blocker antihypertensive	C ₁₂ H ₂₁ ClN ₂ O ₃ S	273.12674	0.9	10.7	1.07	Sigma-Aldrich	98	DMSO
Spirooxamine	Fungicide	C ₁₈ H ₃₅ NO ₂	298.27406	4.2	6.9	8.24	Sigma-Aldrich	98.9	MeOH
Sulfadiazine	Pharmaceutical/ Sulphonamide	C ₁₀ H ₁₀ N ₄ O ₂ S	251.05972	0.4	2.0; 7.0	2.27	Sigma-Aldrich	99	MeOH
Sulfamethazine	Pharmaceutical/ Sulphonamide	C ₁₂ H ₁₄ N ₄ O ₂ S	279.09102	0.3	2.7; 7.7	3.59	Sigma-Aldrich	100	MeOH
Sulfamethoxazole	Pharmaceutical/ Sulphonamide	C ₁₀ H ₁₁ N ₃ O ₃ S	254.05939	0.8	2.0; 6.2	4.80	Sigma-Aldrich	99	MeOH
Sulfapyridine	Pharmaceutical/ Sulphonamide	C ₁₁ H ₁₁ N ₃ O ₂ S	250.06447	0.9	8.4	2.54	Sigma-Aldrich	99.8	MeOH
Sulfathiazole	Pharmaceutical/ Sulphonamide	C ₉ H ₉ N ₃ O ₂ S ₂	256.02089	0.1	2.2; 7.2	2.38	Sigma-Aldrich	100	MeOH
Tamoxifen	Pharmaceutical/ Estrogenic receptor	C ₂₆ H ₂₉ NO	372.23219	7.1	8.9	10.39	Sigma-Aldrich	100	MeOH
Tebuconazole	Fungicide	C ₁₆ H ₂₂ ClN ₃ O	308.15242	3.7	2.3	12.22	Sigma-Aldrich	99.3	MeOH
Telmisartan	Pharmaceutical/ Hypertensive	C ₃₃ H ₃₀ N ₄ O ₂	515.24415	6.1	3.6; 4.7; 5.9	7.75	Boehringer	99	MeOH
Terbinafine	Pharmaceutical/ Antifungal	C ₂₁ H ₂₆ ClN	292.20598	5.5	8.9	8.33	Sigma-Aldrich	100	EtOH
Terbuthylazine	Herbicide	C ₉ H ₁₆ ClN ₅	230.11670	3.1	2.0	11.11	Sigma-Aldrich	99.4	EtOH
Terbutryn	Herbicide	C ₁₀ H ₁₉ N ₅ S	242.14339	3.7	4.3	8.70	Sigma-Aldrich	99.1	MeOH
Testosterone	Hormone	C ₁₉ H ₂₈ O ₂	289.21621	4.2	-0.9	10.46	Sigma-Aldrich	99	MeOH
Thiabendazole	Pharmaceutical/ Anthelmintic	C ₁₀ H ₇ N ₃ S	202.04334	2.5	4.6	1.80	Sigma-Aldrich	100	MeOH
Thiacloprid	Insecticide	C ₁₀ H ₉ ClN ₄ S	253.03092	1.3	12.4	6.18	Sigma-Aldrich	99.9	AcN
Thiamethoxam	Fungicide	C ₈ H ₁₀ ClN ₅ O ₃ S	292.02656	1.5	13.6	3.45	Sigma-Aldrich	99.3	MeOH
Tramadol	Pharmaceutical/ Analgesic	C ₁₆ H ₂₆ ClNO ₂	264.19581	3.0	9.2; 13.1	3.17	Sigma-Aldrich	99	EtOH
Triadimenol	Fungicide	C ₁₄ H ₁₈ ClN ₃ O ₂	296.11603	3.1	13.3	10.87	Sigma-Aldrich	98.2	AcN
Triamcinolone	Pharmaceutical/ corticoid	C ₂₁ H ₂₇ FO ₆	395.18644	1.2	13.4	5.46	Sigma-Aldrich	100	DMSO
Triethyl phosphate	Industrial chemicals/ Catalyst	C ₆ H ₁₅ O ₄ P	183.07807	0.8	4.9	5.70	Sigma-Aldrich	99.8	EtOH
Trimethoprim	Pharmaceutical/ Antibiotic	C ₁₄ H ₁₈ N ₄ O ₃	291.14517	1.3	7.2	1.92	Fluka	99	MeOH
Triphenyl phosphate	Industrial chemical/Flame retardant	C ₁₈ H ₁₅ O ₄ P	327.07807	4.6	10	13.10	Sigma-Aldrich	100	Acetone
Valsartan	Pharmaceutical/ Antihypertensive	C ₂₄ H ₂₉ N ₅ O ₃	436.23432	5.3	4.4; 8.3	11.30	Boehringer	99	MeOH
Verapamil	Pharmaceutical/ Blood	C ₂₇ H ₃₈ N ₂ O ₄	455.29043	3.8	8.9	7.11	Sigma-Aldrich	95	MeOH

Abbreviations (NEG): 2,6-Di-tert-butyl-4-(dimethylaminomethyl)phenol (2,6-Di-tB-4-DMAMP), Bisphenol A (BPA), Methyl butyl phthalate (MBP), Perfluorobutanesulfonic acid (PFBS), Perfluorooctanoic acid (PFOA), Perfluorooctanesulfonic acid (PFOS), Perfluorooctanesulfonamide (PFPSA), **Abbreviations (POS):** 4,4'-bis(dimethylamino)benzophenone (4,4-BDMABP), 4-methylbenzophenone (4-MBP), 4-phenylbenzophenone (4-PBZ), Benzyl butyl phthalate (BBP), Bis(2-ethylhexyl)adipate (BEHA), Bis(2-ethylhexyl)phthalate (BEHP), Bis(methylglycol)phthalate (BMGP), Dibutyl phthalate (DBP), Dibutyl phthalate (DCHP), 4,4'-bis(diethylamino)benzophenone (DEAB), Diethyl phthalate (DEP), 2,4-Diethyl-9H-thioxanthen-9-one (DETX), Di-n-octyl phthalate (DOP), Ethyl-4-dimethylaminobenzoate (EDAB), 2-Ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine (EDDP), 17- α -ethynylestradiol (EE2), 2-ethylhexyl-4-dimethylaminobenzoate (EHDAB), 2-isopropylthioxanthone (ITX), Methyl 3,5-di-tert-butyl-4-hydroxybenzoate (MBHB).

Table 2. S. Validation results for the target 245 analytes: instrumental (UHPLC-qOrbitrap) and procedural (Vortex – CaptivaND-Lipids – UHPLC-qOrbitrap) figures of merit.

Compound	UHPLC - qOrbitrap				Vortex - Captiva ND-Lipids - UHPLC-qOrbitrap													
					Low-concentration (10 ng/g)							High-concentration (40 ng/g)						
	LOQ _{inst} (ng/g)	RSD (%)	LOI _{inst} (ng/g)	Extern. cal. (r ²)	LOQ _{pro} c (ng/g)	LOI _{proc} (ng/g)	Matrix- match. cal. (r ²)	Abs Rec. (%)	RSD (%)	Apparent recovery		Abs Rec. (%)	RSD (%)	Apparent recovery				
										Surr. corr.	Matrix- match.	RSD (%)			Surr. corr.	Matrix- match.	RSD (%)	
[M-H] ⁺																		
2,4-Dinitrophenol ^b	10.36	2	4.71	0.9981	1.54	0.77	0.9943	69	4	90	90	4	84	2	107	101	2	
2,6-Di-tB-4-DMAMP ^a	43.44	2	175.16	0.9702	28.04	29.13	0.9542	94	21	-	72	25	144	7	-	129	7	
Atorvastatin ^a	12.11	1	12.11	0.9922	0.90	9.85	0.9841	16	12	22	98	7	67	1	92	123	7	
Bentazone	10.25	3	4.65	0.9940	1.52	1.52	0.9957	-	-	-	94	3	-	-	-	102	1	
Bicalutamide ^b	8.19	2	1.33	0.9951	0.61	0.61	0.9954	66	3	93	91	3	80	3	103	107	1	
BPA ^a	146.77	4	26.59	0.9991	1.53	3.85	0.9915	-	-	-	56	4	-	-	-	111	2	
Butylparaben	9.15	1	1.48	0.9987	0.68	0.68	0.9939	66	1	-	91	1	104	3	-	108	1	
Clofibric acid	46.01	2	9.46	0.9990	0.70	3.53	0.9961	55	2	-	95	2	98	2	-	108	1	
Efavirenz ^a	9.86	1	1.60	0.9985	1.46	0.73	0.9955	62	4	88	85	3	71	3	97	108	2	
Estriol ^a	48.36	1	9.94	0.9970	1.47	16.17	0.9940	-	-	-	-	-	-	-	-	-	-	
Flufenoxuron ^a	10.16	3	10.16	0.9947	3.71	3.79	0.9840	29	10	41	71	7	76	3	104	106	5	
Flutamide ^d	165.85	10	1.89	0.9972	0.86	0.75	0.9983	-	-	24	-	15	93	1	99	-	10	
Furosemide ^a	49.43	2	26.23	0.9970	0.75	8.27	0.9925	48	4	68	96	3	39	5	54	110	2	
Hydrochlorothiazide ^d	10.52	4	51.18	0.9967	1.56	17.11	0.9975	32	2	45	99	2	84	3	90	105	2	
MBP ^a	46.59	1	9.58	0.9985	0.71	0.71	0.9922	-	-	-	-	-	-	-	-	-	-	
Mecoprop	8.74	2	8.74	0.9990	0.65	3.26	0.9961	-	-	-	95	2	-	-	-	108	1	
Monensin ^a	4.45	2	9.80	0.9957	1.45	15.93	0.9906	37	17	53	80	14	131	2	72	120	5	
Monobenzylphthalate ^{a,a}	8.87	2	8.87	0.9974	0.66	3.31	0.9970	56	3	79	96	3	-	-	31	106	1	
Nitrofurantoin ^a	14.84	2	6.74	0.9935	0.00	5.54	0.9970	43	3	61	104	3	51	2	70	104	2	
Nonylphenol ^{a,a}	16.46	4	1.03	0.6720	12.07	0.47	0.7132	-	-	-	-	-	43	1	59	67	4	
PFBS ^a	24.51	3	1.54	0.9892	1.41	0.70	0.9971	72	2	101	100	2	73	3	100	104	1	
PFOA ^a	8.66	2	22.34	0.9891	0.64	3.23	0.9890	66	2	93	89	2	84	3	115	105	2	
PFOS ^a	9.39	16	1.52	0.9969	0.70	0.70	0.9950	53	6	75	91	6	65	11	89	139	15	
PFOSA ^a	25.12	2	1.58	0.9798	1.44	0.72	0.9928	-	-	-	-	-	67	6	92	107	1	
Pravastatin ^a	10.04	3	10.04	0.9943	0.74	3.75	0.9942	48	3	68	99	2	130	1	71	107	1	
Propanil	8.58	1	1.39	0.9985	0.64	0.64	0.9939	-	-	-	91	1	-	-	-	107	1	
Propofol	9.77	14	25.21	0.9787	1.45	6.98	0.9916	-	-	-	68	13	-	-	-	117	12	
Valsartan ^a	4.14	1	23.50	0.9945	0.67	7.41	0.9912	47	4	66	95	4	59	5	82	118	2	
[M+H] ⁺																		
2-HBT ^c	1.51	1	-	0.9996	0.69	0.00	0.9989	74	2	97	94	2	55	1	70	109	3	
4,4-BDMABP ^a	9.88	2	4.49	0.9929	1.47	1.47	0.9981	81	2	107	100	2	78	2	101	105	1	
4-Hydroxytamoxifen ^c	9.80	2	1.59	0.9974	1.45	0.73	0.9957	70	1	92	96	1	77	8	99	105	1	

4-MBP ^{*a}	4.36	4	24.79	0.9996	3.58	7.81	0.9923	56	3	79	88	3	-	-	28	109	2
4-PBZ [*]	3.99	3	1.42	0.9994	0.65	0.65	0.9949	50	8	-	79	8	102	1	-	111	3
Acetaminophen	4.08	2	8.98	0.9951	3.35	0.67	0.9963	127	2	-	103	2	75	1	-	103	3
Acetamiprid ^b	10.31	1	4.68	0.9987	0.76	0.76	0.9987	78	2	103	96	2	-	-	72	105	2
Acetochlor ^a	4.01	1	4.01	0.9988	1.31	0.65	0.9969	65	1	92	91	1	-	-	96	104	3
Acyclovir ^a	1.96	9	12.12	0.9981	19.71	59.27	0.9633	-	-	-	-	-	65	1	90	68	10
Alachlor ^d	4.49	1	4.49	0.9990	1.47	0.73	0.9969	65	1	70	91	1	94	2	101	104	3
Albendazole ^b	12.07	2	1.96	0.9979	0.89	0.89	0.9990	80	3	105	98	3	78	1	100	104	1
Amantadine	2.36	4	5.20	0.9952	0.38	4.23	0.9932	59	9	-	87	9	148	3	-	113	5
Ambroxol	9.30	2	24.00	0.9961	1.38	15.12	0.9923	-	-	-	108	25	99	2	-	135	10
Ametryn ^a	10.54	2	1.71	0.9989	0.78	0.78	0.9980	68	1	96	89	1	21	26	29	103	3
Amiodarone ^b	4.50	2	4.50	0.9959	1.47	1.47	0.9889	45	4	60	87	4	77	1	99	124	3
Amitriptyline ^a	1.53	1	1.43	0.9982	0.70	0.70	0.9916	52	11	74	97	11	83	2	115	118	11
Anastrozole	6.55	1	6.55	0.9988	1.07	1.07	0.9975	-	-	-	98	2	-	-	-	102	2
Atenolol ^b	10.53	1	4.78	0.9940	8.56	0.00	0.9953	-	-	-	79	6	81	2	104	-	5
Atrazine ^a	4.14	2	1.48	0.9993	1.35	0.68	0.9978	71	2	100	93	2	75	6	101	103	2
Azelastine ^b	8.72	2	3.96	0.9961	0.65	0.65	0.9890	74	5	98	110	5	-	-	107	116	3
Azithromycin	9.66	9	4.39	0.9954	1.43	0.72	0.9926	51	7	-	71	7	111	2	-	95	6
Azoxystrobin	10.70	3	4.86	0.9987	0.79	0.79	0.9985	103	3	-	86	3	89	6	-	98	1
BBP [*]	9.61	3	4.37	0.9962	3.59	3.59	0.9955	61	10	-	87	10	98	1	-	113	5
BEHA ^{*a}	24.41	8	9.46	0.9818	30.87	0.70	0.6154	24	1	34	95	1	52	9	72	-	5
BEHP [*]	45.26	19	1.51	0.8449	45.50	0.69	0.6925	107	1	-	-	-	37	4	-	-	-
Bendicarb ^a	7.11	3	7.11	0.9968	0.53	1.05	0.9946	62	4	88	92	4	131	2	71	106	5
Benzethonium ^a	4.39	1	-	0.9981	0.72	0.00	0.9931	63	2	89	96	2	-	-	123	118	2
Benzophenone [*]	4.40	5	4.40	0.9991	1.44	0.72	0.9655	54	13	-	81	13	123	9	-	86	11
Benzothiazole ^a	27.00	11	149.03	0.9988	0.00	0.78	-	-	-	95	-	29	42	9	57	-	29
Bezafibrate ^d	4.39	1	9.66	0.9990	0.72	1.43	0.9984	88	2	96	98	2	67	1	72	103	1
Bisoprolol ^d	4.42	2	4.42	0.9976	0.72	0.72	0.9966	86	3	93	95	3	72	2	77	102	2
BMGP [*]	4.24	1	45.44	0.9950	1.39	61.18	0.9958	71	4	-	91	4	121	10	-	102	1
Boscalid ^a	4.92	3	27.93	0.9992	0.80	4.04	0.9981	70	4	98	90	4	85	2	116	113	1
Bosentan	9.22	1	23.78	0.9971	0.68	3.44	0.9937	77	4	-	97	4	91	7	-	113	3
Bupropion ^a	9.25	1	4.20	0.9987	3.45	1.37	0.9944	17	30	23	98	29	-	-	29	141	26
Caffeine ^b	9.19	2	9.19	0.9976	0.68	1.36	0.9979	73	4	96	95	3	82	4	105	107	2
Caprolactam [*]	8.92	2	-	0.9896	29.12	0.50	0.9465	-	-	-	-	-	60	1	82	75	19
Captopril	1.74	2	10.73	0.9966	52.44	52.44	-	-	-	-	-	-	-	-	-	-	-
Carbamazepine	9.34	1	1.51	0.9961	1.38	0.69	0.9991	87	1	-	102	1	163	10	-	105	2
Carbaryl ^a	10.23	3	26.41	0.9922	0.76	8.36	0.9965	73	3	103	97	3	86	5	93	106	2
Carbendazim	11.68	3	5.31	0.9944	0.87	0.87	0.9982	-	-	-	98	1	-	-	-	102	1
Celecoxib ^a	5.59	1	59.81	0.9966	1.82	10.00	0.9954	71	4	100	91	3	53	14	72	103	2
Cetirizine ^a	1.96	2	12.10	0.9992	1.79	1.79	0.9839	62	5	88	118	5	20	16	28	155	6
Chloridazon ^b	2.37	2	6.65	0.9994	5.46	1.09	0.9967	77	2	102	109	3	50	3	69	108	1
Chloroxuron	9.88	1	4.49	0.9981	0.73	0.73	0.9985	84	2	-	96	2	110	1	-	104	1
Chlortoluron ^b	10.73	2	1.74	0.9966	0.80	0.80	0.9990	79	2	104	99	1	33	14	45	104	2
Ciprofloxacin ^c	47.96	10	140.46	0.9199	48.21	16.03	0.9972	165	26	85	80	26	70	5	96	114	7
Clarithromycin ^a	5.52	1	12.14	0.9936	1.80	1.80	0.9943	64	3	91	95	3	67	2	93	102	4
Clomazone ^a	4.29	1	9.44	0.9995	1.40	3.52	0.9963	68	3	97	95	3	90	3	96	103	5
Clomipramine ^b	3.93	1	3.93	0.9984	1.29	0.64	0.9960	69	2	91	96	2	81	2	104	104	2
Clonidine ^d	4.39	2	4.39	0.9958	0.72	0.72	0.9559	90	13	97	119	13	85	3	91	156	10
Clopidrogel ^a	9.36	2	4.25	0.9986	0.69	0.69	0.9983	50	4	71	82	4	61	3	84	109	1
Clozapine	10.34	1	4.70	0.9937	1.53	0.77	0.9957	-	-	-	102	5	-	-	-	-	-
Cortisone ^b	10.38	29	26.79	0.9829	3.87	3.87	0.9933	-	-	108	105	10	-	-	99	100	7
Cotinine	9.69	7	4.40	0.9944	1.44	15.74	0.9924	-	-	-	86	8	-	-	-	-	-
Crotamiton ^a	4.45	1	1.59	0.9990	0.73	0.73	0.9955	66	3	94	95	3	74	5	102	106	4
Cyclophosphami de ^b	4.25	2	9.36	0.9988	1.39	1.39	0.9984	77	1	102	93	1	82	2	105	103	1
Cyproterone ^a	4.37	4	4.37	0.9978	1.43	0.71	0.9984	67	6	95	91	6	56	5	77	102	1
Danofloxacin	43.30	7	126.79	0.9558	29.05	3.32	0.9921	-	-	162	78	15	73	11	100	103	5
DBP [*]	8.30	9	1.34	0.9789	27.08	0.62	0.7530	-	-	-	-	-	-	-	-	-	-
DCHIP ^{*,d}	4.36	6	24.78	0.9937	0.71	7.81	0.9904	30	25	43	79	23	88	2	95	111	9
DEAB ^{*,a}	10.11	1	-	0.9964	0.75	0.00	0.9988	62	10	88	84	8	38	12	52	103	5
DEP [*]	22.43	5	1.41	0.9789	28.36	0.64	-	-	-	-	-	-	-	-	-	-	-

Desloratadine	24.11	3	9.34	0.9927	1.39	0.69	0.9707	-	-	-	90	27	-	-	-	120	13
DETX* ^e	9.14	3	1.48	0.9930	1.36	1.36	0.9967	-	-	-	-	-	144	1	79	130	15
Dexamethasone ^b	4.09	2	9.01	0.9959	1.34	3.36	0.9979	74	1	97	95	1	49	6	67	104	3
Diazepam	4.79	2	4.79	0.9991	0.78	0.78	0.9967	95	1	-	98	1	64	5	-	104	1
Dichlorvos	1.43	3	22.75	0.9993	1.31	7.17	0.9824	-	-	-	109	14	-	-	-	111	14
Diethyl Toluamide ^b	1.65	1	1.61	0.9979	0.74	0.74	0.9944	61	3	81	91	3	82	1	105	102	5
Diflufenican	4.63	3	10.19	0.9977	1.51	8.29	0.9975	-	-	-	77	4	-	-	-	113	6
Dimethachlor ^a	4.58	2	4.58	0.9985	1.49	0.75	0.9951	67	3	94	90	3	59	13	81	102	2
Dimethoate	9.96	1	9.96	0.9971	0.74	1.48	0.9971	71	4	93	95	4	89	2	114	106	3
Diphenhydramin ^{e,d}	4.15	2	4.15	0.9972	0.68	0.68	0.9964	64	4	70	95	4	94	1	101	110	2
Diuron ^d	9.38	2	4.26	0.9987	0.69	1.39	0.9991	78	2	110	95	2	76	5	104	101	3
Domperidone	6.91	1	39.23	0.9988	1.13	5.67	0.9984	119	2	-	105	2	54	1	-	108	3
DOP*	46.24	16	46.24	0.8664	46.48	46.48	0.7336	102	1	-	-	-	51	4	-	-	-
Drospirenone ^a	9.69	3	4.40	0.9980	0.72	0.72	0.9985	64	5	91	101	5	63	5	86	111	5
Duloxetine	23.92	2	23.92	0.9949	0.69	7.54	0.9975	66	6	-	101	5	99	4	-	112	1
EDAB*	3.65	2	1.30	0.9994	0.60	0.60	0.9985	57	5	-	95	5	98	1	-	109	5
EDDP* ^a	1.63	1	1.63	0.9982	0.75	0.75	0.9929	52	11	74	-	11	-	-	91	123	11
EHDAB* ^a	4.20	2	1.50	0.9961	0.69	3.45	0.9974	26	13	36	69	12	67	2	92	103	12
Enoxacin	47.20	1	138.22	0.9214	15.78	31.67	0.8082	-	-	-	-	-	-	-	-	-	-
Enrofloxacin ^c	22.47	3	124.04	0.9966	7.08	3.25	0.9406	-	-	101	132	6	137	1	75	146	1
Eprosartan	4.14	5	4.14	0.9975	0.68	3.40	0.9967	44	5	-	105	5	-	-	-	112	6
Equilin*	4.58	2	25.99	0.9951	1.49	16.37	0.9976	61	5	-	95	5	101	2	-	98	4
Erythromycine	4.20	2	23.84	0.9966	7.51	30.14	0.9754	-	-	-	-	-	108	3	-	-	-
Ethion	4.25	6	183.50	0.9963	3.49	45.74	0.9961	37	15	-	75	12	103	2	-	107	13
Exemestane ^a	1.65	3	4.61	0.9990	0.75	1.51	0.9963	72	3	101	84	3	41	2	57	102	2
Fenoxycarb ^a	4.52	3	25.68	0.9993	0.74	3.71	0.9993	68	1	96	90	1	82	3	106	110	1
Fenpropidin ^a	4.18	2	1.49	0.9987	0.68	0.68	0.9917	63	4	89	98	4	18	23	25	114	5
Fenpropimorph	3.72	1	3.72	0.9982	0.61	0.61	0.9936	47	7	-	82	7	106	1	-	119	3
Fenthion ^a	26.04	8	143.71	0.9962	3.76	16.40	0.9905	42	23	60	80	19	65	8	89	119	24
Finasteride ^a	4.57	1	4.57	0.9984	0.74	0.74	0.9975	70	1	99	95	1	78	2	107	104	1
Fluconazole	3.96	1	8.73	0.9986	0.65	1.29	0.9990	95	1	-	98	1	112	3	-	102	2
Flumequine ^b	9.85	2	9.85	0.9991	0.73	3.67	0.9978	79	4	104	96	4	-	-	33	108	3
Flusilazole ^b	4.13	1	-	0.9994	0.67	0.00	0.9984	72	1	95	92	1	84	4	90	109	1
Fluvoxamine ^b	9.36	2	4.25	0.9978	1.39	0.69	0.9939	46	12	61	103	11	83	2	106	117	8
Gabapentin ^b	4.25	3	1.52	0.9963	45.74	1.39	0.8696	-	-	-	-	-	76	1	97	-	22
Genistein ^a	6.09	2	13.41	0.9984	0.99	5.00	0.9975	73	2	103	92	2	-	-	-	111	1
Genistin ^a	6.12	3	65.55	0.9973	1.00	10.96	0.9974	70	5	99	94	5	54	1	74	107	3
Glibenclamide ^b	5.12	4	29.06	0.9971	0.83	4.20	0.9945	77	3	101	92	3	38	11	49	106	1
Glimepiride ^b	5.36	3	11.80	0.9976	0.87	4.40	0.9954	75	2	98	96	2	55	2	71	109	3
Glycitin ^a	13.75	1	66.89	0.9987	2.04	22.36	0.9959	69	5	97	99	5	61	2	83	112	1
Hexazinone ^d	10.66	2	1.73	0.9957	1.58	0.79	0.9988	84	2	91	100	1	-	-	-	105	2
Hydrocortisone	4.43	1	9.75	0.9983	0.72	3.64	0.9979	80	4	-	98	4	105	3	-	107	3
Hydroxychloroquine	43.03	12	43.03	0.9700	43.26	28.88	0.9734	-	-	-	-	-	150	13	82	97	23
Ifosfamide	4.37	2	9.62	0.9988	1.43	1.43	0.9984	77	1	-	93	1	102	3	-	103	1
Imatinib ^b	9.45	2	4.29	0.9933	30.82	0.70	0.9487	52	10	68	118	8	89	2	114	136	8
Imazalil	4.34	1	4.34	0.9980	0.71	0.71	0.9974	67	1	-	98	1	159	4	-	117	2
Imidacloprid ^d	10.39	2	26.82	0.9987	0.77	3.88	0.9977	89	3	97	101	3	75	2	81	104	3
Iminostilbene ^b	3.94	2	1.40	0.9987	1.29	0.64	0.9960	-	-	33	-	15	80	2	103	-	5
Imipramine ^b	4.25	2	1.52	0.9982	0.69	0.69	0.9971	67	3	89	100	3	79	1	101	120	4
Indometacin ^b	4.25	5	276.86	0.9968	0.69	45.74	0.9968	72	3	95	92	3	82	15	105	106	2
Irbersartan ^b	4.22	3	4.22	0.9983	0.69	0.69	0.9992	65	3	85	97	3	75	7	96	112	1
Isoproturon ^d	9.50	2	1.54	0.9961	0.70	0.70	0.9987	68	2	74	98	2	94	2	101	104	1
ITX*	1.46	4	1.46	0.9983	0.67	0.67	0.9973	-	-	-	77	10	-	-	-	108	11
Ketoconazole ^a	8.60	5	3.90	0.9932	0.64	0.64	0.9985	66	1	93	102	1	70	1	96	108	2
Ketoprofen	1.54	1	4.32	0.9984	0.71	0.71	0.9966	77	2	-	95	2	92	3	-	108	2
Lenacil ^b	11.77	3	11.77	0.9961	0.87	1.75	0.9997	75	2	98	92	2	59	5	76	102	3
Levofloxacin	39.33	3	20.87	0.9888	0.60	3.02	0.9993	125	15	-	84	15	89	1	-	111	13
Lidocaine	3.63	4	1.30	0.9954	0.59	6.51	0.9945	102	6	-	99	6	129	1	-	118	3

Linuron ^b	57.00	4	10.06	0.9994	0.75	3.75	0.9976	70	4	92	92	4	82	1	106	109	2
Lomefloxacin ^c	43.01	6	43.01	0.9713	3.30	3.30	0.9994	142	10	78	89	10	88	2	95	108	4
Lorazepam ^b	1.44	2	8.86	0.9985	0.66	3.31	0.9972	76	2	100	96	2	-	-	-	110	2
Losartan ^b	1.53	2	9.42	0.9981	1.40	1.40	0.9949	60	2	79	94	2	83	1	107	112	2
MBHB ^{*,b}	4.22	2	23.97	0.9988	3.47	7.55	0.9977	48	12	67	76	12	78	3	99	113	4
Mebendazole	5.17	4	5.17	0.9989	0.84	0.84	0.9991	78	2	-	98	2	-	-	-	111	2
Mebeverine ^b	10.40	2	4.72	0.9985	0.77	0.77	0.9960	74	1	97	97	1	63	4	81	109	2
Meclocycline ^b	130.83	16	271.86	0.9398	44.91	44.91	-	-	-	-	-	-	82	6	105	-	7
Medroxyprogesterone ^b	10.28	1	10.28	0.9980	0.76	3.83	0.9990	70	5	92	90	5	76	5	98	103	3
Mefenamic acid ^b	1.96	1	12.10	0.9985	0.90	1.80	0.9978	74	2	98	94	2	86	1	111	111	1
Memantine ^a	4.42	2	-	0.9989	1.44	0.00	0.9851	54	10	77	101	9	72	1	100	124	5
Metalaxyl ^a	3.79	2	1.35	0.9989	0.62	0.62	0.9977	72	4	102	93	4	79	3	102	105	1
Metamitron	9.63	2	4.38	0.9972	1.43	0.71	0.9994	100	1	-	99	1	87	2	-	104	1
Metazachlor ^a	4.36	2	4.36	0.9983	0.71	1.42	0.9945	72	3	101	93	3	71	5	98	109	1
Metconazole ^a	1.47	2	4.12	0.9982	0.67	1.34	0.9975	72	1	102	93	1	68	1	94	108	2
Metformin ^b	9.15	1	1.48	0.9968	3.41	14.87	0.9478	-	-	-	-	-	83	4	106	128	18
Methiocarb	4.21	2	9.27	0.9987	0.69	3.46	0.9962	70	3	-	92	3	-	-	-	108	1
Methotrexate	4.61	5	-	0.9942	49.56	0.00	-	-	-	-	-	-	92	1	-	-	-
Methylparaben ^b	4.25	5	45.55	0.9993	3.50	15.23	0.9901	58	4	77	74	4	90	4	115	99	6
Metolachlor ^a	9.90	1	4.50	0.9990	0.73	0.73	0.9988	69	3	97	94	3	61	2	84	103	4
Metoprolol ^d	4.61	5	4.61	0.9982	0.75	0.75	0.9959	92	4	100	99	4	27	28	37	109	1
Metribuzin ^c	122.90	1	41.97	0.9815	28.16	7.02	0.8556	-	-	-	-	-	-	-	122	102	1
Miconazole ^b	3.97	1	8.73	0.9987	0.65	1.29	0.9957	51	6	77	86	6	87	3	112	123	3
Mirtazapine ^b	9.11	5	4.14	0.9947	1.35	0.67	0.9838	75	7	99	118	6	81	3	104	142	2
Montelukast	4.61	3	26.19	0.9971	1.51	33.12	0.9962	53	9	-	85	8	-	-	-	112	4
Myclobutanil ^b	1.67	2	1.67	0.9990	0.77	0.77	0.9968	79	2	104	89	2	-	-	32	100	1
Mycophenolic acid	3.61	2	7.95	0.9964	0.59	1.22	0.9965	78	4	-	93	4	129	1	-	108	3
Naproxen ^a	10.03	13	296.80	0.9917	8.16	49.03	0.9927	60	22	85	64	22	35	16	49	87	4
Norfloxacin ^c	44.12	7	-	0.8962	3.38	-	0.9982	170	27	94	88	27	79	5	-	116	13
Norgestimate ^a	1.71	2	4.78	0.9979	0.78	3.93	0.9966	55	10	77	90	9	56	9	76	112	3
Nortriptyline ^b	9.31	2	1.51	0.9973	0.69	0.69	0.9935	67	6	95	107	6	82	2	106	120	3
Ofloxacin ^a	47.89	6	25.41	0.9779	8.01	3.67	0.7882	-	-	25	-	15	-	-	60	-	13
Omeprazole	4.25	1	9.36	0.9990	0.69	7.61	0.9953	-	-	-	-	-	88	3	-	-	-
Ondansetron ^b	1.93	5	5.41	0.9975	0.88	0.88	0.9950	76	3	100	103	3	137	11	75	119	1
Orlistat ^a	4.09	4	9.00	0.9970	1.33	7.32	0.9913	23	24	32	68	16	66	7	91	98	14
Oryzalin ^a	23.67	5	130.67	0.9985	3.42	29.94	0.9961	55	5	77	81	5	163	1	89	118	5
Oxazolam ^b	8.90	2	22.96	0.9972	0.66	14.46	0.9954	50	16	66	86	14	81	2	104	102	9
Oxybutynin ^b	4.20	1	4.20	0.9986	0.69	0.69	0.9964	69	2	91	97	2	78	1	100	112	2
Parathion	192.23	17	-	0.9661	31.98	0.00	0.9325	-	-	-	-	-	131	28	-	-	-
Paroxetine ^a	9.88	2	4.49	0.9962	0.73	0.73	0.9954	70	5	99	104	5	171	1	93	120	3
Pefloxacin ^c	24.89	4	46.90	0.9908	31.47	7.84	0.9867	128	12	71	92	10	67	3	92	108	11
Pendimethalin ^a	9.21	8	131.12	0.9967	1.37	3.43	0.9920	41	17	59	76	15	62	1	85	110	7
Pentoxifylline	14.92	1	6.78	0.9958	2.21	1.11	0.9981	98	5	-	106	4	39	1	-	107	1
Pindolol ^d	8.89	4	8.89	0.9971	29.01	3.32	0.9777	-	-	58	-	30	91	4	97	83	28
Pipamperone ^c	11.38	3	5.17	0.9953	0.84	0.84	0.9948	136	1	75	106	1	57	2	78	111	1
Pirimicarb ^a	8.50	2	1.38	0.9989	0.63	0.63	0.9977	59	7	83	92	7	89	1	96	112	3
Pirimiphos-methyl ^a	3.59	1	-	0.9984	0.59	0.00	0.9976	46	7	65	83	6	122	1	-	118	1
Prednisone	9.83	1	9.83	0.9980	0.73	3.67	0.9986	74	1	-	98	1	-	-	-	69	5
Primidone ^d	1.22	2	19.42	0.9990	0.56	2.81	0.9982	79	1	86	97	1	90	5	97	108	2
Prochloraz ^a	1.33	1	-	0.9978	0.61	0.00	0.9972	74	4	104	89	4	61	13	84	111	1
Progesterone ^c	4.30	1	9.46	0.9987	3.53	0.70	0.9606	154	3	85	106	5	79	4	101	108	1
Propachlor ^a	9.50	1	4.31	0.9988	1.41	0.70	0.9955	60	5	84	95	4	104	1	-	103	5
Propamocarb ^a	4.32	1	4.32	0.9959	1.41	1.41	0.9694	38	19	54	120	19	63	12	87	163	13
Propanil	1.39	1	8.58	0.9992	0.64	1.27	0.9955	71	2	-	87	2	96	2	-	105	4
Propiconazole ^b	4.60	2	4.60	0.9964	0.75	1.50	0.9989	82	1	108	94	1	82	3	105	109	1
Propranolol ^b	9.52	2	1.54	0.9978	0.71	0.71	0.9956	77	4	101	101	4	75	2	96	110	2
Propyphenazone ^a	4.56	1	1.63	0.9990	0.74	0.74	0.9975	69	3	97	93	3	61	16	84	108	3
Propyzamide	4.06	2	23.09	0.9985	1.33	7.28	0.9957	63	3	-	87	3	-	-	-	109	2

Prosulfocarb	8.55	4	8.55	0.9943	0.63	6.95	0.9950	43	14	-	79	13	121	5	-	119	16
Pyrantel	6.62	4	2.36	0.9962	5.44	47.55	0.9854	-	-	-	95	8	-	-	-	100	2
Pyrazophos ^d	4.29	2	4.29	0.9972	0.70	1.40	0.9977	87	11	95	89	11	60	4	65	112	5
Quinmerac	3.90	2	8.58	0.9989	1.27	3.20	0.9872	17	8	-	108	8	98	2	-	147	8
Quinoxifen	9.06	1	4.11	0.9944	0.67	3.38	0.9960	38	17	-	82	13	-	-	-	111	4
Raloxifene ^d	10.26	4	4.66	0.9941	0.76	0.76	0.9960	69	1	73	97	1	86	4	93	110	2
Ranitidine	4.24	3	24.09	0.9900	15.18	45.65	0.9437	-	-	-	-	-	-	-	-	-	-
Risperidone ^a	5.15	2	5.15	0.9984	1.68	0.84	0.9894	65	6	92	113	6	67	6	92	137	4
Ropinirole ^e	4.20	5	4.20	0.9987	30.21	0.69	0.9874	148	13	82	95	11	76	4	98	102	3
Roxithromycin ^b	4.18	3	4.18	0.9966	0.68	0.68	0.9944	74	2	97	101	2	84	2	108	113	6
Sertraline ^a	4.19	1	4.19	0.9969	1.37	1.37	0.9893	63	6	89	111	6	-	-	58	136	4
Simazine ^a	9.27	1	4.21	0.9989	0.69	0.69	0.9985	72	1	102	94	1	82	5	105	106	2
Sotalol ^a	11.94	7	11.94	0.9894	1.77	58.35	0.9753	31	17	44	82	12	65	15	90	-	14
Spiroamine ^a	4.54	2	4.54	0.9984	1.48	1.48	0.9901	62	2	88	108	2	63	10	87	136	5
Sulfadiazine ^a	4.39	2	9.66	0.9988	0.72	3.61	0.9863	58	13	82	92	12	72	6	99	119	15
Sulfamethazine ^a	1.37	2	8.44	0.9998	1.25	3.15	0.9953	57	13	80	83	13	158	18	86	109	10
Sulfamethoxazole ^a	4.41	1	9.70	0.9990	1.44	3.62	0.9985	61	10	86	89	9	52	14	71	96	6
Sulfapyridine ^a	4.82	1	27.36	0.9994	0.79	3.96	0.9752	86	15	94	97	14	68	1	73	135	18
Sulfathiazole ^b	1.47	4	44.01	0.9990	0.67	14.71	0.9892	43	17	57	96	16	81	2	104	118	14
Tamoxifen ^a	4.03	2	4.03	0.9985	0.66	0.66	0.9965	64	2	90	98	2	134	2	73	124	1
Tebuconazole ^b	3.77	2	3.77	0.9992	1.23	1.23	0.9970	74	1	98	92	1	79	3	102	102	2
Telmisartan ^a	9.20	6	4.18	0.9970	1.36	0.68	0.9970	116	1	-	97	1	85	2	-	108	2
Terbinafine ^a	4.58	2	1.63	0.9989	0.75	0.75	0.9975	41	11	57	78	10	53	2	73	114	3
Terbutylazine ^a	4.30	1	1.53	0.9991	0.70	0.70	0.9973	68	1	96	92	1	90	2	97	110	2
Terbutryn	2.98	1	1.06	0.9991	0.49	0.49	0.9970	62	3	-	88	3	100	2	-	110	2
Testosterone ^d	9.56	3	4.38	0.9976	0.71	0.71	0.9995	75	3	98	97	3	90	1	96	109	2
Thiabendazole ^b	6.87	2	3.12	0.9966	0.51	0.51	0.9959	83	2	109	96	2	148	1	81	107	2
Thiacloprid	3.75	1	8.27	0.9985	0.61	1.23	0.9996	97	2	-	97	1	108	3	-	101	1
Thiamethoxam	8.27	1	21.35	0.9984	1.23	3.09	0.9955	107	4	-	104	4	92	2	-	120	1
Tramadol	1.60	4	4.49	0.9974	0.73	0.73	0.9965	77	7	-	96	7	103	1	-	112	3
Triadimenol	3.72	1	39.82	0.9986	0.61	6.66	0.9989	75	2	-	95	2	-	-	-	116	2
Triamcinolone ^b	1.98	4	31.53	0.9976	1.81	1.81	0.9982	77	1	101	101	1	31	14	42	113	1
Triethylphosphat ^e	4.30	2	1.53	0.9996	7.70	0.70	0.9902	39	17	56	110	17	143	13	78	110	14
Trimethoprim	4.38	5	4.38	0.9897	1.43	0.71	0.9824	114	15	-	86	15	79	2	-	107	12
Triphenylphosph ^a	3.76	1	3.76	0.9994	0.61	0.61	0.9986	73	6	96	90	6	79	1	101	113	2
Valsartan ^b	4.14	1	9.11	0.9985	0.67	3.40	0.9971	60	8	79	101	8	61	2	78	122	1
Verapamil ^b	4.23	1	4.23	0.9985	0.69	0.69	0.9983	75	4	99	98	3	88	1	110	114	1

Superscripts: (a) [²H₅]-atrazine, (b) [¹³C₃]-caffeine, (c) [²H₈]-ciprofloxacin, (d) [²H₆]-diuron, (e) [²H₅]-enrofloxacin, (*) Not included in the optimization, only at validation. *Abbreviations (NEG):* 2,6-Di-tert-butyl-4-(dimethylaminomethyl)phenol (2,6-Di-tB-4-DMAMP), Bisphenol A (BPA), Methyl butyl phthalate (MBP), Perfluorobutanesulfonic acid (PFBS), Perfluorooctanoic acid (PFOA), Perfluorooctanesulfonic acid (PFOS), Perfluorooctanesulfonamide (PFPSA), *Abbreviations (POS):* 4,4'-bis(dimethylamino)benzophenone (4,4'-BDMABP), 4-methylbenzophenone (4-MBP), 4-phenylbenzophenone (4-PBZ), Benzyl butyl phthalate (BBP), Bis(2-ethylhexyl)adipate (BEHA), Bis(2-ethylhexyl)phthalate (BEHP), Bis(methylglycol)phthalate (BMGP), Dibutyl phthalate (DBP), Dibutyl phthalate (DCHP), 4,4'-bis(diethylamino)benzophenone (DEAB), Diethyl phthalate (DEP), 2,4-Diethyl-9H-thioxanthene-9-one (DETX), Di-n-octyl phthalate (DOP), Ethyl-4-dimethylaminobenzoate (EDAB), 2-Ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine (EDDP), 17- α -ethynylestradiol (EE2), 2-ethylhexyl-4-dimethylaminobenzoate (EHDAB), 2-isopropylthioxanthone (ITX), Methyl 3,5-di-tert-butyl-4-hydroxybenzoate (MBHB).

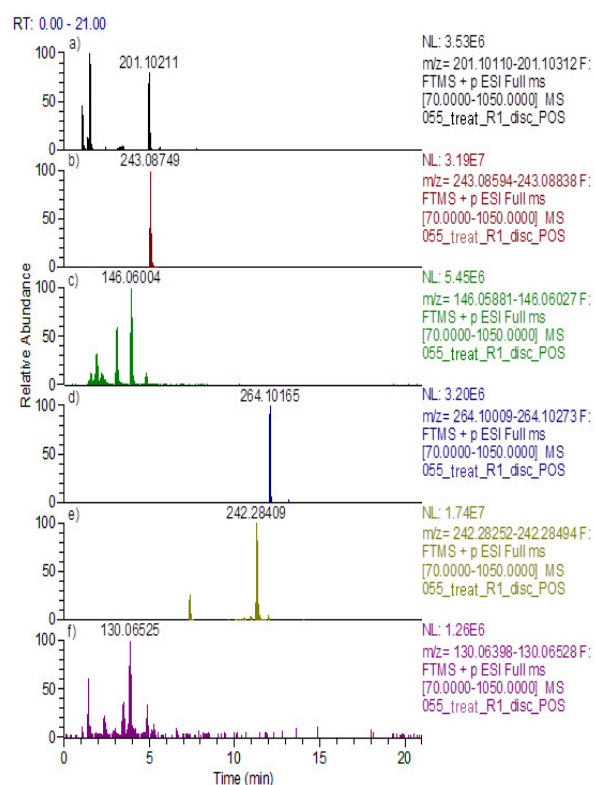


Figure S1. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 1 and 2a in commercial treated milk by suspect screening in positive ionization modes. (a) 1,2,3,9-tetrahydro-4H-carbazol-4-one oxime; (b) 3-amino-2-phenyl-2H-pyrazolo[4,3-c]pyridine-4,6-diol; (c) 4-Indolecarbaldehyde; (d) 7-Methyl-2-phenylquinoline-4-carboxylic acid; (e) Bis(2-ethylhexyl) amine; (f) Isoquinoline.

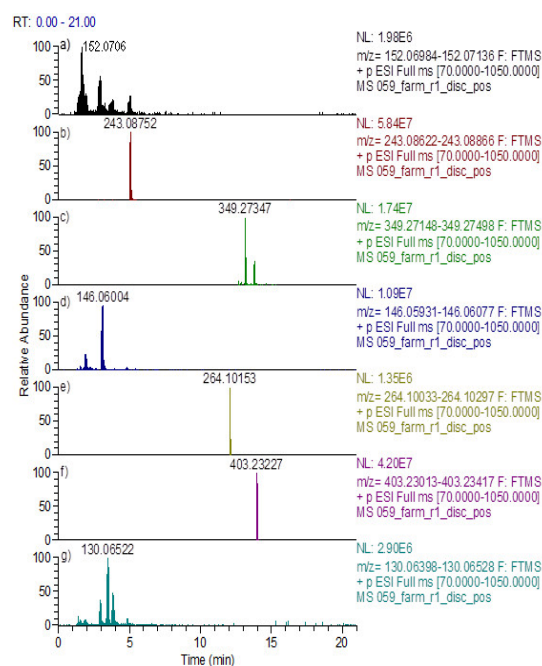


Figure S2. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 1 and 2a in commercial raw milk by suspect screening in positive ionization modes. (a) acetaminophen; (b) 3-amino-2-phenyl-2H-pyrazolo[4,3-c]pyridine-4,6-diol; (c) 3-Methyl-5-(5,5,8a-trimethyl-2-methylene-7-oxodecahydro-1-naphthalenyl)pentyl acetate; (d) 4-Indolecarbaldehyde; (e) 7-Methyl-2-phenylquinoline-4-carboxylic acid; (f) Citroflex A-4; (g) Isoquinoline.

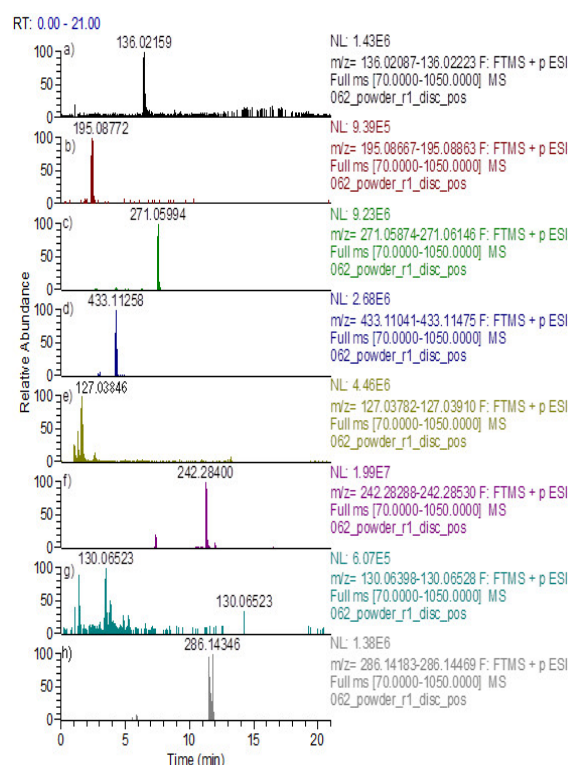


Figure S3. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 1 and 2a in commercial powder milk by suspect screening in positive ionization modes. (a) Benzothiazole; (b) Caffeine; (c) Genistein; (d) Genistin; (e) 5-Hydroxymethyl-2-furaldehyde; (f) Bis(2-ethylhexyl) amine; (g) Isoquinoline; (h) Piperine.

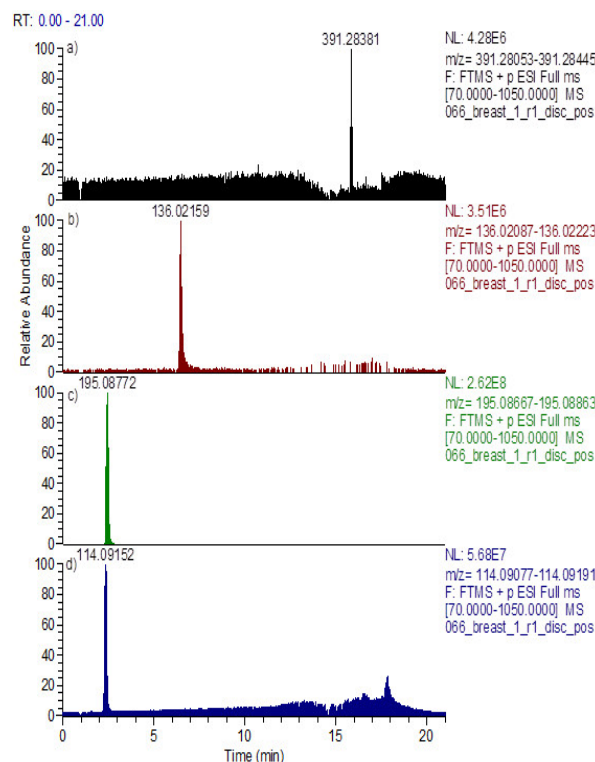


Figure S4. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 1 in breast milk A by suspect screening in positive ionization modes. (a) BEHP; (b) Benzothiazole; (c) Caffeine; (d) Caprolactam.

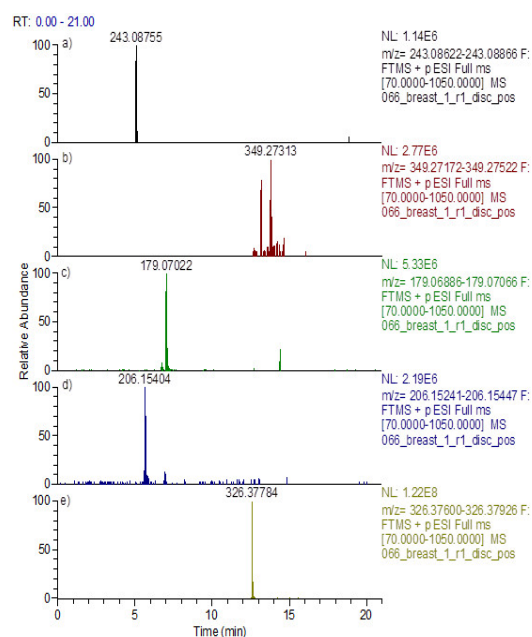


Figure S5. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 2a in breast milk A by suspect screening in positive ionization modes. (a) 3-amino-2-phenyl-2H-pyrazolo[4,3-c]pyridine-4,6-diol; (b) 3-Methyl-5-(5,5,8a-trimethyl-2-methylene-7-oxodecahydro-1-naphthalenyl)pentyl acetate; (c) 4-Methoxycinnamic acid; (d) Amfepramone; (e) Didecyldimethylammonium.

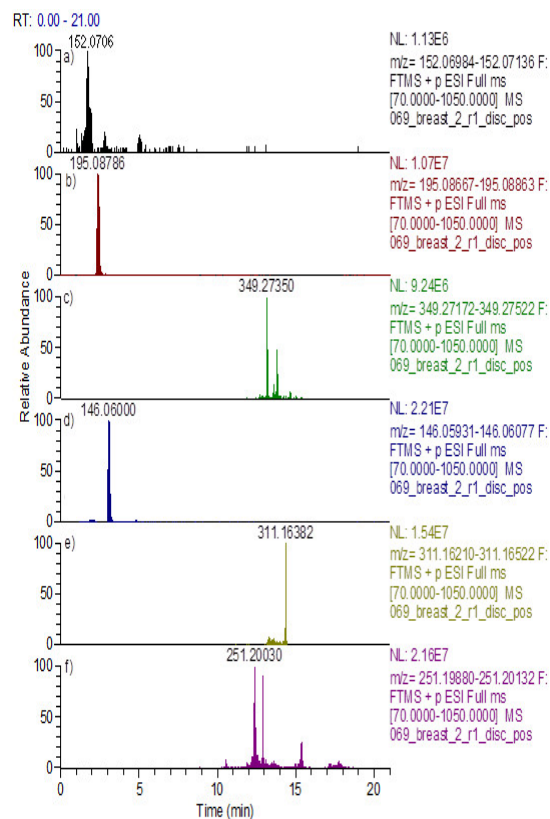


Figure S6. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 1 and 2a in breast milk B by suspect screening in positive ionization modes. (a) Acetaminophen; (b) Caffeine; (c) 3-Methyl-5-(5,5,8a-trimethyl-2-methylene-7-oxodecahydro-1-naphthalenyl)pentyl acetate; (d) 4-Indolecarbaldehyde; (e) Avobenzone; (f) OPEO.

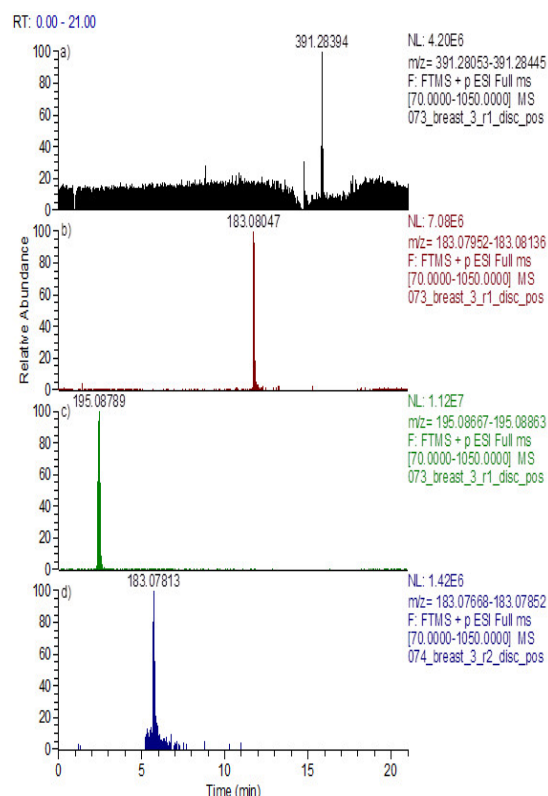


Figure S7. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 1 in breast milk C by suspect screening in positive ionization modes. (a) BEHP; (b) Benzophenone; (c) Caffeine; (d) Triethyl phosphate.

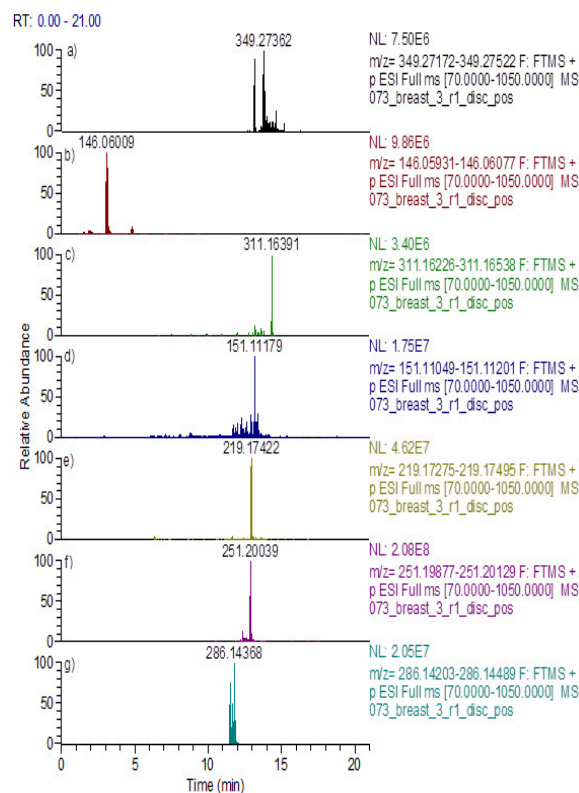


Figure S8. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 2a in breast milk C by suspect screening in positive ionization modes. (a) BEHP; (b) Benzophenone; (c) Caffeine; (d) Avobenzone; (e) Nootkatone; (f) OPEO; (g) Piperine.

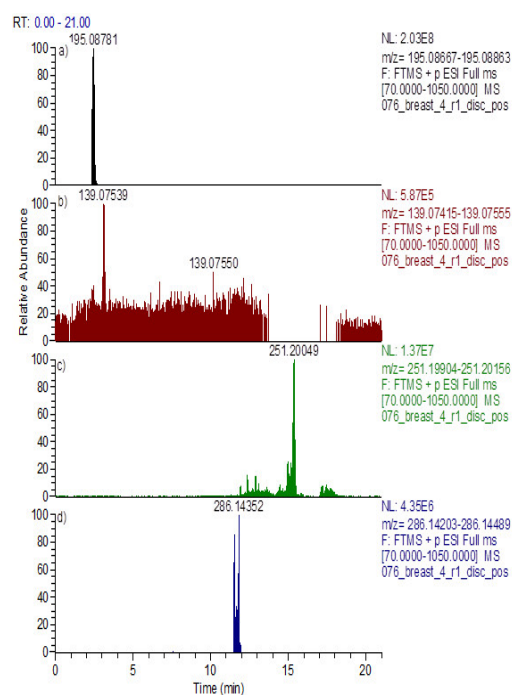


Figure S9. Extracted ion chromatograms (EICs) of the identified compounds at confidence level 1 and 2a in breast milk D by suspect screening in positive ionization modes. (a) Caffeine; (b) 3-Acetyl-2,5-dimethylfuran; (c) OPEO; (d) Piperine.