

Multi-Step Subcritical Water Extracts of *Fucus vesiculosus* L. and *Codium tomentosum* Stackhouse: Composition, Health-Benefits and Safety

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Table S1. Pharmaceuticals, metabolites, transformation products, isotopically labelled internal standards (ILIS), chemical abstracts service (CAS), formula, molecular weight, supplier company, and solvent used for the preparation of each stock solution.

Pharmaceuticals, metabolites, transformation products, and Isotopically Labelled Internal Standards (ILIS) ^{Note 1}	CAS ^{Note 2,3}	Formula (Molecular Weight) ^{Note 3}	Supplier Company	Solvent used for the preparation of each stock solution
Acetaminophen	103-90-2	C ₈ H ₉ NO ₂ (MW=151.165 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile
Acetylsalicylic acid	50-78-2	C ₉ H ₈ O ₄ (MW= 180.159 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile
Alprazolam	28981-97-7	C ₁₇ H ₁₃ ClN ₄ (MW= 308.77 g/mol)	Lipomed AG (Arllesheim, Switzerland)	Methanol
Amfepramone	134-80-5 90-84-6	C ₁₃ H ₂₀ CINO (Amfepramone hydrochloride) (MW= 241.76 g/mol) C ₁₃ H ₁₉ NO (MW= 205.301 g/mol)	Lipomed AG (Arllesheim, Switzerland)	Methanol
Amoxicillin	61336-70-7 26787-78-0	C ₁₆ H ₂₅ N ₃ O ₆ S (Amoxicillin trihydrate) (MW= 419.449 g/mol) C ₁₆ H ₁₉ N ₃ O ₆ S (MW= 365.404 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol-Milli-Q water (2:1, v/v)
Ampicillin	7177-48-2	C ₁₆ H ₁₉ N ₃ O ₄ S (MW= 349.5 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1, v/v)
Atenolol	29122-68-7	C ₁₄ H ₂₂ N ₂ O ₃ (MW= 266.341 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Atorvastatin	344423-98-9 134523-00-5	C ₆₆ H ₇₄ CaF ₂ N ₄ O ₁₃ (Atorvastatin calcium trihydrate) (MW= 1209.408 g/mol) C ₃₃ H ₃₆ FN ₂ O ₅ (MW= 558.65 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-5% acetic acid in Milli-Q water
Azithromycin	83905-01-5	C ₃₈ H ₇₂ N ₂ O ₁₂ (MW= 748.996 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Bupropion	31677-93-7 34911-55-2	C ₁₃ H ₁₉ Cl ₂ NO (Bupropion hydrochloride) (MW= 276.201 g/mol) C ₁₃ H ₁₈ CINO (MW= 239.743 g/mol)	Lipomed AG (Arllesheim, Switzerland)	Methanol
Caffeine	58-08-2	C ₈ H ₁₀ N ₄ O ₂ (MW= 194.194 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Carbamazepine	298-46-4	C ₁₅ H ₁₂ N ₂ O (MW= 236.274 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Carboxybupropfen	15935-54-3	C ₁₃ H ₁₆ O ₄ (MW= 236.267 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile
Chlorpromazine	69-09-0 318.863	C ₁₇ H ₂₀ Cl ₂ N ₂ S (Chlorpromazine hydrochloride) (MW= 355.321 g/mol) C ₁₇ H ₁₉ CIN ₂ S (MW= 318.863 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol-Milli-Q water
Chlortetracycline	64-72-2 57-62-5	C ₂₂ H ₂₄ Cl ₂ N ₂ O ₈ (Chlortetracycline hydrochloride) (MW= 515.34 g/mol) C ₂₂ H ₂₃ CIN ₂ O ₈ (MW= 478.882 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1, v/v)
Ciprofloxacin	85721-33-1	C ₁₇ H ₁₈ FN ₃ O ₃ (MW= 331.347 g/mol)	Sigma-Aldrich (Madrid, Spain)	Milli-Q Water-10% acetic acid in Milli-Q water (1:1, v/v)
Citalopram	59729-33-8	C ₂₀ H ₂₁ FN ₂ O (MW= 324.399 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Citalopram N-oxide	62498-71-9 917482-45-2	C ₂₀ H ₂₂ ClFN ₂ O ₂ (Citalopram N-oxide hydrochloride) (MW= 376.856 g/mol) C ₂₀ H ₂₁ FN ₂ O ₂ (MW= 340.398 g/mol)	H. Lundbeck (Copenhagen, Denmark)	Methanol
Citalopram propionic acid*	Not Available	C ₁₈ H ₁₄ FNO ₃ (MW= 311.312 g/mol)	H. Lundbeck (Copenhagen, Denmark)	Methanol
Clarithromycin	81103-11-9	C ₃₈ H ₆₉ NO ₁₃ (MW= 747.964 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Clobenzorex	5843-53-8 13364-32-4	C ₁₆ H ₁₉ Cl ₂ N (Clobenzorex hydrochloride) (MW= 296.235 g/mol) C ₁₆ H ₁₈ CIN (MW= 259.777 g/mol)	LGC (Middlesex, UK)	Methanol
d-Cathine	2153-98-2	C ₉ H ₁₄ CINO (d-Cathine hydrochloride) (MW= 187.667 g/mol)	Lipomed AG (Arllesheim, Switzerland)	Methanol
Demethylcitalopram	97743-99-2 62498-67-3	C ₁₉ H ₂₀ ClFN ₂ O (Demethylcitalopram hydrochloride) (MW= 346.83 g/mol) C ₁₉ H ₁₉ FN ² O	H. Lundbeck (Copenhagen, Denmark)	Methanol
Diazepam	439-14-5	C ₁₆ H ₁₃ CIN ₂ O (MW= 284.743 g/mol)	Lipomed AG (Arllesheim, Switzerland)	Methanol
Diclofenac	15307-79-6	C ₁₄ H ₁₀ Cl ₂ NNaO ₂ (Diclofenac sodium salt) (MW= 318.12 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1, v/v)

	15307-86-5	C ₁₄ H ₁₁ Cl ₂ NO ₂			
Didemethylcitalopram	1189694-81-2	C ₁₈ H ₁₈ ClFN ₂ O (Didemethylcitalopram hydrochloride) (MW= 332.803 g/mol)	H. Lundbeck (Copenhagen, Denmark)	Methanol	
	62498-69-5	C ₁₈ H ₁₇ FN ₂ O (MW= 296.3 g/mol)			
Diltiazem	33286-22-5	C ₂₂ H ₂₇ ClN ₂ O ₄ S (Diltiazem hydrochloride) (MW= 450.978 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol	
	42399-41-7	C ₂₂ H ₂₆ N ₂ O ₄ S (MW= 414.5 g/mol)			
Doxycycline	24390-14-5	C ₂₂ H ₂₄ N ₂ O ₈ HCl 0.5H ₂ O 0.5C ₂ H ₆ O (Doxycycline hyclate) (MW= 512.94 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1, v/v)	
	564-25-0	C ₂₂ H ₂₄ N ₂ O ₈ (MW= 444.44 g/mol)			
Enrofloxacin	93106-60-6	C ₁₉ H ₂₂ FN ₃ O ₃ (MW= 359.401 g/mol)	Sigma-Aldrich (Madrid, Spain)	Milli-Q Water-10% acetic acid in Milli-Q water (1:1, v/v)	
(+)-Ephedrine	134-71-4	C ₁₀ H ₁₆ CINO ((+)-Ephedrine hydrochloride) (MW= 201.694 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Methanol	
	134-72-5	C ₁₀ H ₁₅ NO (MW= 165.236 g/mol)			
10,11-Epoxy carbamazepine	36507-30-9	C ₁₅ H ₁₂ N ₂ O ₂ (MW= 252.273 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol	
Erythromycin	643-22-1	C ₃₇ H ₆₇ NO ₁₃ (MW= 733.937 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol	
Fenfluramine	404-82-0	C ₁₂ H ₁₇ ClF ₃ N (Fenfluramine hydrochloride) (MW= 267.72 g/mol)	LGC (Middlesex, UK)	Methanol	
	404-82-0	C ₁₂ H ₁₆ F ₃ N (MW= 231.262 g/mol)			
Fenofibrate	49562-28-9	C ₂₀ H ₂₁ ClO ₄ (MW= 360.834 g/mol)	Sigma-Aldrich (Madrid, Spain)		
Fluoxetine	56296-78-7	C ₁₇ H ₁₉ ClF ₃ NO (Fluoxetine hydrochloride) (MW= 345.79 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol	
	54910-89-3	C ₁₇ H ₁₈ F ₃ NO (MW= 309.332 g/mol)			
Gemfibrozil	25812-30-0	C ₁₅ H ₂₂ O ₃ (MW= 250.338 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol	
2-Hydroxyibuprofen	51146-55-5	C ₁₃ H ₁₈ O ₃ (MW= 222.284 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile	
Ibuprofen	15687-27-1	C ₁₃ H ₁₈ O ₂ (MW= 206.285 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile	
Ketoprofen	22071-15-4	C ₁₆ H ₁₄ O ₃ (MW= 254.285 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile	
Lansoprazole	103577-45-3	C ₁₆ H ₁₄ F ₃ N ₃ O ₂ S (MW= 369.362 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol	
Lomefloxacin hydrochloride	8079-52-8	C ₁₇ H ₂₀ ClF ₂ N ₃ O ₃ (MW= 387.812 g/mol)	Sigma-Aldrich (Madrid, Spain)	Milli-Q Water-10% acetic acid in Milli-Q water (1:1, v/v)	
Lomefloxacin	98079-51-7	C ₁₇ H ₁₉ F ₂ N ₃ O ₃ (MW= 351.354 g/mol)			
Lorazepam	846-49-1	C ₁₅ H ₁₀ Cl ₂ N ₂ O ₂ (MW= 321.157 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Methanol	
Mazindol	22232-71-9	C ₁₆ H ₁₃ CIN ₂ O (MW= 284.743 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Methanol	
Metformin	1115-70-4	C ₄ H ₁₂ ClN ₅ (Metformin hydrochloride) (MW= 165.625 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol	
	657-24-9	C ₄ H ₁₁ N ₅ (MW= 129.167 g/mol)			
d,l-Methamphetamine	300-42-5	C ₁₀ H ₁₆ CIN (d,l-Methamphetamine hydrochloride) (MW= 185.70 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Methanol	
	7632-10-2	C ₁₀ H ₁₅ N (MW= 149.237 g/mol)			
Moxifloxacin	186826-86-8	C ₂₁ H ₂₆ ClFN ₃ O ₄ (Moxifloxacin hydrochloride) (MW= 437.896 g/mol)	Sigma-Aldrich (Madrid, Spain)	Milli-Q Water-10% acetic acid in Milli-Q water (1:1, v/v)	
	151096-09-2	C ₂₁ H ₂₄ FN ₃ O ₄ (MW= 401.438 g/mol)			
Naproxen	22204-53-1	C ₁₄ H ₁₄ O ₃ (MW= 230.263 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1,v/v)	
Nimesulide	51803-78-2	C ₁₃ H ₁₂ N ₂ O ₅ S (MW= 308.308 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile	
d,l-Norephedrine	154-41-6	C ₉ H ₁₄ CINO (d,l-Norephedrine hydrochloride) (MW= 187.667 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Methanol	
	37577-28-9	C ₉ H ₁₃ NO (MW= 151.209 g/mol)			
Norfloxacin	70458-96-7	C ₁₆ H ₁₈ FN ₃ O ₃ (MW= 319.33 g/mol)	Sigma-Aldrich (Madrid, Spain)	Milli-Q Water-10% acetic acid in Milli-Q water (1:1, v/v)	
Norfluooxetine	57226-68-3	C ₁₆ H ₁₇ ClF ₃ NO (Norfluooxetine hydrochloride) (MW= 331.763 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol	
	83891-03-6	C ₁₆ H ₁₆ F ₃ NO (MW= 295.305 g/mol)			
Norsertaline	675126-08-6	C ₁₆ H ₁₆ Cl ₃ N (Norsertaline hydrochloride) (MW= 328.661 g/mol)	Cerilliant-Certified Reference Materials (Texas, USA)	Purchased as methanolic solution	
	87857-41-8	C ₁₆ H ₁₅ Cl ₂ N (MW= 292.203 g/mol)			
O-Desmethylvenlafaxine	93413-62-8	C ₁₆ H ₂₅ NO ₂ (MW= 263.381 g/mol)	Sigma-Aldrich (Madrid, Spain)	Purchased as methanolic solution	
Ofloxacin	82419-36-1	C ₁₈ H ₂₀ FN ₃ O ₄ (MW= 361.373 g/mol)	Sigma-Aldrich (Madrid, Spain)	Milli-Q Water-10% acetic acid in Milli-Q water (1:1, v/v)	
Oxytetracycline	2058-46-0	C ₂₂ H ₂₅ CIN ₂ O ₉ (Oxytetracycline hydrochloride) (MW= 496.897 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1, v/v)	

	2058-46-0	C ₂₂ H ₂₄ N ₂ O ₉ (MW= 460.439 g/mol)		
Paroxetine	78246-49-8	C ₁₉ H ₂₁ ClFNO ₃ (Paroxetine hydrochloride) (MW= 365.829 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
	110429-35-1	C ₁₉ H ₂₀ FNO ₃ (MW= 329.371 g/mol)		
Phenolphthalein	77-09-8	C ₂₀ H ₁₄ O ₄ (MW= 318.328 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Phentermine	1197-21-3	C ₁₀ H ₁₆ CIN (Phentermine hydrochloride) (MW= 185.695 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Methanol
	122-09-8	C ₁₀ H ₁₅ N (MW= 149.237 g/mol)		
Pravastatin	81131-70-6	C ₂₃ H ₃₆ NaO ₇ (Pravastatin sodium salt hydrate) (MW= 446.516 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
	81093-37-0	C ₂₃ H ₃₆ O ₇ (MW= 424.534 g/mol)		
Propranolol	318-98-9	C ₁₆ H ₂₂ ClNO ₂ (Propranolol hydrochloride) (MW= 295.807 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
	525-66-6	C ₁₆ H ₂₁ NO ₂ (MW= 259.349 g/mol)		
Prulifloxacin	123447-62-1	C ₂₁ H ₂₆ FN ₃ O ₆ S (MW= 461.464 g/mol)	Toronto Research Chemicals Inc. (Ontario, Canada)	Milli-Q Water-10% acetic acid in Milli-Q water (1:1, v/v)
Rimionabant	168273-06-1	C ₂₂ H ₂₁ Cl ₃ N ₄ O (MW= 463.787 g/mol)	LGC (Middlesex, UK)	Methanol
Salicylic acid	69-72-7	C ₇ H ₆ O ₃ (MW= 138.122 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile
Sertraline	79559-97-0	C ₁₇ H ₁₈ Cl ₃ N (Sertraline hydrochloride) (MW= 342.688 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
	79617-96-2	C ₁₇ H ₁₇ Cl ₂ N (MW= 306.23 g/mol)		
Sibutramine	84485-00-7	C ₁₇ H ₂₇ Cl ₂ N (Sibutramine hydrochloride) (MW= 316.31 g/mol)	LGC (Middlesex, UK)	Purchased as methanolic solution
	106650-56-0	C ₁₇ H ₂₆ CIN (MW= 279.852 g/mol)		
Simvastatin	79902-63-9	C ₂₈ H ₃₈ O ₅ (MW= 418.574 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Sulfadiazine	68-35-9	C ₁₀ H ₁₀ N ₄ O ₂ S (MW= 250.276 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Sulfadimethoxine	122-11-2	C ₁₂ H ₁₄ N ₄ O ₄ S (MW= 310.328 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Sulfamethazine	57-68-1	C ₁₂ H ₁₄ N ₄ O ₂ S (MW= 278.33 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Sulfamethizole	144-82-1	C ₉ H ₁₀ N ₄ O ₂ S ₂ (MW= 270.325 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1, v/v)
Sulfamethoxazole	723-46-6	C ₁₀ H ₁₁ N ₃ O ₃ S (MW= 253.276 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Sulfamethoxypyridazine	80-35-3	C ₁₁ H ₁₂ N ₄ O ₃ S (MW= 280.302 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Sulfapyridine	144-83-2	C ₁₁ H ₁₁ N ₃ O ₂ S (MW= 249.288 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Sulfaquinoxaline	59-40-5	C ₁₄ H ₁₂ N ₄ O ₂ S (MW= 300.336 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Sulfathiazole	144-74-1	C ₉ H ₈ N ₃ NaO ₂ S ₂ (Sulfathiazole sodium salt) (MW= 277.292 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1, v/v)
	72-14-0	C ₉ H ₈ N ₃ O ₂ S ₂ (MW= 255.31 g/mol)		
Synephrine	94-07-5	C ₉ H ₁₃ NO ₂ (MW= 167.208 g/mol)	LGC (Middlesex, UK)	Methanol
Tetracycline	64-75-5	C ₂₂ H ₂₆ ClN ₂ O ₈ (Tetracycline hydrochloride) (MW=480.898 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile-metanol (1:1, v/v)
	64-75-5	C ₂₂ H ₂₄ N ₂ O ₈ (MW= 444.44 g/mol)		
Topiramate	97240-79-4	C ₁₂ H ₂₁ NO ₈ S (MW= 339.359 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Methanol
Trazodone	19666-36-5	C ₁₉ H ₂₃ Cl ₂ N ₅ O (Trazodone hydrochloride) (MW= 408.327 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
	19794-93-5	C ₁₉ H ₂₂ ClN ₅ O (MW= 371.869 g/mol)		
Trimethoprim	738-70-5	C ₁₄ H ₁₈ N ₄ O ₃ (MW= 290.323 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
Venlafaxine	99300-78-4	C ₁₇ H ₂₈ ClNO ₂ (Venlafaxine hydrochloride) (MW= 313.866 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
	93413-69-5	C ₁₇ H ₂₇ NO ₂ (MW= 277.408 g/mol)		
Zonisamide	68291-97-4	C ₈ H ₈ N ₂ O ₃ S (MW= 212.223 g/mol)	LGC (Middlesex, UK)	Methanol
ILIS, Acetaminophen-d4	64315-36-2	C ₈ H ₅ D ₄ NO ₂ (MW= 155.189 g/mol)	Toronto Research Chemicals Inc. (Ontario, Canada)	Acetonitrile
ILIS, Atenolol-d7	1202864-50-3	C ₁₄ H ₁₅ D ₇ N ₂ O ₃ (MW= 273.384 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
ILIS, Azithromycin-d3	163921-65-1	C ₃₈ H ₆₉ D ₃ N ₂ O ₁₂ (MW= 752.014 g/mol)	Toronto Research Chemicals Inc. (Ontario, Canada)	Methanol
ILIS, Caffeine ¹³ C ₃	78072-66-9	¹³ C ₃ C ₅ H ₁₀ N ₄ O ₂ (MW= 197.17 g/mol)	Sigma-Aldrich (Madrid, Spain)	Purchased as methanolic solution
ILIS, Carbamazepine-d10	132183-78-9	C ₁₅ H ₂ D ₁₀ N ₂ O (MW= 246.33 g/mol)	Cerilliant-Certified Reference Materials (Texas, USA)	Purchased as methanolic solution
ILIS, Ciprofloxacin-d8 hydrochloride	1216659-54-9	C ₁₇ H ₁₁ D ₈ ClFN ₃ O ₃ (MW= 375.85 g/mol)	Toronto Research Chemicals Inc. (Ontario, Canada)	Milli-Q Water-10% acetic acid in Milli-Q water (1:1, v/v)

ILIS , d,l-Methamphetamine-d5 hydrochloride	60124-88-1	C ₁₀ H ₁₁ ClD ₅ N (MW= 190.74 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Methanol
ILIS , Diazepam-d5	65854-76-4	C ₁₆ H ₈ D ₅ ClN ₂ O (MW= 289.77 g/mol)	Lipomed AG (Arlesheim, Switzerland)	Purchased as methanolic solution
ILIS , Fluoxetine-d5 hydrochloride	1173020-43-3	C ₁₇ H ₁₄ D ₅ ClF ₃ NO (MW= 350.821 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
ILIS , Gemfibrozil-d6	1184986-45-5	C ₈ H ₅ D ₄ NO ₂ (MW= 256.37 g/mol)	Toronto Research Chemicals Inc. (Ontario, Canada)	Methanol
ILIS , Ibuprofen-d3	121662-14-4	C ₁₃ H ₁₈ D ₃ O ₂ (MW= 209.30 g/mol)	Sigma-Aldrich (Madrid, Spain)	Acetonitrile
ILIS , Metformin-(dimethyl-d6) hydrochloride	1185166-01-1	C ₄ D ₆ H ₆ ClN ₅ (MW= 171.66 g/mol)	Sigma-Aldrich (Madrid, Spain)	Methanol
ILIS , Propranolol-d7	344298-99-3	C ₁₆ H ₂₁ D ₇ NO ₂ (MW= 266.39 g/mol)	LGC (Middlesex, UK)	Methanol
ILIS , Salicylic acid-d4	97781-16-3	C ₉ H ₄ D ₄ O ₄ (MW= 184.18 g/mol)	Toronto Research Chemicals Inc. (Ontario, Canada)	Acetonitrile
ILIS , Sulfamethoxazole-d4	1020719-86-1	C ₁₀ H ₇ D ₄ N ₃ O ₃ S (MW= 257.3 g/mol)	Toronto Research Chemicals Inc. (Ontario, Canada)	Methanol
ILIS , Topiramate-d12	1279037-95-4	C ₁₂ H ₅ D ₁₂ NO ₆ S (MW= 351.44 g/mol)	LGC (Middlesex, UK)	Purchased as methanolic solution
ILIS , Venlafaxine-d6	1062606-12-5	C ₁₇ H ₂₂ ClD ₆ NO ₂ (MW= 319.90 g/mol)	Cerilliant-Certified Reference Materials (Texas, USA)	Purchased as methanolic solution

* for the compound Citalopram propionic acid, the information of CAS is not available.

Note 1: Pharmaceuticals organized in the table by alphabetic order. **Note 2:** Chemical Abstracts Service, CAS (a unique numerical identifier assigned by the Chemical Abstracts Service to every chemical substance described in the open scientific literature).

Note 3: CAS, formula, and molecular weight for all the compounds were obtained in the web site of PubChem (PubChem is an open chemistry database at the National Institutes of Health (NIH) [Available at: <https://pubchem.ncbi.nlm.nih.gov/>], with exception for citalopram propionic acid [Available at: <http://www.hmdb.ca/metabolites/HMDB60463>].

Table S2. Pesticides, transformation products, isotopically labelled internal standards (ILIS), chemical abstracts service (CAS), formula, molecular weight, supplier company, and solvent used for the preparation of each stock solution.

Pesticides, transformation products, and isotopically Labelled Internal Standard (ILIS) ^{Note 1}	CAS ^{Note 2,3}	Formula (Molecular Weight) ^{Note 3}	Supplier Company	Solvent used for the preparation of each stock solution
Alachlor	15972-60-8	C ₁₄ H ₂₀ ClNO ₂ (MW= 269.8 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Ametryn	384-12-8	C ₉ H ₁₁ N ₅ S (MW= 227.12 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Asulam	3337-71-1	C ₈ H ₁₀ N ₂ O ₄ S (MW= 230.2 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Atrazine	1912-24-9	C ₈ H ₁₄ ClN ₅ (MW= 175.8 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Atrazine-desethyl	6190-65-4	C ₈ H ₁₀ ClN ₅ (MW= 187.63 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Atrazine-desisopropyl	1007-28-9	C ₈ H ₈ ClN ₅ (MW= 173.6 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Azinphos-methyl	86-50-0	C ₁₀ H ₁₂ N ₃ O ₃ PS ₂ (MW= 317.32 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Azoxystrobin	131860-33-8	C ₂₂ H ₁₇ N ₃ O ₅ (MW= 403.4 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Bensulfuron-methyl	83055-99-6	C ₁₆ H ₁₈ N ₄ O ₇ S (MW= 410.4 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Bentazone	25057-89-0	C ₁₀ H ₁₂ N ₂ O ₃ S (MW= 240.3 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Carbaryl	63-25-2	C ₁₂ H ₁₁ NO ₂ (MW= 201.2 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Carbofuran	1563-66-2	C ₁₂ H ₁₅ NO ₃ (MW= 221.3 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Chlorfenvinphos	470-90-6	C ₁₂ H ₁₄ Cl ₂ O ₄ P (MW= 359.6 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Chlortoluron	15545-48-9	C ₁₀ H ₁₃ ClN ₂ O (MW= 212.7 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Chlorpropham	101-21-3	C ₁₀ H ₁₂ ClNO (MW= 213.7 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Dimethoate	60-51-5	C ₅ H ₁₂ NO ₃ PS ₂ (MW= 229.3 g/mol)	Fluka™ (Seelze, Germany)	Methanol
Diuron	330-54-1	C ₉ H ₁₀ Cl ₂ N ₂ O (MW= 233.1 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Imidacloprid	138261-41-3	C ₉ H ₁₀ ClN ₃ O ₂ (MW= 255.7 g/mol)	Sigma Aldrich (Madrid, Spain)	Acetonitrile
Isoproturon	34123-59-6	C ₁₂ H ₁₈ N ₂ O (MW= 206.3 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Linuron	330-55-2	C ₈ H ₁₀ Cl ₂ N ₂ O ₂ (MW= 249.1 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Malathion	121-75-5	C ₁₀ H ₁₉ O ₆ PS ₂ (MW= 330.3 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Metalaxyl	57837-19-1	C ₁₅ H ₂₁ NO ₄ (MW= 379.3 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Metolachlor	51218-45-2	C ₁₅ H ₂₂ ClNO ₂ (MW= 283.79 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
Methiocarb	2032-65-7	C ₁₁ H ₁₅ NO ₂ S (MW= 225.3 g/mol)	Fluka™ (Seelze, Germany)	Methanol
Methiocarb sulfone	2179-25-1	C ₁₁ H ₁₅ NO ₄ S (MW= 257.3 g/mol)	Fluka™ (Seelze, Germany)	Methanol
Methiocarb sulfoxide	2635-10-1	C ₁₁ H ₁₅ NO ₃ S (MW= 241.3 g/mol)	Fluka (Seelze, Germany)	Methanol
Metobromuron	3060-89-7	C ₈ H ₁₁ BrN ₂ O ₂ (MW= 259.1 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Monolinuron	1746-81-2	C ₉ H ₁₁ ClN ₂ O ₂ (MW= 214.6 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Pirimicarb	23103-28-2	C ₁₁ H ₁₈ NaO ₂ (MW= 238.3 g/mol)	Fluka™ (Seelze, Germany)	Acetonitrile
Propoxur	114-26-1	C ₁₁ H ₁₅ NO ₃ (MW= 209.2 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Acetonitrile
Pyrimethanil	53112-28-0	C ₁₂ H ₁₃ N ₃ (MW= 199.3 g/mol)	Fluka™ (Seelze, Germany)	Methanol
Terbuthylazine	5915-41-3	C ₉ H ₁₆ ClN ₅ (MW= 229.7 g/mol)	Sigma Aldrich (Madrid, Spain)	Acetonitrile
Thiobencarb	28249-77-6	C ₁₂ H ₁₆ ClNOS (MW= 257.8 g/mol)	Riedel-de-Haën™ (Seelze, Germany)	Methanol
ILIS, Diuron-d6	1007536-67-5	C ₉ H ₄ D ₆ Cl ₂ N ₂ O (MW= 239.13 g/mol)	Sigma Aldrich (Madrid, Spain)	Methanol

Note 1: Pesticides organized in the table by alphabetic order. **Note 2:** Chemical Abstracts Service, CAS (a unique numerical identifier assigned by the Chemical Abstracts Service to every chemical substance described in the open scientific literature). **Note 3:** CAS, formula, and molecular weight for all the compounds were obtained in the web site of PubChem (PubChem is an open chemistry database at the National Institutes of Health (NIH) [Available at: <https://pubchem.ncbi.nlm.nih.gov/>].

Table S3. Concentration in the standards and in the analysed samples of the fifteen isotopically labelled internal standards (ILIS).

Isotopically Labelled Internal Standards (ILIS) ^{Note 1}	Final concentration (µg/L)
Acetaminophen-d4	800
Azithromycin-d3	900
Caffeine ¹³ C ₃	400
Carbamazepine-d10	100
d,l-Methamphetamine-d5 hydrochloride	200
Diuron-d6	1000
Diazepam-d5	200
Fluoxetine-d5 hydrochloride	60
Gemfibrozil-d6	250
Ibuprofen-d3	1000
Metformin-(dimethyl-d6) hydrochloride	50
Salicylic acid-d4	55
Sulfamethoxazole-d4	400
Topiramate-d12	150
Venlafaxine-d6	100

Note1: the fifteen isotopically labelled internal standards are listed in the table by alphabetic order.

Table S4. Therapeutic class, pharmaceuticals, ionization mode, precursor and product ions, mass spectrometry conditions, ion ratio, and isotopically labelled internal standards (ILIS) for each pharmaceutical in study. Legend: P- Chromatographic program.

Therapeutic class	Pharmaceuticals, metabolites, transformation products, and isotopically labelled internal standards (ILIS) <i>Note 1</i>	ESI	Precursor (m/z)	Quantitation product				Qualifier Product				Dwell Time (msec)	ILIS	P
				m/z	Q1	CE	Q3	m/z	Q1	CE	Q3			
					Pre Bias (V)		Pre Bias (V)		Pre Bias (V)		Pre Bias (V)			
Analgesic	Acetaminophen	ESI-	150.20	107.15	16.0	20.0	17.0		Note 2			25.0	2	PI
NSAIDs	Acetylsalicylic acid	ESI-	179.30	137.15	20.0	10.0	21.0	92.90	19.0	22.0	10.0	25.0	1	PI
NSAIDs-metabolite	Carboxyibuprofen	ESI-	235.20	191.25	25.0	9.0	16.0	72.90	24.0	17.0	11.0	25.0	3	PI
NSAIDs	Diclofenac	ESI-	294.10	250.20	11.0	11.0	14.0	35.05	14.0	24.0	11.0	25.0	3	PI
NSAIDs-metabolite	2-Hydroxyibuprofen	ESI-	221.20	177.30	23.0	8.0	10.0		Note 2			25.0	3	PI
NSAIDs	Ibuprofen	ESI-	205.20	161.30	21.0	10.0	23.0		Note 2			25.0	3	PI
	Ketoprofen	ESI-	253.20	209.20	27.0	7.0	12.0		Note 2			25.0	3	PI
	Naproxen	ESI-	229.20	170.00	24.0	16.0	17.0	169.25	25.0	31.0	17.0	25.0	3	PI
	Nimesulide	ESI-	307.00	229.15	15.0	16.0	17.0	79.05	15.0	26.0	29.0	25.0	3	PI
NSAIDs-transformation product	Salicylic acid	ESI-	137.30	93.10	15.0	17.0	14.0	65.10	15.0	30.0	10.0	25.0	1	PI
Antibiotic	Azithromycin	ESI+	749.30	158.00	-28.0	-45.0	-16.0	116.10	-38.0	-55.0	-11.0	10.0	9	PII
	Ciprofloxacin	ESI+	332.00	314.05	-17.0	-22.0	-22.0	231.00	-24.0	-39.0	-16.0	10.0	10	PII
	Clarithromycin	ESI+	748.30	158.05	-28.0	-34.0	-10.0	83.00	-28.0	-54.0	-17.0	10.0	9	PII
	Enrofloxacin	ESI+	360.00	316.10	-18.0	-21.0	-15.0	342.10	-27.0	-23.0	-24.0	10.0	10	PII
	Erythromycin	ESI+	734.40	158.00	-28.0	-33.0	-10.0	83.00	-28.0	-55.0	-19.0	10.0	9	PII
	Lomefloxacin	ESI+	352.00	264.95	-29.0	-25.0	-19.0	333.95	-18.0	-22.0	-24.0	10.0	10	PII
	Moxifloxacin	ESI+	402.05	384.05	-21.0	-23.0	-26.0	95.95	-15.0	-48.0	-20.0	10.0	10	PII
	Norfloxacin	ESI+	320.00	302.05	-27.0	-22.0	-21.0	231.00	-26.0	-43.0	-16.0	10.0	10	PII
	Ofloxacin	ESI+	362.00	318.10	-29.0	-21.0	-15.0	260.95	-29.0	-29.0	-18.0	10.0	10	PII
	Prulifloxacin	ESI+	462.00	443.95	-17.0	-22.0	-22.0	360.00	-24.0	-32.0	-24.0	10.0	10	PII
	Sulfadiazine	ESI+	250.90	155.90	-18.0	-18.0	-10.0	91.95	-19.0	-30.0	-19.0	10.0	10	PII
	Sulfadimethoxine	ESI+	310.90	155.90	-24.0	-23.0	-15.0	91.95	-25.0	-38.0	-18.0	10.0	10	PII
	Sulfamethazine	ESI+	278.90	185.90	-23.0	-19.0	-12.0	91.95	-22.0	-36.0	-19.0	10.0	10	PII
	Sulfamethoxazole	ESI+	253.95	155.90	-29.0	-18.0	-16.0	91.95	-20.0	-32.0	-18.0	10.0	10	PII
	Sulfamethoxypyridazine	ESI+	280.90	155.95	-14.0	-19.0	-10.0	92.00	-14.0	-32.0	-18.0	10.0	10	PII
	Sulfapyridine	ESI+	249.90	155.95	-18.0	-18.0	-16.0	91.95	-28.0	-31.0	-20.0	10.0	10	PII
	Trimethoprim	ESI+	291.00	230.00	-23.0	-25.0	-15.0	123.00	-23.0	-27.0	-12.0	10.0	10	PII
Pshychiatric drugs	Carbamazepine	ESI+	236.95	193.95	-18.0	-21.0	-23.0	193.00	-26.0	-36.0	-13.0	10.0	11	PII
	Citalopram	ESI+	325.05	108.95	-16.0	-29.0	-23.0	261.95	-16.0	-22.0	-18.0	10.0	12	PII
	Diazepam	ESI+	284.95	153.90	-23.0	-29.0	-10.0	192.95	-23.0	-33.0	-23.0	10.0	7	PII
Pshychiatric drugs-metabolite	10,11-Epoxy carbamazepine	ESI+	253.00	179.95	-21.0	-27.0	-12.0	235.90	-21.0	-12.0	-16.0	10.0	11	PII

Pshychiatric drugs	Fluoxetine	ESI+	309.95	44.00	-25.0	-14.0	-18.0		Note 2		10.0	12	PII	
Pshychiatric drugs -metabolite	Norfluoxetine	ESI+	296.00	134.0	-23.0	-8.0	-13.0	30.20	-24.0	-15.0	-12.0	10.0	12	PII
	Norsertraline	ESI+	291.90	274.90	-23.0	-11.0	-19.0	158.95	-22.0	-24.0	-10.0	10.0	12	PII
Pshychiatric drugs	Paroxetine	ESI+	330.00	70.0	-27.0	-34.0	-14.0	44.0	-37.0	-28.0	-14.0	10.0	12	PII
	Sertraline	ESI+	305.95	158.90	-15.0	-26.0	-15.0	274.95	-25.0	-13.0	-19.0	10.0	12	PII
	Trazodone	ESI+	372.05	175.95	-19.0	-26.0	-11.0	147.95	-19.0	-40.0	-15.0	10.0	12	PII
	Venlafaxine	ESI+	278.10	58.00	-20.0	-25.0	-20.0	260.05	-23.0	-14.0	-12.0	10.0	13	PII
Antibiotic	Ampicillin	ESI+	348.00	307.05	-17.0	-10.0	-21.0		Note 2		15.0	12	PII	
Lipid regulator and cholesterol lowering statin drugs	Atorvastatin	ESI+	559.10	440.05	-20.0	-24.0	-16.0	250.00	-20.0	-47.0	-16.0	15.0	12	PII
β-blockers	Atenolol	ESI+	267.05	144.95	-10.0	-28.0	-15.0	56.00	-22.0	-34.0	-11.0	15.0	12	PII
Stimulant	Caffeine	ESI+	194.95	138.00	-22.0	-21.0	-13.0	42.00	-23.0	-41.0	-16.0	15.0	8	PII
Antibiotic	Chlorocycline	ESI+	479.00	444.00	-24.0	-24.0	-15.0	462.00	-24.0	-20.0	-22.0	15.0	12	PII
Antipsychotic drugs	Chlorpromazine	ESI+	319.00	85.95	-22.0	-21.0	-18.0	58.00	-25.0	-43.0	-12.0	15.0	12	PII
Pshychiatric drugs -metabolite	Demethylcitalopram	ESI+	352.05	311.00	-29.0	-8.0	-15.0	108.95	-18.0	-34.0	-22.0	15.0	12	PII
	Didemethylcitalopram	ESI+	297.00	108.95	-25.0	-23.0	-10.0	262.00	-23.0	-15.0	-18.0	15.0	12	PII
	Citalopram N-oxide	ESI+	341.05	108.95	-17.0	-26.0	-10.0	261.95	-28.0	-19.0	-18.0	15.0	12	PII
	O-Desmethylvenlafaxine	ESI+	264.00	58.00	-20.0	-25.0	-20.0	246.05	-21.0	-13.0	-17.0	15.0	13	PII
Calcium channel blocker	Diltiazem	ESI+	415.05	178.00	-20.0	-30.0	-20.0	150.00	-13.0	-48.0	-15.0	15.0	12	PII
Antibiotic	Doxycycline	ESI+	445.05	428.05	-17.0	-21.0	-15.0	97.95	-17.0	-47.0	-20.0	15.0	12	PII
Fibrate lipid lowering agent	Fenofibrate	ESI+	361.00	232.855	-29.0	-16.0	-16.0	138.95	-18.0	-35.0	-13.0	15.0	12	PII
Proton pump inhibitor	Lanzoprazole	ESI+	370.00	251.90	-19.0	-13.0	-17.0	118.90	-30.0	-17.0	-12.0	15.0	12	PII
Antidiabetic drugs	Metformin	ESI+	129.50	70.95	-10.0	-24.0	-14.0	59.95	-10.0	-15.0	-13.0	15.0	16	PII
Antibiotic	Oxytetracycline	ESI+	460.95	425.95	-23.0	-20.0	-15.0	443.05	-17.0	-15.0	-22.0	15.0	12	PII
β-blockers	Propanolol	ESI+	301.00	260.00	-25.0	-8.0	-18.0		Note 2		15.0	12	PII	
Lipid regulator and cholesterol lowering statin drugs	Simvastatin	ESI+	419.15	199.00	-15.0	-15.0	-13.0	285.00	-16.0	-13.0	-20.0	15.0	12	PII
Antibiotic	Sulfamethizole	ESI+	270.85	155.95	-13.0	-16.0	-19.0	92.00	-21.0	-31.0	-19.0	15.0	10	PII
	Sulfaquinoxaline	ESI+	300.90	155.95	-25.0	-19.0	-10.0	92.00	-25.0	-37.0	-18.0	15.0	10	PII
	Sulfathiazole	ESI+	255.85	155.90	-19.0	-17.0	-16.0	92.00	-19.0	-29.0	-18.0	15.0	10	PII
	Tetracycline	ESI+	445.05	410.00	-13.0	-22.0	-20.0	153.95	-22.0	-29.0	-15.0	15.0	12	PII
Antibiotic	Amoxicillin	ESI-	364.10	223.00	17.0	11.0	12.0	205.95	18.0	18.0	28.0	25.0	5	PIII
Pshychiatric drugs- metabolite	Citalopram propionic acid	ESI-	310.05	266.10	15.0	11.0	11.0	236.20	30.0	18.0	10.0	25.0	5	PIII
Lipid regulator and cholesterol lowering statin drugs	Gemfibrozil	ESI-	249.20	120.95	26.0	13.0	11.0	105.95	27.0	50.0	15.0	25.0	5	PIII
Stimulant, anorectic, anxiolytics, laxatives	Phenolphthalein	ESI-	317.20	93.10	30.0	14.0	10.0	273.20	28.0	18.0	15.0	25.0	4	PIII
Lipid regulator and cholesterol lowering statin drugs	Pravastatin	ESI-	423.15	101.15	21.0	30.0	15.0	58.85	20.0	24.0	17.0	25.0	5	PIII
Stimulant, anorectic, anxiolytics, laxatives	Topiramate	ESI-	338.10	78.05	21.0	31.0	13.0	95.85	16.0	25.0	10.0	25.0	4	PIII
	Zonisamide	ESI-	211.10	118.95	22.0	15.0	18.0	147.20	22.0	11.0	11.0	25.0	4	PIII
Stimulant, anorectic, anxiolytics, laxatives	Alprazolam	ESI+	308.50	280.90	-25.0	-29.0	-19.0	205.05	-12.0	-43.0	-14.0	15.0	7	PIV
	Anfepramone	ESI+	205.80	105.00	-24.0	-24.0	-20.0	100.00	-10.0	-25.0	-20.0	15.0	6	PIV
	Bupropion	ESI+	239.90	184.00	-29.0	-14.0	-20.0	130.95	-27.0	-30.0	-12.0	15.0	6	PIV

	<i>d</i> -Cathine	ESI+	151.90	134.00	-17.0	-15.0	-13.0	116.95	-17.0	-20.0	-11.0	15.0	6	PIV
	Clobenzorex	ESI+	260.00	91.00	-17.0	-27.0	-18.0	119.00	-21.0	-17.0	-11.0	15.0	6	PIV
	(+)-Ephedrine	ESI+	165.90	148.00	-20.0	-15.0	-16.0	116.95	-18.0	-22.0	-11.0	15.0	6	PIV
	Fenfluramine	ESI+	231.90	159.90	-27.0	-230	-10.0	109.00	-26.0	-48.0	-10.0	15.0	6	PIV
	Lorazepam	ESI+	320.90	274.85	-26.0	-24.0	-18.0	302.90	-26.0	-17.0	-14.0	15.0	7	PIV
	Mazindol	ESI+	284.90	44.00	-23.0	-27.0	-17.0	Note 2				15.0	6	PIV
	<i>d,l</i> -Methamphetamine	ESI+	149.80	91.05	-11.0	-22.0	-17.0	119.10	-11.0	-17.0	-24.0	15.0	6	PIV
	<i>d,l</i> -Norephedrine	ESI+	151.80	134.10	-10.0	-15.0	-14.0	117.05	-10.0	-21.0	-23.0	15.0	6	PIV
	Phentermine	ESI+	149.90	90.95	-17.0	-22.0	-20.0	18.05	-17.0	-9.0	-20.0	15.0	6	PIV
	Rimonabant	ESI+	462.90	362.90	-23.0	-30.0	-25.0	84.00	-23.0	-28.0	-18.0	15.0	6	PIV
	Sibutramine	ESI+	279.90	124.90	-23.0	-26.0	-13.0	139.00	-19.0	-17.0	-14.0	15.0	6	PIV
	Synephrine	ESI+	167.90	149.95	-19.0	-12.0	18.0	90.95	-19.0	-23.0	-19.0	15.0	6	PIV
Isotopically labelled internal standards (ILIS)	1-Salicylin acid-d4 (ILIS 1)	ESI-	141.00	97.05	16.0	17.0	20.0	Note 3				25.0	-	PI
	2-Acetaminophen-d4 (ILIS 2)	ESI-	154.10	111.05	20.0	20.0	20.0	Note 3				25.0	-	PI
	3-Ibuprofen-d3 (ILIS 3)	ESI-	208.00	164.00	21.0	10.0	23.0	Note 3				25.0	-	PI
	4-Topiramate-d12 (ILIS 4)	ESI-	350.20	77.95	21.0	31.0	13.0	Note 3				25.0	-	PIII
	5-Gemfibrazil-d6 (ILIS 5)	ESI-	255.20	121.10	26.0	13.0	11.0	Note 3				25.0	-	PIII
	6-d,l-Methamphetamine-d5 (ILIS 6)	ESI+	154.70	92.10	-11.0	-21.0	-17.0	Note 3				15.0	-	PIV
	7-Diazepam-d5** (ILIS 7)	ESI+	289.90	154.05	-23.0	-31.0	-10.0-	Note 3				10.0	--	PII
	7-Diazepam-d5*** (ILIS 7)	ESI+	289.90	154.05	-23.0	-31.0	10.0	Note 3				15.0	-	PIV
	8-Caffeine ¹³ C ₃ (ILIS 8)	ESI+	197.95	140.05	-22.0	-22.0	-14.0	Note 3				10.0	-	PII
	9-Azithromycin-d3 (ILIS 9)	ESI+	752.30	83.15	-38.0	-55.0	-11.0	Note 3				10.0	-	PII
	10-Sulfamethoxazole-d4 (ILIS 10)	ESI+	258.00	96.10	-29.0	-18.0	-16.0	Note 3				10.0	-	PII
	11-Carbamazepine-d10 (ILIS 11)	ESI+	246.95	204.10	-18.0	-22.0	-23.0	Note 3				10.0	-	PII
	12-Fluoxetine-d5 (ILIS 12)	ESI+	315.05	44.05	-25.0	-15.0	-20.0	Note 3				10.0	-	PII
	13-Venlafaxine-d6 (ILIS 13)	ESI+	283.80	64.05	-20.0	-25.0	-20.0	Note 3				10.0	-	PII
	14-Metformin-d6 (ILIS 14)	ESI+	135.95	60.10	-10.0	-16.0	-13.0	Note 3				10.0	-	PII

** Conditions of diazepam-d5 in program II; *** Conditions of diazepam-d5 in program IV

Note 1: Pharmaceuticals organized in the table by alphabetic order in each chromatographic program; **Note 2:** Only one transition could be recorded due to the poor fragmentation of the compound [Gros M, Petrović M, Barceló D. Development of a multi-residue analytical methodology based on liquid chromatography–tandem mass spectrometry (LC–MS/MS) for screening and trace level determination of pharmaceuticals in surface and wastewaters. Talanta 2006; 70: 678-690]; **Note 3:** For the isotopically labelled internal standards only one transition is needed.

Table S5. Chemical family, pesticides type, name of each pesticides, ionization mode, precursor and product ions, mass spectrometry conditions, ion ratio, and isotopically labelled internal standards (ILIS). Legend: P- Chromatographic program.

Chemical Family, Pesticide Type	Pesticides, transformation products, and isotopically labelled internal standards (ILIS) ^{Note 1}	ESI	Precursor (m/z)	Quantitation product				Qualifier Product				Dwell Time (msec)	ILIS	P
				m/z	Q1	CE	Q3	m/z	Q1	CE	Q3			
					Pre Bias (V)		Pre Bias (V)			Pre Bias (V)				
Chloroacetanilide, Herbicide	Alachlor	ESI+	270.00	238.05	-21.0	-13.0	-16.0	45.00	-30.0	-30.0	-17.0	2.5	15	PV
1,3,5-triazine, Herbicide	Ametryn	ESI+	228.00	185.95	-22.0	-21.0	-21.0	67.95	-27.0	-41.0	-14.0	2.5	15	PV
Carbamate, Herbicide	Asulam	ESI+	230.90	155.95	-18.0	-13.0	-16.0	91.90	-19.0	-28.0	-19.0	2.5	15	PV
1,3,5-triazine, Herbicide	Atrazine	ESI+	215.95	173.95	-25.0	-19.0	-11.0	43.00	-25.0	-44.0	-16.0	2.5	15	PV
1,3,5-triazine, atrazine degradation product	Atrazine-desethyl	ESI+	187.95	145.95	-16.0	-19.0	-15.0	43.00	-22.0	-38.0	-17.0	2.5	15	PV
1,3,5-triazine, atrazine degradation product	Atrazine-desisopropyl	ESI+	173.90	43.00	-21.0	-34.0	-17.0	67.95	-20.0	-30.0	-12.0	2.5	15	PV
Organophosphorus, Insecticide; acaricide; molluscicide	Azinphos-methyl	ESI+	317.90	159.95	-26.0	-10.0	-10.0	131.95	-15.0	-18.0	-14.0	2.5	15	PV
Strobilurin analog, Fungicide	Azoxystrobin	ESI+	403.95	372.05	-21.0	-16.0	-26.0	329.00	-20.0	-32.0	-15.0	2.5	15	PV
Sulfonylurea, Herbicide	Bensulfuron-methyl	ESI+	410.95	148.95	-20.0	-23.0	-16.0	182.00	-20.0	-21.0	-12.0	2.5	15	PV
Benzothiazinone, Herbicide	Bentazon	ESI-	239.15	132.20	26.0	26.0	14.0	175.20	25.0	19.0	10.0	2.5	15	PV
Carbamate, Insecticide; plant growth regulator	Carbaryl	ESI+	201.90	145.00	-22.0	-12.0	-17.0	127.00	-25.0	-32.0	-12.0	2.5	15	PV
Carbamate, Insecticide; nematocide	Carbofuran	ESI+	221.95	165.05	-26.0	-13.0	-11.0	122.95	-27.0	-23.0	-12.0	2.5	15	PV
Organophosphorus, Insecticide; acaricide	Chlorfenvinphos	ESI+	360.85	98.90	-29.0	-32.0	-20.0	155.00	-18.0	-15.0	-10.0	2.5	15	PV
Urea, Herbicide	Chlortoluron	ESI+	212.95	71.95	-14.0	-21.0	-15.0	46.00	-18.0	-17.0	-18.0	2.5	15	PV
Carbamate, Herbicide; plant growth regulator	Chlorpropham	ESI+	212.90	71.95	-24.0	-24.0	-15.0	46.00	-25.0	-18.0	-18.0	2.5	15	PV
Organophosphorus, Insecticide, acaricide	Dimethoate	ESI+	229.90	198.80	-19.0	-10.0	-14.0	124.95	-11.0	-23.0	-12.0	2.5	15	PV
Urea, Herbicide	Diuron	ESI+	232.90	71.95	-28.0	-22.0	-15.0	46.00	-28.0	-18.0	-16.0	2.5	15	PV
Urea, Herbicide	Imidacloprid	ESI+	255.95	209.10	-29.0	-16.0	-14.0	175.10	-20.0	-19.0	-11.0	2.5	15	PV
Urea, Herbicide	Isoproturon	ESI+	207.00	71.95	-25.0	-22.0	-15.0	46.00	-24.0	-21.0	-18.0	2.5	15	PV
Urea, Herbicide	Linuron	ESI+	249.05	208.00	-28.0	-7.0	-15.0	159.95	-27.0	-19.0	-18.0	2.5	15	PV
Organophosphorus, Insecticide; acaricide; veterinary substance	Melathion	ESI+	332.90	127.00	-25.0	-14.0	-13.0	286.80	-28.0	-9.0	-20.0	2.5	15	PV
Phenylamide (acylalanine type), Fungicide	Metolachlor	ESI+	284.00	252.00	-14.0	-16.0	-18.0	176.05	-24.0	-27.0	-11.0	2.5	15	PV
Carbamate, Molluscicide; insecticide; acaricide; bird repellent	Metalaxyl	ESI+	218.10	42.90	-11.0	-32.0	-15.0	Note 2					15	PV
Carbamate, metabolite	Methiocarb	ESI+	226.10	169.05	-15.0	-12.0	-15.0	121.00	-19.0	-21.0	-12.0	2.5	15	PV
Carbamate, metabolite	Methiocarbe sulfone	ESI+	282.90	242.10	-23.0	-8.0	-16.0	185.10	-22.0	-20.0	-12.0	2.5	15	PV
Urea, Herbicide	Methiocarbe sulfoxide	ESI+	241.95	185.10	-29.0	-15.0	-23.0	122.10	-28.0	-32.0	-11.0	2.5	15	PV
Urea, Herbicide	Metobromuron	ESI+	258.90	148.00	-19.0	-16.0	-14.0	170.00	-20.0	-21.0	-11.0	2.5	15	PV
Carbamate, Insecticide	Monolinuron	ESI+	215.05	125.90	-14.0	-18.0	-12.0	148.00	-22.0	-16.0	-18.0	2.5	15	PV
Carbamate, Insecticide	Pirimicarb	ESI+	239.05	71.95	-20.0	-22.0	-20.0	182.00	-18.0	-17.0	-12.0	2.5	15	PV
Anilinopyrimidine, Fungicide	Propoxur	ESI+	210.00	111.00	-17.0	-16.0	-10.0	168.00	-14.0	-10.0	-11.0	2.5	15	PV
1,3,5-traizine, Herbicide	Pyrimethanil	ESI+	200.00	106.95	-13.0	-27.0	-10.0	82.00	-16.0	-29.0	-17.0	2.5	15	PV
Thiocarbamate, Herbicide	Terbutylazine	ESI+	229.95	174.00	-20.0	-19.0	-20.0	95.90	-27.0	-30.0	-19.0	2.5	15	PV
Chloroacetanilide, Herbicide	Thiobencarb	ESI+	257.95	124.95	-22.0	-17.0	-11.0	88.90	-13.0	-50.0	-17.0	2.5	15	PV
Isotopically labelled internal standards (ILIS)	Diuron-d6 (ILIS 15)	ESI+	240.95	78.00	-28.0	-25.0	-16.0	Note 3				2.5	15	PV

P-Chromatographic program. **Note 1:** Pesticides organized by alphabetic order; **Note 2:** Only one transition could be recorded due to the poor fragmentation of the compound. **Note 3:** For the Isotopically labelled internal standards only one transition is needed.

Table S6. Chromatographic programs and mass spectrometry conditions used in the negative and positive ionization modes for pharmaceutical and pesticides analysis.

Chromatographic program	ESI mode	Compounds	Chromatographic Column	Eluents	Mode of elution	Source dependent parameters	
Program I	Negative	Pharmaceuticals	Column: Kinetex C18 column (2.6 x 150 mm i.d., 1.7 μm particle size) from Phenomenex, Inc. (California, USA). Flow rate: 0.22 mL/min Oven temperature=30°C Injection volume= 5 μL	Eluent A Ultra-pure water	Time (min)	%Acetonitrile	NGF=2.6 L/min DGF=12.5 L/min IV=5.0 kV DLT=250°C HBT=300°C
					0.0	30.0	
				Eluent B Acetonitrile	1.0	35.6	
					2.0	100	
					6.0	100	
					6.5	30.0	
					10.5	30.0	
Program II	Positive	Pharmaceuticals	Column: Cortecs™ UPLC® C18+ column (100 x 2.1 mm i.d.; 1.6 μm particle size) from Waters (Milford, Massachusetts, USA) Flow rate: 0.30 mL/min Oven temperature=30°C Injection volume= 5 μL	Eluent A 0.1% formic acid in ultrapure water	Time (min)	%Acetonitrile	NGF=2.6 L/min DGF=15 L/min IV=5.0 kV DLT=300°C HBT=425°C
					0.0	5	
					3.0	100	
				Eluent B acetonitrile	3.5	100	
					4.0	5	
					7.0	5	
Program III	Negative	Pharmaceuticals	Column: Kinetex C18 column (2.6 x 150 mm i.d., 1.7 μm particle size) from Phenomenex, Inc. (California, USA) Flow rate: 0.30 mL/min Oven temperature=30°C Injection volume= 5 μL	Eluent A Ultra-pure water	Time (min)	%Acetonitrile	NGF=2.6 L/min DGF=15 L/min IV=5.0 kV DLT=300°C HBT=425°C
					0.0	10	
				Eluent B Acetonitrile	5.5	100	
					6.5	100	
					7.0	10	
					9.0	10	
Program IV	Positive	Pharmaceuticals	Column: Kinetex C18 column (2.6 x 150 mm i.d., 1.7 μm particle size) from Phenomenex, Inc. (California, USA) Flow rate: 0.30 mL/min Oven temperature=30°C Injection volume= 5 μL	Eluent A 0.1% formic acid in ultrapure water	Time (min)	%Acetonitrile	NGF=2.6 L/min DGF=15 L/min IV=5.0 kV DLT=300°C HBT=425°C
					0.0	5	
					1.0	5	
				Eluent B acetonitrile	2.0	100	
					7.0	100	
					8.5	5	
					11.0	5	
Program V	Positive	Pesticides	Column: Luna OMEGA C18 column (2.1 x 150 mm i.d., 1.6 μm particle size) from Phenomenex, Inc. (California, USA) Flow rate: 0.30 mL/min Oven temperature=30°C Injection volume= 5 μL	Eluent A 0.1% formic acid in ultrapure water	Time (min)	%Acetonitrile	NGF=3.0 L/min DGF=16 L/min IV=5.0 kV DLT=200°C HBT=250°C
					0.0	5	
					3.0	100	
				Eluent B acetonitrile	5.0	100	
					6.0	5	
					10.0	5	

NGF-Nebulizing gas flow (nitrogen), DGF-Drying gas flow (nitrogen), IV-Interface voltage, DLT-Desolvation line temperature, and HBT-Heat block temperature.

Table S7. Retention time, regression, detection and quantitation limits for each transition and ion ratio for each pharmaceutical.

Pharmaceutical	MRM	Retention time			Regression		LOD (µg/L)	LOQ (µg/L)	Ion Ratio				
		Average (min)	RSD (%)	n	Equation	R			Average	RSD (%)	n	-20% ion ratio	+ 20% ion ratio
Acetaminophen	Quantitation	1.661	3.39	34	$Y = (1.12153)X + (-0.00489729)$	0.999910	3.48	10.56	Note 1				
Acetylsalicylic acid	Quantitation	1.677	6.55	35	$Y = (0.0231806)X + (0.0124567)$	0.999210	0.140	0.410	2.03	4.75	23	1.62	2.43
	Qualifier	1.685	6.42	34	$Y = (0.0120497)X + (0.00565358)$	0.999887	0.050	0.170					
Alprazolam	Quantitation	3.599	0.156	35	$Y = (0.179327)X + (0.0469456)$	0.999757	0.010	0.050	1.88	4.95	14	1.50	2.25
	Qualifier	3.599	0.136	33	$Y = (0.108434)X + (0.0108339)$	0.999802	0.070	0.240					
Amoxicillin	Quantitation	1.281	1.61	32	$Y = (0.0393282)X + (0.000213570)$	0.999854	0.090	0.280	2.61	4.03	18	2.09	3.14
	Qualifier	1.281	1.55	31	$Y = (0.0152365)X + (0.000264637)$	0.999890	0.010	0.040					
Ampicillin	Quantitation	2.816	0.364	35	$Y = (0.205343)X + (0.0100769)$	0.999977	0.090	0.320	Note 1				
Anfepramone	Quantitation	3.277	0.115	36	$Y = (13.0628)X + (0.0752357)$	0.999995	0.030	0.120	1.39	2.79	28	1.11	1.66
	Qualifier	3.279	0.157	36	$Y = (9.71745)X + (-0.0243496)$	0.999993	0.010	0.030					
Astorvatatin	Quantitation	3.538	0.055	36	$Y = (0.872547)X + (-0.158568)$	0.999626	0.020	0.080	1.84	2.44	24	1.47	2.20
	Qualifier	3.538	0.055	36	$Y = (0.462852)X + (-0.0728353)$	0.999674	0.040	0.140					
Atenolol	Quantitation	0.913	0.532	35	$Y = (0.283783)X + (-0.0167443)$	0.999853	2.95	9.82	1.05	5.64	20	0.84	1.26
	Qualifier	0.911	0.966	35	$Y = (0.246228)X + (0.00427671)$	0.999991	3.74	12.5					
Azithromycin	Quantitation	2.777	0.243	36	$Y = (8.14492)X + (0.0328438)$	0.999952	0.160	0.520	2.70	3.24	19	2.16	3.25
	Qualifier	2.777	0.235	26	$Y = (7.94994)X + (0.0420264)$	0.999863	0.170	0.580					
Bupropion	Quantitation	3.356	0.249	36	$Y = (53.4663)X + (1.84361)$	0.999831	0.010	0.030	2.16	3.58	30	1.73	2.59
	Qualifier	3.356	0.253	36	$Y = (26.1419)X + (0.488269)$	0.999942	0.010	0.020					
Caffeine	Quantitation	2.473	0.121	36	$Y = (2.26155)X + (0.0252275)$	0.999966	0.890	2.98	1.22	4.96	33	0.97	1.46
	Qualifier	2.473	0.079	36	$Y = (1.77883)X + (0.0352183)$	0.999940	0.190	0.650					
Carbamazepine	Quantitation	3.110	0.134	36	$Y = (2.66887)X + (0.0835463)$	0.999968	0.010	0.050	4.16	2.16	27	3.33	4.99
	Qualifier	3.110	0.115	36	$Y = (0.617467)X + (0.0286352)$	0.999905	0.030	0.110					
Carboxybuprofen	Quantitation	2.905	8.194	35	$Y = (1.20617)X + (-0.0157709)$	0.999517	0.810	2.45	1.4	1.95	28	1.1	1.7
	Qualifier	2.875	9.158	36	$Y = (0.842636)X + (-0.00953159)$	0.999375	1.05	3.17					
d-Cathine	Quantitation	3.251	0.077	36	$Y = (13.3899)X + (-0.302528)$	0.999891	0.220	0.730	2.3	3.47	35	1.8	2.7
	Qualifier	3.250	0.122	36	$Y = (5.84737)X + (-0.114523)$	0.999908	0.240	0.790					
Chlorocycline	Quantitation	2.498	0.273	25	$Y = (0.0481730)X + (-0.0419264)$	0.999303	1.09	3.63	1.17	4.58	11	0.94	1.40
	Qualifier	2.484	1.220	30	$Y = (0.0403372)X + (-0.0257034)$	0.999248	2.01	6.69					
Chlorpromazine	Quantitation	2.821	0.025	36	$Y = (3.43548)X + (0.350571)$	0.999800	0.010	0.050	1.49	3.26	29	1.19	1.79
	Qualifier	2.821	0.028	36	$Y = (2.28472)X + (0.212035)$	0.999909	0.010	0.050					

Ciprofloxacin	Quantitation	2.379	0.445	27	$Y = (12.9303)X + (-0.0352396)$	0.999933	0.280	0.930	2.09	2.73	25	1.67	2.50
	Qualifier	2.379	0.301	36	$Y = (6.70863)X + (-0.0485370)$	0.999952	0.180	0.610					
Citalopram	Quantitation	2.655	0.166	36	$Y = (2.24008)X + (0.102021)$	0.999846	0.040	0.140	3.20	2.83	31	2.56	3.84
	Qualifier	2.655	0.165	36	$Y = (0.690305)X + (0.0263768)$	0.999712	0.050	0.180					
Clarithromycin	Quantitation	2.777	0.200	27	$Y = (34.8012)X + (0.167270)$	0.999909	0.010	0.030	3.05	2.29	25	2.44	3.66
	Qualifier	2.776	0.179	36	$Y = (11.3813)X + (0.0418367)$	0.999865	0.040	0.130					
Clobenzorex	Quantitation	3.449	0.371	36	$Y = (69.1496)X + (1.37955)$	0.999777	0.010	0.030	1.81	4.98	25	1.45	2.18
	Qualifier	3.449	0.383	36	$Y = (35.6033)X + (1.37644)$	0.999751	0.010	0.020					
Citalopram demethyl	Quantitation	2.621	0.126	36	$Y = (1.00555)X + (-0.196766)$	0.999427	1.21	4.04	2.82	3.37	25	2.26	3.39
	Qualifier	2.622	0.239	36	$Y = (0.366526)X + (-0.0688258)$	0.999365	0.510	1.71					
Citalopram didemethyl	Quantitation	2.599	0.150	36	$Y = (0.536276)X + (-0.179748)$	0.999600	3.40	11.3	1.6	3.49	28	1.3	1.9
	Qualifier	2.601	0.134	36	$Y = (0.321850)X + (-0.0586333)$	0.999402	5.83	19.4					
Citalopram N-oxide	Quantitation	2.676	0.087	36	$Y = (1.97530)X + (-0.234162)$	0.999786	0.780	2.61	1.38	3.94	27	1.11	1.66
	Qualifier	2.676	0.047	35	$Y = (1.37189)X + (-0.0962831)$	0.999878	0.020	0.050					
Citalopram propionic acid	Quantitation	4.286	0.347	36	$Y = (0.584889)X + (0.00541258)$	0.999943	0.280	0.850	2.3	2.57	28	1.9	2.8
	Qualifier	4.284	0.437	36	$Y = (0.250762)X + (0.00249637)$	0.999847	0.020	0.060					
O-Desmethylvenlafaxine	Quantitation	2.339	0.350	36	$Y = (8.71572)X + (0.737690)$	0.999599	0.020	0.070	4.01	2.05	30	3.21	4.81
	Qualifier	2.339	0.410	36	$Y = (2.11473)X + (0.218518)$	0.999224	0.080	0.260					
Diazepam	Quantitation	3.529	0.128	36	$Y = (2.94716)X + (0.0754380)$	0.999823	0.010	0.050	1.27	3.95	29	1.02	1.52
	Qualifier	3.528	0.133	36	$Y = (2.51630)X + (0.0323572)$	0.999827	0.030	0.110					
Diclofenac	Quantitation	4.169	0.423	36	$Y = (1.62888)X + (-0.00466846)$	0.999758	0.080	0.240	10.18	3.51	31	8.14	12.21
	Qualifier	4.171	0.533	35	$Y = (0.155517)X + (-0.000301460)$	0.999947	0.110	0.330					
Diltiazem	Quantitation	2.654	0.116	36	$Y = (3.31104)X + (0.111262)$	0.999936	0.010	0.020	3.19	3.48	30	2.55	3.82
	Qualifier	2.653	0.122	36	$Y = (1.07378)X + (0.0114945)$	0.999926	0.010	0.030					
Doxycycline	Quantitation	2.526	0.318	34	$Y = (0.365737)X + (-0.338747)$	0.999551	1.66	5.54	5.21	3.65	19	4.17	6.25
	Qualifier	2.392	1.37	29	$Y = (0.0725768)X + (-0.0635292)$	0.999452	1.75	5.84					
Enrofloxacin	Quantitation	2.406	0.283	36	$Y = (12.4283)X + (0.000749846)$	0.999883	0.070	0.250	1.32	4.21	22	1.06	1.59
	Qualifier	2.403	0.335	27	$Y = (8.89786)X + (0.0666777)$	0.999838	0.090	0.310					
(+)-Ephedrine	Quantitation	3.257	0.091	36	$Y = (16.0764)X + (-0.0192273)$	0.999972	0.460	1.55	3.96	2.19	30	3.16	4.75
	Qualifier	3.257	0.085	36	$Y = (4.08274)X + (-0.00595158)$	0.999996	0.030	0.090					
10,11-Epoxy carbamazepine	Quantitation	2.899	0.109	36	$Y = (1.50960)X + (0.104813)$	0.999803	0.010	0.020	1.09	2.03	30	0.87	1.31
	Qualifier	2.899	0.116	36	$Y = (1.36043)X + (0.113039)$	0.999820	0.010	0.030					
Erythromycin	Quantitation	2.634	0.148	27	$Y = (6.87316)X + (0.0784127)$	0.999876	0.020	0.070	2.69	3.79	26	2.15	3.23
	Qualifier	2.634	0.198	36	$Y = (2.47205)X + (0.0396889)$	0.999864	0.030	0.100					
Fenfluramine	Quantitation	3.372	0.234	36	$Y = (20.4009)X + (0.309775)$	0.999932	0.210	0.720	3.24	1.93	33	2.59	3.89
	Qualifier	3.372	0.259	36	$Y = (6.34855)X + (0.0792328)$	0.999956	0.020	0.070					

Fenofibrate	Quantitation	4.450	0.106	35	$Y = (0.167823)X + (-0.0254142)$	0.999681	1.67	5.58	1.15	3.42	25	0.92	1.38
	Qualifier	4.453	0.246	35	$Y = (0.144540)X + (-0.0199009)$	0.999565	2.08	6.92					
Fentermine	Quantitation	3.257	0.080	36	$Y = (35.7513)X + (0.116920)$	0.999952	0.010	0.040	16.96	4.17	23	13.57	20.36
	Qualifier	3.255	0.146	36	$Y = (2.21057)X + (-0.0196968)$	0.999921	0.190	0.630					
Fluoxetine	Quantitation	2.804	0.151	36	$Y = (3.40022)X + (-0.0761480)$	0.999963	0.020	0.070	54.1	2.45	25	43.3	64.9
	Qualifier	2.804	0.189	32	$Y = (0.0619889)X + (-0.000721706)$	0.999934	0.310	1.04					
Gemfibrozil	Quantitation	5.677	0.408	36	$Y = (1.15599)X + (0.000273772)$	0.999984	0.080	0.260	52.36	2.07	20	41.89	62.83
	Qualifier	5.670	0.398	32	$Y = (0.0225317)X + (-0.000253063)$	0.999965	0.120	0.370					
2-Hydroxyibuprofen	Quantitation	3.012	6.122	34	$Y = (1.07445)X + (-0.0228344)$	0.999507	1.62	4.92	Note 1				
Ibuprofen	Quantitation	4.307	0.220	36	$Y = (0.736439)X + (-0.000436140)$	0.999915	0.150	0.450	Note 1				
Ketoprofen	Quantitation	3.890	0.309	36	$Y = (2.18857)X + (-0.00732679)$	0.999960	0.160	0.490	Note 1				
Lanzoprazole	Quantitation	2.838	0.060	36	$Y = (0.917109)X + (0.100898)$	0.999684	0.010	0.020	2.89	3.07	23	2.32	3.47
	Qualifier	2.838	0.091	36	$Y = (0.332633)X + (0.0221102)$	0.999823	0.030	0.100					
Lomefloxacin	Quantitation	2.391	0.336	32	$Y = (3.10848)X + (0.0385129)$	0.999813	0.120	0.410	1.22	3.95	15	0.98	1.47
	Qualifier	2.391	0.774	23	$Y = (2.54572)X + (0.00724765)$	0.999650	0.250	0.820					
Lorazepam	Quantitation	3.554	0.084	36	$Y = (3.01194)X + (-0.0652863)$	0.999869	0.010	0.040	2.24	2.73	25	1.79	2.69
	Qualifier	3.555	0.397	36	$Y = (1.37350)X + (-0.0339598)$	0.999791	0.700	2.35					
Mazindol	Quantitation	3.356	0.227	36	$Y = (36.9371)X + (3.73131)$	0.999742	0.010	0.040	Note 1				
Metformin	Quantitation	0.660	1.27	36	$Y = (0.321469)X + (-0.00730507)$	0.999958	0.140	0.470	1.21	2.95	24	0.97	1.45
	Qualifier	0.661	1.51	24	$Y = (0.270374)X + (-0.0108923)$	0.999958	0.130	0.440					
d,l-Methamphetamine	Quantitation	3.257	0.099	36	$Y = (13.4285)X + (0.128715)$	0.999892	0.110	0.380	4.90	2.99	31	3.92	5.88
	Qualifier	3.258	0.174	36	$Y = (2.75210)X + (0.00866900)$	0.999993	0.010	0.040					
Moxifloxacin	Quantitation	2.469	0.250	27	$Y = (9.64109)X + (-0.290050)$	0.999598	0.110	0.360	3.30	3.41	19	2.64	3.97
	Qualifier	2.469	0.334	36	$Y = (2.86333)X + (-0.0623552)$	0.999574	0.140	0.450					
Naproxen	Quantitation	3.948	0.303	36	$Y = (1.09789)X + (-0.00144390)$	0.999853	0.010	0.030	1.84	3.74	32	1.47	2.21
	Qualifier	3.946	0.220	36	$Y = (0.608148)X + (-0.000377853)$	0.999735	0.020	0.050					
Nimesulide	Quantitation	4.133	0.133	36	$Y = (4.48427)X + (-0.0139536)$	0.999888	0.020	0.060	8.82	0.97	24	7.06	10.59
	Qualifier	4.136	0.603	36	$Y = (0.507141)X + (-0.00109917)$	0.999952	0.030	0.090					
d,l-Norephedrine	Quantitation	3.251	0.082	36	$Y = (5.07146)X + (-0.0480787)$	0.999980	0.260	0.870	2.10	2.96	30	1.68	2.52
	Qualifier	3.250	0.123	36	$Y = (2.47466)X + (-0.0307268)$	0.999985	0.230	0.770					
Norfloxacin	Quantitation	2.375	1.23	27	$Y = (10.6605)X + (-0.157677)$	0.999798	1.60	5.34	5.84	2.25	17	4.67	7.01
	Qualifier	2.370	0.430	31	$Y = (1.91040)X + (-0.0472131)$	0.999629	0.700	2.32					
Norfluoxetine	Quantitation	2.778	0.212	36	$Y = (0.197050)X + (-0.00653015)$	0.999554	0.090	0.310	1.09	3.90	29	0.87	1.31
	Qualifier	2.778	0.213	35	$Y = (0.175225)X + (-0.00339312)$	0.999865	0.130	0.430					
Norserttraline	Quantitation	2.801	0.493	36	$Y = (0.124385)X + (0.00244630)$	0.999969	5.33	17.8	1.39	3.24	19	1.11	1.67
	Qualifier	2.803	0.735	34	$Y = (0.0883889)X + (-0.00587728)$	0.999715	3.04	10.1					

Ofloxacin	Quantitation	2.371	0.276	27	Y = (17.1323)X + (0.185203)	0.999869	0.180	0.620	1.29	4.44	26	1.03	1.55
	Qualifier	2.371	0.275	36	Y = (13.5243)X + (0.0635528)	0.999905	0.040	0.140					
Oxytetracycline	Quantitation	2.357	0.198	24	Y = (0.0419188)X + (-0.0469376)	0.999598	1.25	4.15	2.48	3.10	13	1.98	2.98
	Qualifier	2.360	0.704	25	Y = (0.0182545)X + (-0.0205711)	0.999498	13.69	45.6					
Paroxetine	Quantitation	2.717	0.149	36	Y = (0.910500)X + (-0.130027)	0.999670	0.410	1.370	1.39	2.87	29	1.11	1.67
	Qualifier	2.717	0.152	36	Y = (0.644454)X + (-0.0992948)	0.999683	0.150	0.500					
Phenolphthalein	Quantitation	4.531	0.240	36	Y = (3.54539)X + (0.196511)	0.999736	0.010	0.030	5.11	1.25	25	4.09	6.57
	Qualifier	4.529	0.277	36	Y = (0.680798)X + (0.0498404)	0.999505	0.040	0.120					
Pravastatin	Quantitation	3.535	0.667	33	Y = (0.0492404)X + (-8.75910e-005)	0.999971	0.070	0.210	1.15	2.71	23	0.92	1.38
	Qualifier	3.530	0.932	35	Y = (0.0432767)X + (0.000122420)	0.999875	0.030	0.080					
Propanolol	Quantitation	2.632	0.337	36	Y = (0.729575)X + (-0.0566092)	0.999881	2.11	7.03	Note 1				
Prulifloxacin	Quantitation	2.741	0.219	27	Y = (8.79816)X + (-0.0517378)	0.999910	0.090	0.280	1.18	3.55	26	0.94	1.41
	Qualifier	2.739	0.145	36	Y = (7.19572)X + (0.0152447)	0.999838	0.080	0.270					
Rimonabant	Quantitation	4.337	0.146	36	Y = (12.1388)X + (4.94926)	0.999782	0.010	0.020	4.70	2.10	30	3.76	5.64
	Qualifier	4.336	0.138	36	Y = (2.66341)X + (1.05284)	0.999562	0.010	0.040					
Salicylic acid	Quantitation	1.601	4.14	36	Y = (0.508232)X + (-0.0217815)	0.999766	3.63	11.0	9.74	3.61	23	7.79	11.69
	Qualifier	1.612	3.26	36	Y = (0.0539851)X + (-0.00165165)	0.999944	8.44	25.6					
Sertraline	Quantitation	2.822	0.199	36	Y = (1.36293)X + (-0.0902651)	0.999891	0.080	0.260	1.41	2.82	23	1.13	1.69
	Qualifier	2.823	0.242	36	Y = (0.993422)X + (-0.0739301)	0.999911	0.080	0.250					
Sibutramine	Quantitation	3.721	1.58	30	Y = (75.2990)X + (-2.91407)	0.999800	0.190	0.650	2.09	3.17	27	1.67	2.50
	Qualifier	3.735	1.76	34	Y = (36.4190)X + (-1.20229)	0.999871	0.210	0.690					
Simvastatin	Quantitation	4.259	0.058	35	Y = (0.285996)X + (-0.0157286)	0.999913	0.040	0.120	1.22	3.33	29	0.97	1.46
	Qualifier	4.259	0.035	36	Y = (0.232151)X + (-0.0125086)	0.999958	0.050	0.170					
Sulfadiazine	Quantitation	2.554	0.262	27	Y = (14.6384)X + (0.110844)	0.999732	0.030	0.110	1.26	2.01	24	1.01	1.51
	Qualifier	2.553	0.245	35	Y = (11.4754)X + (0.0602667)	0.999814	0.100	0.340					
Sulfadimethoxine	Quantitation	3.008	0.186	27	Y = (41.4033)X + (-0.591546)	0.999833	0.080	0.270	2.03	2.98	25	1.62	2.43
	Qualifier	3.010	0.574	36	Y = (21.0089)X + (-0.323471)	0.999823	0.370	1.23					
Sulfamethazine	Quantitation	2.702	0.167	27	Y = (23.5234)X + (0.301930)	0.999731	0.000	0.000	1.43	3.11	27	1.15	1.72
	Qualifier	2.702	0.201	36	Y = (15.2144)X + (0.316772)	0.999689	0.010	0.020					
Sulfamethizole	Quantitation	2.666	0.051	36	Y = (32.8790)X + (-0.0905455)	0.999945	0.040	0.130	1.93	4.46	25	1.54	2.31
	Qualifier	2.666	0.087	36	Y = (16.9662)X + (0.0469254)	0.999986	0.020	0.050					
Sulfamethoxazole	Quantitation	2.891	0.153	27	Y = (18.3074)X + (0.0322277)	0.999946	0.020	0.060	1.20	2.96	30	0.96	1.43
	Qualifier	2.890	0.134	36	Y = (15.7580)X + (-0.0672412)	0.999911	0.040	0.120					
Sulfamethoxypyridazine	Quantitation	2.695	0.201	27	Y = (29.2260)X + (0.187498)	0.999761	0.020	0.080	1.15	2.73	24	0.92	1.38
	Qualifier	2.694	0.188	36	Y = (24.3340)X + (0.263906)	0.999899	0.020	0.080					
Sulfapyridine	Quantitation	2.581	0.249	27	Y = (18.5438)X + (-0.142218)	0.999905	0.180	0.610	1.31	3.18	28	1.04	1.57

	Qualifier	2.582	0.244	36	$Y = (13.1512)X + (-0.00755633)$	0.999730	0.060	0.190					
Sulfaquinoxaline	Quantitation	2.995	0.049	36	$Y = (33.1310)X + (-0.231374)$	0.999877	0.080	0.270	1.56	3.82	27	1.25	1.88
	Qualifier	2.996	0.146	36	$Y = (21.7703)X + (-0.153190)$	0.999921	0.060	0.190					
Sulfaquinoxaline	Quantitation	4.004	0.319	34	$Y = (0.0867622)X + (0.00123453)$	0.999863	0.050	0.160	2.49	3.27	22	1.99	2.98
	Qualifier	3.998	0.728	31	$Y = (0.0368467)X + (-1.75817e-005)$	0.999959	0.100	0.300					
Sulfathiazole	Quantitation	2.511	0.083	36	$Y = (25.3266)X + (-0.0420419)$	0.999982	0.040	0.120	1.74	3.92	26	1.40	2.09
	Qualifier	2.511	0.118	35	$Y = (14.5806)X + (0.0595692)$	0.999922	0.030	0.100					
Synephrine	Quantitation	1.294	0.423	36	$Y = (9.89755)X + (-0.0989919)$	0.999852	0.750	2.50	4.45	2.53	28	3.56	5.34
	Qualifier	1.293	0.413	36	$Y = (2.21955)X + (-0.0240835)$	0.999880	0.520	1.72					
Tetracycline	Quantitation	2.384	0.170	27	$Y = (0.246994)X + (-0.232154)$	0.999694	0.350	1.16	2.00	3.59	14	1.60	2.41
	Qualifier	2.392	1.271	28	$Y = (0.122908)X + (-0.113980)$	0.999302	5.16	17.2					
Topiramate	Quantitation	4.229	0.261	36	$Y = (2.31447)X + (0.000881671)$	0.999995	0.020	0.050	5.54	3.13	18	4.43	6.65
	Qualifier	4.228	0.312	33	$Y = (0.431505)X + (-0.0113229)$	0.999958	1.52	4.61					
Trazodone	Quantitation	2.546	0.174	36	$Y = (1.03567)X + (-0.0195913)$	0.999972	0.040	0.130	1.22	2.43	29	0.98	1.47
	Qualifier	2.546	0.160	36	$Y = (0.833718)X + (-0.00775081)$	0.999959	0.270	0.910					
Trimethoprim	Quantitation	2.366	0.291	26	$Y = (5.88940)X + (0.0307121)$	0.999960	0.130	0.430	1.06	3.30	24	0.85	1.28
	Qualifier	2.367	0.399	36	$Y = (6.86695)X + (-0.0650998)$	0.999638	4.17	13.9					
Venlafaxine	Quantitation	2.518	0.173	36	$Y = (13.6715)X + (1.17294)$	0.999661	0.010	0.030	4.84	1.78	24	3.87	5.81
	Qualifier	2.518	0.194	36	$Y = (2.82840)X + (0.267302)$	0.999668	0.030	0.100					
Zonisamide	Quantitation	3.733	0.496	36	$Y = (1.64794)X + (0.0382692)$	0.999924	0.170	0.500	1.81	2.61	27	1.45	2.17
	Qualifier	3.736	0.426	36	$Y = (0.912682)X + (0.0214751)$	0.999876	0.330	1.01					

Pharmaceuticals organized in the table by alphabetic order

Note 1: Only one transition could be recorded due to their poor fragmentation

Table S8. Retention time, regression, detection and quantitation limits for each transition and ion ratio for each pesticide.

Pesticides	MRM	Retention time			Regression		LOD (µg/L)	LOQ (µg/L)	Ion Ratio				
		Average (min)	RSD (%)	n	Equation	R			Average	RSD (%)	n	-20% Ion ratio	+ 20% Ion ratio
Alachlor	Quantitation	4.613	0.25	36	$Y = (5.78558)X + (0.0209059)$	0.99988	0.010	0.030	3.19	3.34	29	2.55	3.83
	Qualifier	4.599	0.28	36	$Y = (1.77551)X + (0.00657384)$	0.99985	0.140	0.440					
Ametryn	Quantitation	3.797	0.04	36	$Y = (51.8106)X + (0.390445)$	0.99953	0.010	0.030	2.16	4.11	17	1.73	2.60
	Qualifier	3.797	0.05	36	$Y = (18.5654)X + (0.650880)$	0.99933	0.010	0.020					
Asulam	Quantitation	3.322	0.10	35	$Y = (1.57017)X + (0.0105356)$	0.99978	0.030	0.080	1.32	2.58	22	1.06	1.58
	Qualifier	3.322	0.08	33	$Y = (1.13570)X + (0.0231755)$	0.99971	0.010	0.050					
Atrazine	Quantitation	4.087	0.05	36	$Y = (24.5233)X + (0.0192450)$	0.99983	0.020	0.070	2.01	4.07	23	1.61	2.41
	Qualifier	4.087	0.04	36	$Y = (11.5877)X + (0.00943163)$	0.99985	0.070	0.200					
Atrazine-desethyl	Quantitation	3.516	0.09	36	$Y = (4.72043)X + (-0.00217138)$	0.99988	0.340	1.03	1.63	4.08	21	1.30	1.95
	Qualifier	3.516	0.14	36	$Y = (2.83014)X + (0.00114037)$	0.99989	0.060	0.190					
Atrazine-desisopropyl	Quantitation	3.303	0.25	34	$Y = (0.810192)X + (0.000961784)$	0.99977	1.36	4.13	1.12	4.72	20	0.89	1.34
	Qualifier	3.301	0.07	31	$Y = (0.778505)X + (-0.000709147)$	0.99967	0.570	1.73					
Azinphos-methyl	Quantitation	4.298	0.08	35	$Y = (3.94537)X + (-0.000994027)$	0.99997	0.010	0.030	1.81	4.10	12	1.45	2.17
	Qualifier	4.299	0.07	36	$Y = (2.22658)X + (-0.00130689)$	0.99977	0.130	0.390					
Azoxystrobin	Quantitation	4.312	0.04	36	$Y = (22.3020)X + (0.0291066)$	0.99954	0.020	0.060	5.96	3.26	19	4.77	7.16
	Qualifier	4.312	0.08	36	$Y = (3.61539)X + (0.00416409)$	0.99953	0.030	0.080					
Bensulfuron-methyl	Quantitation	4.077	0.05	36	$Y = (20.1308)X + (0.0110967)$	0.99973	0.020	0.070	2.45	3.62	26	1.96	2.94
	Qualifier	4.076	0.05	36	$Y = (7.87768)X + (0.0100038)$	0.99931	0.010	0.030					
Bentazon	Quantitation	4.020	0.09	33	$Y = (0.691212)X + (0.0127226)$	0.99964	0.250	0.750	2.26	2.73	18	1.81	2.71
	Qualifier	4.021	0.10	32	$Y = (0.307405)X + (0.00367799)$	0.99977	0.140	0.440					
Carbaryl	Quantitation	4.010	0.08	33	$Y = (1.04334)X + (0.00123476)$	0.99982	0.660	1.99	2.68	3.27	17	2.14	3.22
	Qualifier	4.011	0.09	31	$Y = (0.354998)X + (0.00002859)$	0.99951	1.37	4.14					
Carbofuran	Quantitation	3.947	0.05	36	$Y = (16.2178)X + (0.121797)$	0.99975	0.060	0.190	0.99	3.66	35	0.79	1.19
	Qualifier	3.946	0.03	36	$Y = (16.1885)X + (0.127057)$	0.99967	0.070	0.210					
Chlorfenvinphos	Quantitation	4.634	0.12	33	$Y = (1.30320)X + (0.000694796)$	0.99988	0.120	0.370	1.46	5.95	10	1.17	1.75
	Qualifier	4.632	0.07	31	$Y = (0.778240)X + (-0.000135808)$	0.99964	0.230	0.690					
Chlortoluron	Quantitation	3.997	0.05	36	$Y = (26.9005)X + (0.00201672)$	0.99990	0.130	0.400	0.98	4.75	24	0.78	1.17

	Qualifier	3.996	0.06	36	$Y = (28.4796)X + (0.0173369)$	0.99966	0.010	0.030					
Chlorpropham	Quantitation	3.996	0.07	36	$Y = (14.4548)X + (-0.00342676)$	0.99944	0.160	0.490	1.03	2.97	29	0.83	1.24
	Qualifier	3.996	0.06	36	$Y = (13.7213)X + (0.00239978)$	0.99986	0.130	0.400					
Dimethoate	Quantitation	3.539	0.06	36	$Y = (5.30546)X + (0.0170082)$	0.99980	0.210	0.640	1.09	4.62	17	0.87	1.31
	Qualifier	3.538	0.09	35	$Y = (4.69111)X + (0.0110004)$	0.99992	0.230	0.700					
Diuron	Quantitation	4.089	0.04	36	$Y = (2.46995)X + (0.00273755)$	0.99978	0.130	0.390	1.88	4.70	13	1.50	2.25
	Qualifier	4.084	0.38	36	$Y = (1.29231)X + (0.00158067)$	0.99961	0.090	0.270					
Imidacloprid	Quantitation	3.508	0.12	33	$Y = (0.675452)X + (0.000277841)$	0.99973	0.160	0.500	1.86	4.63	13	1.48	2.23
	Qualifier	3.508	0.18	32	$Y = (0.306183)X + (0.00158253)$	0.99984	0.100	0.300					
Isoproturon	Quantitation	4.048	0.04	36	$Y = (46.2430)X + (0.0821940)$	0.99915	0.030	0.090	1.18	3.06	32	0.95	1.42
	Qualifier	4.048	0.04	36	$Y = (39.9800)X + (0.0490080)$	0.99939	0.010	0.020					
Linuron	Quantitation	4.047	0.25	36	$Y = (0.578734)X + (0.00104172)$	0.99973	1.28	3.87	1.81	2.70	13	1.45	2.17
	Qualifier	4.356	0.10	33	$Y = (0.190125)X + (0.00194087)$	0.99978	0.130	0.390					
Melathion	Quantitation	4.487	0.12	23	$Y = (0.0747668)X + (-0.00185515)$	0.99975	2.23	6.75	1.37	3.59	12	1.10	1.64
	Qualifier	4.484	0.08	21	$Y = (0.0544132)X + (0.000586693)$	0.99972	0.920	2.780					
Metolachlor	Quantitation	4.638	0.06	36	$Y = (11.4398)X + (0.0213983)$	0.99990	0.040	0.130	1.45	7.38	7	1.16	1.74
	Qualifier	4.638	0.04	36	$Y = (13.5063)X + (0.00850926)$	0.99979	0.090	0.270					
Metalaxyl	Quantitation	4.088	0.39	36	$Y = (2.76686)X + (-0.00134179)$	0.99990	0.290	0.880	Note 1				
Methiocarb	Quantitation	4.303	0.06	35	$Y = (2.42204)X + (-0.00137898)$	0.99975	0.270	0.820	0.97	4.02	22	0.78	1.17
	Qualifier	4.304	0.18	36	$Y = (2.50719)X + (0.00305352)$	0.99971	0.560	1.680					
Methiocarbe sulfone	Quantitation	3.339	0.06	36	$Y = (20.7890)X + (0.00962249)$	0.99971	0.570	1.720	1.78	2.90	29	1.42	2.13
	Qualifier	3.339	0.06	36	$Y = (11.3291)X + (0.00516808)$	0.99981	0.010	0.040					
Methiocarbe sulfoxide	Quantitation	3.340	0.10	36	$Y = (4.09666)X + (0.00334794)$	0.99960	0.010	0.020	3.54	4.44	17	2.83	4.24
	Qualifier	3.339	0.09	33	$Y = (1.05599)X + (0.000520520)$	0.99972	0.010	0.020					
Metobromuron	Quantitation	4.148	0.42	33	$Y = (0.630688)X + (0.00555753)$	0.99967	0.050	0.160	1.14	3.93	22	0.91	1.36
	Qualifier	4.151	0.07	30	$Y = (0.569507)X + (0.00827548)$	0.99978	0.140	0.430					
Monolinuron	Quantitation	4.088	0.07	36	$Y = (3.52220)X + (-0.000878116)$	0.99998	0.050	0.140	2.43	5.74	14	1.94	2.91
	Qualifier	4.088	0.07	33	$Y = (1.56850)X + (0.00160774)$	0.99938	0.010	0.020					
Pirimicarb	Quantitation	3.296	0.05	36	$Y = (84.1353)X + (-0.0630855)$	0.99974	0.110	0.320	2.33	2.59	36	1.86	2.80
	Qualifier	3.296	0.05	36	$Y = (37.4754)X + (-0.0245084)$	0.99988	0.040	0.120					
Propoxur	Quantitation	3.930	0.05	36	$Y = (37.6386)X + (0.0198632)$	0.99971	0.010	0.030	2.22	2.51	24	1.77	2.66
	Qualifier	3.930	0.08	36	$Y = (18.3003)X + (-0.0128080)$	0.99988	0.060	0.180					
Pyrimethanil	Quantitation	4.136	0.04	36	$Y = (47.8849)X + (-0.0259311)$	0.99976	0.030	0.100	1.33	4.53	30	1.06	1.59

	Qualifier	4.135	0.05	36	$Y = (35.5058)X + (0.00724680)$	0.99985	—	0.020	0.050					
Terbutylazine	Quantitation	4.368	0.03	36	$Y = (192.541)X + (0.164482)$	0.99972		0.030	0.080	6.83	3.84	28	5.46	8.19
	Qualifier	4.368	0.04	36	$Y = (27.2459)X + (0.0325320)$	0.99989		0.050	0.150					
Thiobencarb	Quantitation	4.918	0.06	35	$Y = (2.29223)X + (-0.00454050)$	0.99999		0.350	1.05	17.54	4.53	14	14.03	21.05
	Qualifier	4.916	0.08	24	$Y = (0.131831)X + (-0.00226479)$	0.99972		1.63	4.93					

Pharmaceuticals organized in the table by alphabetic order

Note 1: Only one transition could be recorded due to their poor fragmentation