Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Material

Economically feasible strategy for confirmation of pharmaceuticals in hospital effluent using screening analysis

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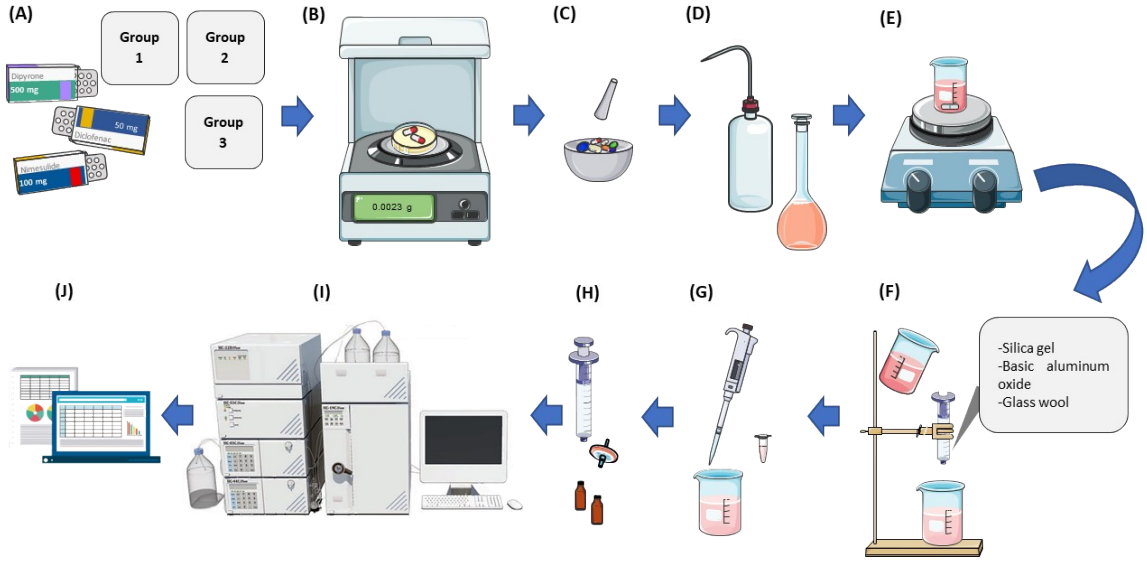
Section S1. Chemical reagents and materials

Commercial pharmaceuticals used were acquired through donation. To clean-upthe commercial pharmaceuticals mix solutions, aluminum oxide 90 active basic (Vetec), silica gel 60 (Macherey-Nagel), commercial 5 mL syringeand glass wool was used. Qualitative filter paper was used to filter raw samples. Afterwards, the samples were filtered with nylon membranes (0.45 µm). SPE cartridges Oasis HLB® (500 mg, 6 mL) from Waters were used. To solid phase extraction (SPE) procedure HPLC grade methanol (PanReac AppliChem), ultrapure water (18.2 MΩ.cm, Millipore, Bedford, USA) and PVDF syringe filters (0.22 µm) was used.

To chromatographic analysis, methanol LC-MS grade (Fluka), ultrapure water, formic acid (98% purity, Sigma Aldrich),ammonium formate and ammonium acetate salts (97%, Sigma Aldrich) was used.

Section S2.Analysis of commercial pharmaceutical compounds



FigureS1. Illustration of the preparation of commercial pharmaceuticals mix solutions: (A) Separation of commercial pharmaceuticals into groups; (B) Weighing of commercial pharmaceuticals; (C) Maceration of commercial pharmaceuticals; (D) Solubilization of commercial pharmaceuticals in ultrapure water; (E) Agitation of the solutions; (F) Clean-up step; (G) 1 mL aliquot; (H) Filtration of the solutions in 0.22 µm PVDF filter; (I) Analysis at UHPLC-QTOF MS; (J) Data processing.

Section S3.Physicochemical characterization of hospital effluent samples studied

Characterization of the samples was carried out by determination the following physicochemical parameters: pH, electrical conductivity, concentrations of total phosphates and chlorides, chemical oxygen demand (COD), biochemical oxygen demand (BOD_5), BOD_5/COD ratio, suspended total solids (STS) and total solids (ST). The methods used in the analysis of characterization of these waste waters were based on Standard Methods for the Examination of Water and Wastewater Analysis, according to American Public Health Association (APHA), 2012.

Table S1. Physicochemical parameters of the samples.

Parameters	Months sampled						LOQ	LOD
	Aug. 17	Sep. 17	Oct. 17	Nov. 17	Dec. 17	Jan. 18		
pH	8.86	8.51	8.98	8.47	8.53	8.23	-	-
Conductivity($\mu S\ cm^{-1}$)	1209.0	427.0	722.0	611.0	114.0	812.0	1.0	0.2
Total chloride ($mg\ L^{-1}$)	98.80	33.90	49.10	44.50	61.70	55.90	0.50	0.02
Total phosphate($mg\ L^{-1}\ PO_4^{3-}$)	53.37	5.39	9.45	5.90	14.58	21.85	0.03	0.01
COD ($mg\ L^{-1}$ de O_2)	571.0	350.0	217.0	209.0	365.0	616.0	5.0	0.8
BOD_5 ($mg\ L^{-1}$ de O_2)	103.0	117.0	69.0	70.0	82.0	312.0	2.0	0.6
BOD_5/COD	0.18	0.33	0.32	0.33	0.22	0.51	-	-
TS ($mg\ L^{-1}$)	60	29	67	76	112	117	10	5
STS ($mg\ L^{-1}$)	654	218	261	317	177	367	10	5

Where: LOQ: Limit of Quantification; LOD: Limit of Detection; COD: Chemical Oxygen Demand; BOD_5: Biochemical Oxygen Demand; STS: Suspended Total Solids; ST: Total Solids.

Physicochemical parameters evaluated were, in general, variable over the monitored time. According to Carraro et al., (2016)[1] the great variability of the characteristics of these effluents is recurrent due to the many variables that influence them, such as the size of the hospital, the number of patients, the number of wards, the number and types of services, country, population and seasonality.

The effluents, according to Resolution 357/2005 of the National Environment Council(CONAMA) from Brazil, must have a pH between 5.0 and 9.0 so that they can be

discharged directly into sewage because at extreme pHs, the physiology of animals and aquatic vegetables can be changed. In this sense, all samples were according CONAMA regulation parameters.

High values of conductivity obtained for the analyzed samples, in the range of 114 to 1209 µS cm^{-1}, are characteristic of the occurrence of high concentration of minerals. High conductivity could mean the risk of salinization of aquatic bodies that receive effluent without treatment.[2]

The BOD_5/COD is a parameter that deserve attention because could reflect in the biodegradability of the matrix under study. According to Kumar et al., (2010),[3]BOD_5/COD close to 1 can be indicative for a biodegradable matrix, even that values close to 0.5 could represent a considerable index of biodegradability according to Esplugas et al., (2004)[4]. With the exception of the January sample, which obtained a value very close to 0.5, the other samples presented BOD_5/COD indexes below 0.5. The possible reduced biodegradability of these samples is an indication of the possible limitation of the treatment performance, of this effluent, in biological treatment systems.

Section S4. Evaluation of solid phase extraction (SPE)

Figure S2 illustrates the two methods tested for the SPE technique. It is possible to verify that the only difference between the two tested method is the elution step. The other steps of SPE occurred equally in both methods.

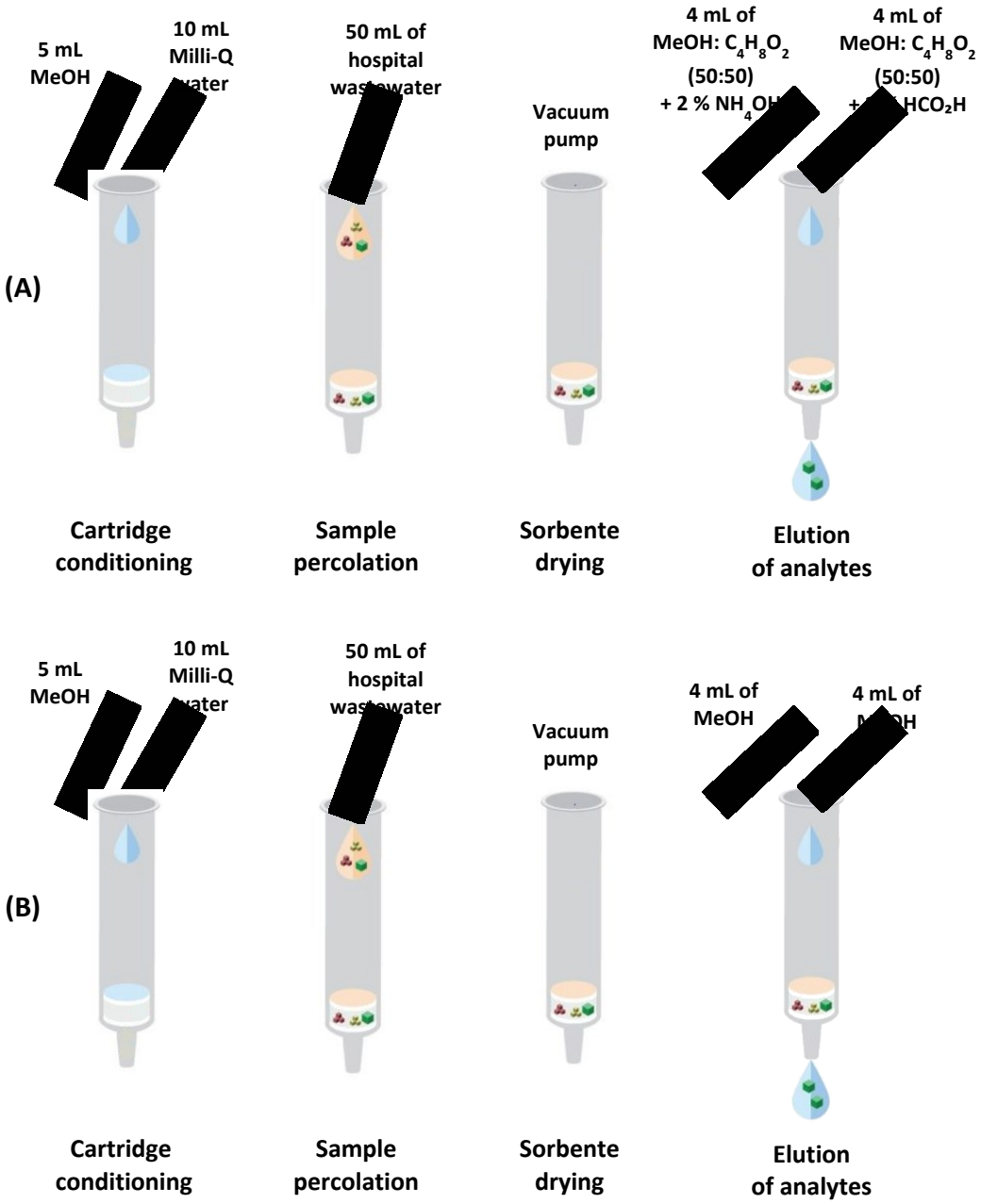


Figure S2. Evaluation of solid phase extraction (SPE):(A) Method A illustration; (B) Method B illustration.

Section S5.Sample preparation

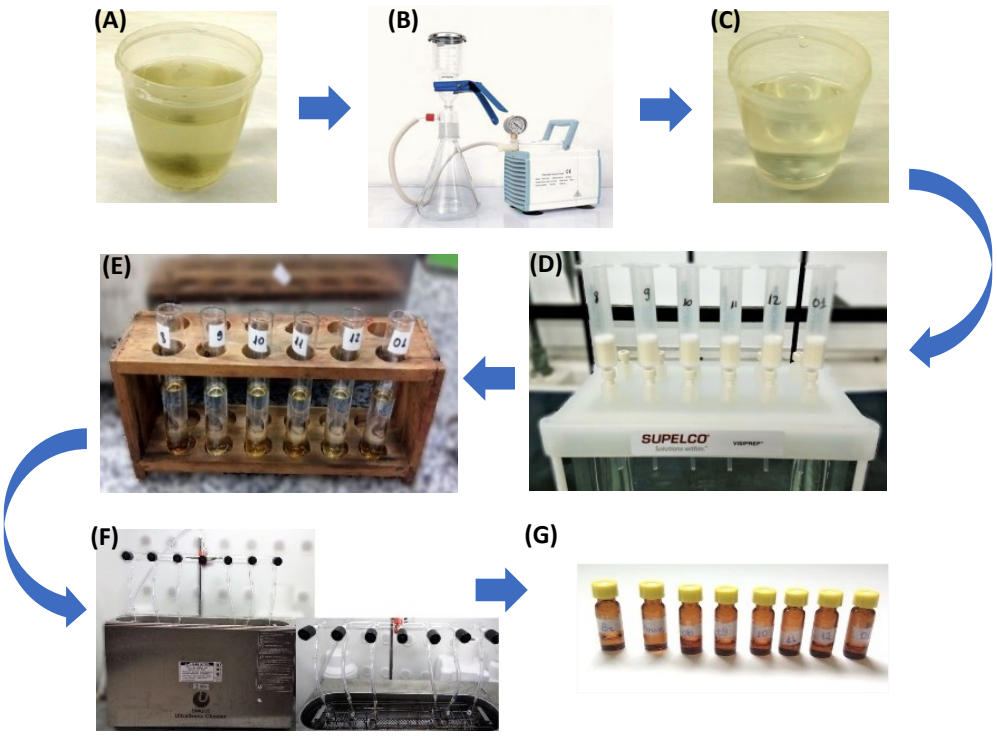


Figure S3 Scheme with photos of the sample preparation step: Figure(A) shows a sample of raw hospital effluent;Figure (B) shows the sample filtration step; Figure(C) shows a sample of hospital wastewater after filtration;Figure(D) shows the stage of conditioning the cartridges and percolating the sample; Figure(E) shows the elution of the analytes; Figure (F) illustrates the drying step of the sample under N_2 flow; Figure (G) illustrates the sample reconstitution step with MeOH:H_2O (10:90), filtration in at 0.22 µm PVDF filter and the conditioning in vials.

Section S6. Construction of pharmaceuticals databases

Table S2. Summarized pharmaceuticals contained in our purpose built-database.

Compound	Ionization mode	rt (min)	Measured *m/z*	Ion formula	Calculated *m/z*	error (ppm)	mSigma*	RDB**
2 - Hydroxyquinoline	Positive	0.9	146.0593	C_9H_8NO	146.0600	5.0	49.7	6.5
8 - Hydroxyquinoline	Positive	0.9	146.0593	C_9H_8NO	146.0600	4.9	49.9	6.5
Aceclofenac	Positive	9.0	354.0298	$C_{16}H_{14}Cl_2NO_4$	354.0294	-1.1	7.0	9.5
Acetaminophen	Positive	2.3	152.0708	$C_8H_{10}NO_2$	152.0706	-1.2	3.1	4.5
	Negative	2.3	150.0560	$C_8H_8NO_2$	150.0561	0.4	4.8	5.5
Albendazole	Positive	8.7	266.0960	$C_{12}H_{16}N_3O_2S$	266.0958	-0.8	6.5	6.5
Amiodarone	Positive	10.6	646.0319	$C_{25}H_{30}I_2NO_3$	646.0310	-1.5	6.6	10.5
Amlodipine	Positive	8.1	409.1528	$C_{20}H_{26}ClN_2O_5$	409.1525	-0.8	5.9	8.5
Amoxicillin	Positive	1.5	366.1123	$C_{16}H_{20}N_3O_5S$	366.1118	-1.2	10.2	8.5
Apresoline	Positive	1.5	161.0822	$C_8H_9N_4$	161.0822	0.1	8.5	6.5
Arginine	Positive	0.9	175.1189	$C_6H_{15}N_4O_2$	171.1900	0.1	7.8	1.5
Atenolol	Positive	2.1	267.1701	$C_{14}H_{23}N_2O_3$	267.1703	0,9	7.2	4.5
Betahistine	Positive	1.0	137.1066	$C_8H_{13}N_2$	137.1073	5.0	49.8	3.5
Betamethasone	Positive	8.2	393.2071	$C_{22}H_{30}FO_5$	393.2072	0.2	0.7	7.5
Bilastine	Positive	7.6	464.2905	$C_{28}H_{38}N_3O_3$	464.2908	0.6	11.7	11.5
Bisacodyl	Positive	8.5	362.1383	$C_{22}H_{20}NO_4$	362.1387	1.0	4.9	13.5
Bromazepam	Positive	7.3	316.0088	$C_{14}H_{11}BrN_3O$	316.0080	-2.5	11.0	10.5
Bupropion	Positive	6.1	240.1150	$C_{13}H_{19}ClNO$	240.1150	0.0	3.0	4.5
Buspirone	Positive	6.1	386.2551	$C_{21}H_{32}N_5O_2$	386.2551	-0.2	12.9	8.5
Caffeine	Positive	4.2	195.0871	$C_8H_{11}N_4O_2$	195.0877	2.6	4.0	5.5
Candesartan Cilexetil	Positive	10.6	611.2620	$C_{33}H_{35}N_6O_6$	611.2613	-1.2	2.6	19.5
Captopril	Positive	4.0	218.0845	$C_9H_{16}NO_3S$	218.0845	0.1	4.8	2.5
Carisoprodol	Positive	8.0	261.1807	$C_{12}H_{25}N_2O_4$	261.1809	0.5	10.3	1.5
Cefadroxil	Positive	1.6	364.0965	$C_{16}H_{18}N_3O_5S$	364.0962	-1.0	7.8	9.5
Celecoxib	Positive	9.4	382.0835	$C_{17}H_{15}F_3N_3O_2S$	382.0832	-1.0	12.4	10.5
	Negative	9.4	380.0686	$C_{17}H_{13}F_3N_3O_2S$	380.0686	0.0	22.4	11.5
Chlormadinone Acetate	Positive	9.7	405.1832	$C_{23}H_{30}ClO_4$	405.1827	-1.2	8.8	8.5
Ciprofloxacin	Positive	5.0	332.1409	$C_{17}H_{19}FN_3O_3$	332.1405	-1.2	4.6	9.5
Citalopram	Positive	6.9	325.1713	$C_{20}H_{22}FN_2O$	325.1711	-0.7	1.8	10.5
Clonazepam	Positive	7.7	316.0479	$C_{15}H_{11}ClN_3O_3$	316.0483	1.5	2.1	11.5
	Negative	7.7	314.0329	$C_{15}H_9ClN_3O_3$	314.0338	2.8	12.2	12.5
Codeine	Positive	2.9	300.1600	$C_{18}H_{22}NO_3$	300.1594	-2.1	7.1	8.5
Cyclobenzaprine	Positive	7.7	276.1746	$C_{20}H_{22}N$	276.1747	0.1	40.8	10.5
Deflazacort	Positive	8.8	442.2227	$C_{25}H_{32}NO_6$	442.2224	-0.6	3.1	10.5
	Negative	8.8	440.2074	$C_{25}H_{30}NO_6$	440.2079	1.0	0.9	11.5
Desloratadine	Positive	7.7	311.1311	$C_{19}H_{20}ClN_2$	311.1310	-0.6	4.4	10.5
Desvenlafaxine	Positive	5.1	264.1958	$C_{16}H_{26}NO_2$	264.1958	0.1	0.7	4.5
Diazepam	Positive	8.9	285.0792	$C_{16}H_{14}ClN_2O$	285.0789	-0.8	6.3	10.5
Diclofenac	Positive	9.6	296.0225	$C_{14}H_{12}Cl_2NO_2$	296.0240	5.0	8.4	8.5
	Negative	8.5	294.0096	$C_{14}H_{10}Cl_2NO_2$	294.0094	-0.6	8.4	9.5
Dimenhydrinate	Positive	4.7	215.0328	$C_7H_8ClN_4O_2$	215.0330	1.1	6.3	5.5
Dipyrone	Positive	4.2	218.1284	$C_{12}H_{16}N_3O$	218,1288	2.0	9.4	6.5

	Negative	4.2	310.0864	$C_{13}H_{16}N_3O_4S$	310.0867	0.9	16.4	7.5
Divalproate	Positive	9.0	145.1222	$C_8H_{17}O_2$	145.1223	0.7	1.0	0.5
Donepezil	Positive	6.2	380.2221	$C_{24}H_{30}NO_3$	380.2220	-0.1	1	10.5
Doxycycline	Positive	7.1	445.1616	$C_{22}H_{25}N_2O_8$	445.1605	-2.3	18.3	11.5
Duloxetine	Positive	7.9	298.1257	$C_{18}H_{20}NOS$	298.1260	1	9.9	9.5
Dydrogesterone	Positive	9.6	313.2167	$C_{21}H_{29}O_2$	313.2162	-1.6	3.4	7.5
Enalapril	Positive	7.1	377.2055	$C_{20}H_{29}N_2O_5$	377.2071	4.1	13.3	7.5
Escitalopram	Positive	6.9	325.1712	$C_{20}H_{22}FN_2O$	325.1711	-0.3	3.5	10.5
Estradiol	Positive	10.5	273.1849	$C_{18}H_{25}O_2$	273.1849	-0.1	15.3	6.5
Etodolac	Positive	9.5	288.1594	$C_{17}H_{22}NO_3$	288.1594	0.1	3.2	7.5
	Negative	8.7	286.1446	$C_{17}H_{20}NO_3$	286.1449	0.8	6.6	8.5
Fexofenadine	Positive	7.8	502.2950	$C_{32}H_{40}NO_4$	502.2952	0.4	13.7	13.5
	Negative	7.7	500.2796	$C_{32}H_{38}NO_4$	500.2806	2.0	5.4	14.5
Fluoxetine	Positive	8.4	310.1412	$C_{17}H_{19}F_3NO$	310.1413	0.3	4.3	7.5
Furosemide	Positive	6.3	331.0153	$C_{12}H_{12}ClN_2O_5S$	331.0150	-1.0	14.6	7.5
	Negative	5.4	329.0004	$C_{12}H_{10}ClN_2O_5S$	329.0004	0.2	5.3	8.5
Galantamine	Positive	3.0	288.1595	$C_{17}H_{22}NO_3$	288.1594	-0.4	13.6	7.5
Hydrochlorothiazide	Positive	2.2	297.9719	$C_7H_9ClN_3O_4S_2$	297.9718	-0.6	10.0	4.5
	Negative	2.2	295.9567	$C_7H_7ClN_3O_4S_2$	295.9572	1.8	5.5	5.5
Hydroxyzine	Positive	8.0	375.1842	$C_{21}H_{28}ClN_2O_2$	375.1834	-2.2	5.0	8.5
Ibuprofen	Positive	10.0	207.1376	$C_{13}H_{19}O_2$	207.1380	1.8	1.5	4.5
	Negative	8.6	205.1235	$C_{13}H_{17}O_2$	205.1234	-0.4	1.2	5.5
Isometheptene	Positive	5.3	142.1591	$C_9H_{20}N$	142.1590	-0.7	1.5	0.5
Ketoprofen	Positive	8.4	255.1014	$C_{16}H_{15}O_3$	255.1016	0.7	3.3	9.5
	Negative	7.0	253.0874	$C_{16}H_{13}O_3$	253.0870	-1.5	6.0	10.5
Ketorolac	Positive	8.7	256.0967	$C_{15}H_{14}NO_3$	256.0968	0.5	1.8	9.5
	Negative	6.2	254.0818	$C_{15}H_{12}NO_3$	254.0823	1.7	11.2	10.5
Lamotrigine	Positive	5.6	256.0151	$C_9H_8Cl_2N_5$	256.0151	-0.0	4.8	7.5
	Negative	5.9	254.0009	$C_9H_6Cl_2N_5$	254.0006	-1.3	5.8	8.5
Lansoprazole	Positive	7.6	370.0835	$C_{16}H_{15}F_3N_3O_2S$	370.0832	-1.0	6.2	9.5
Levodropropizine	Positive	3.0	237.1598	$C_{13}H_{21}N_2O_2$	237.1598	-0.2	15.7	4.5
Loperamide	Positive	8.2	477.2323	$C_{29}H_{34}ClN_2O_2$	477.2303	-4.0	18.2	13.5
Loratadine	Positive	10.3	383.1529	$C_{22}H_{24}ClN_2O_2$	383.1521	-2.2	7.9	11.5
Losartan	Positive	8.3	423.1700	$C_{22}H_{24}ClN_6O$	423.1695	-1.2	2.2	13.5
Lysine	Positive	0.7	147.1128	$C_6H_{15}N_2O_2$	147.1128	0	7.6	0.5
Meclizine	Positive	9.0	391.1945	$C_{25}H_{28}N_2Cl$	391.1936	-2.5	11.6	12.5
Mefenamic acid	Positive	10.4	242.1172	$C_{15}H_{16}NO_2$	242,1176	5	3.9	8.5
	Negative	8.8	240.1031	$C_{15}H_{14}NO_2$	240.1030	-0.4	7.8	9.5
Meloxicam	Positive	9.0	352.0422	$C_{14}H_{14}N_3O_4S_2$	352.0420	-0.6	11.4	9.5
	Negative	6.7	350.0272	$C_{14}H_{12}N_3O_4S_2$	350.0275	0.8	12.0	10.5
Mesalazine	Positive	1.2	154.0503	$C_7H_8NO_3$	154.0499	-3.1	13.4	4.5
Metformin	Positive	1.1	130.1087	$C_4H_{12}N_5$	130.1087	0.4	7.9	1.5
Metoclopramide	Positive	4.8	300.1482	$C_{14}H_{23}ClN_3O_2$	300.1473	-2.9	20.0	4.5
Metronidazole	Positive	2.6	172.0717	$C_6H_{10}N_3O_3$	172.0717	-0.4	2.4	3.5
Naproxen	Positive	8.8	231.1014	$C_{14}H_{15}O_3$	231.1016	0.6	1.2	7.5
	Negative	6.9	229.0867	$C_{14}H_{13}O_3$	229.0870	1.4	5.0	8.5
Naratriptan	Positive	4.0	336.1752	$C_{17}H_{26}N_3O_2S$	336.1740	-3.5	7.4	6.5
Nimesulide	Positive	8.3	309.0542	$C_{13}H_{13}N_2O_5S$	309.0540	-0.7	8.5	8.5
	Negative	8.0	307.0389	$C_{13}H_{11}N_2O_5S$	307.0394	1.5	8.0	9.5
Nitazoxanide	Positive	7.9	308.0337	$C_{12}H_{10}N_3O_5S$	308.0336	-0.3	9.4	9.5
	Negative	6.7	306.0190	$C_{12}H_8N_3O_5S$	306.0190	-0.1	7.8	10.5

Nitrofurantoin	Positive	3.6	239.0406	$C_8H_7N_4O_5$	239.0411	1.9	3.2	7.5
	Negative	3.3	237.0265	$C_8H_5N_4O_5$	237.0265	0.1	7.0	8.5
Norethisterone	Positive	8.9	299.2009	$C_{20}H_{27}O_2$	299.2006	-1.2	0.7	7.5
Norfloxacin	Positive	4.8	320.1413	$C_{16}H_{19}FN_3O_3$	320.1405	-2.4	3.4	8.5
Nortriptyline	Positive	8.6	264.1747	$C_{19}H_{22}N$	264.1747	-0.2	1.7	9.5
Omeprazole	Positive	7.6	346.1224	$C_{17}H_{20}N_3O_3S$	346.1220	-1.1	17.0	9.5
	Negative	7.7	344.1072	$C_{17}H_{18}N_3O_3S$	344.1074	0.8	13.3	10.5
Ondansetron	Positive	5.6	294.1603	$C_{18}H_{20}N_3O$	294.1601	-0.8	5.2	10.5
Oxomemazine	Positive	6.3	331.1474	$C_{18}H_{23}N_2O_2S$	331.1475	0.3	11.7	8.5
Oxymetazoline	Positive	7.3	261.1964	$C_{16}H_{25}N_2O$	261.1961	-1.0	1.5	5.5
Pantoprazole	Positive	7.5	384.0831	$C_{16}H_{16}F_2N_3O_4S$	384.0824	-1.7	8.0	9.5
Papaverine	Positive	5.8	340.1548	$C_{20}H_{22}NO_4$	340.1543	-1.2	1.8	10.5
Prednisolone	Positive	7.7	361.2013	$C_{21}H_{29}O_5$	361.2010	-0.9	3.4	7.5
	Negative	7.7	359.1853	$C_{21}H_{27}O_5$	359.1864	3.0	22.2	8.5
Prednisone	Positive	7.4	359.1859	$C_{21}H_{27}O_5$	359.1853	-1.7	2.9	8.5
	Negative	7.3	357.1708	$C_{22}H_{21}N_4O$	357.1721	3.7	19.3	14.5
Progesterone	Positive	9.9	315.2323	$C_{21}H_{31}O_2$	315.2319	-1.4	3.6	6.5
Propranolol	Positive	6.8	260.1646	$C_{16}H_{22}NO_2$	260.1645	-0.3	21.6	6.5
Pseudoephedrine	Positive	3.1	166.1225	$C_{10}H_{16}NO$	166.1226	0.9	1.1	3.5
Pyridoxine	Positive	1.2	170.0811	$C_8H_{12}NO_3$	170.0812	0.2	6.3	3.5
	Negative	1.6	168.0666	$C_8H_{10}NO_3$	168.0666	0.1	18.3	4.5
Quetiapine	Positive	7.5	384.,1742	$C_{21}H_{26}N_3O_2S$	384.1740	-0.4	9.9	10.5
Racecadotril	Positive	9.1	386.1426	$C_{21}H_{24}NO_4S$	386.1421	-1.5	16.1	10.5
Ranitidine	Positive	2.3	315.1490	$C_{13}H_{23}N_4O_3S$	315.1485	-1.5	7.4	4.5
	Negative	4.5	313.1336	$C_{13}H_{21}N_4O_3S$	313.1340	1.2	4.3	5.5
Rifamycin	Positive	10.3	698.3144	$C_{37}H_{48}NO_{12}$	698.3171	3.9	30.0	14.5
Rosuvastatin	Positive	8.2	482.1755	$C_{22}H_{29}FN_3O_6S$	482.1756	0.0	10.5	9.5
	Negative	7.6	480.1602	$C_{22}H_{27}FN_3O_6S$	480.1610	1.7	11.0	10.5
Secnidazole	Positive	3.9	186.0873	$C_7H_{12}N_3O_3$	186.0873	0.3	5.2	3.5
Sertraline	Positive	8.4	306.0810	$C_{17}H_{18}Cl_2N$	306.0811	0.2	8.1	8.5
Simvastatin	Positive	10.8	419.2790	$C_{25}H_{39}O_5$	419.2792	0.5	5.7	6.5
Sotalol	Positive	1.7	273.1269	$C_{12}H_{21}N_2O_3S$	273.1267	-0.7	6.2	3.5
Sumatriptan	Positive	3.0	296.1430	$C_{14}H_{22}N_3O_2S$	296.1427	-1.0	6.3	5.5
Tadalafil	Positive	8.2	390.1456	$C_{22}H_{20}N_3O_4$	390.1448	-1.9	1.0	14.5
	Negative	8.2	388.1301	$C_{22}H_{18}N_3O_4$	388.1303	0.4	17.0	15.5
Thiamine	Positive	0.8	265.1116	$C_{12}H_{17}N_4OS$	265.1118	0.6	12.1	6.5
Thioridazine	Positive	8.6	371.1609	$C_{21}H_{27}N_2S_2$	371.1610	0.2	14.8	9.5
Tianeptine	Positive	7.5	437.1297	$C_{21}H_{26}ClN_2O_4S$	437.1296	-0.2	3.2	9.5
	Negative	8.2	435.1150	$C_{21}H_{24}ClN_2O_4S$	435.1151	0.1	17.0	10.5
Tibolone	Positive	9.6	313.2158	$C_{21}H_{29}O_2$	313.2162	1.3	7.4	7.5
Topiramate	Positive	6.2	340.1060	$C_{12}H_{22}NO_8S$	340.1061	0.1	8	2.5
	Negative	6.3	338.0912	$C_{12}H_{20}NO_8S$	338.0915	1.0	8.8	3.5
Tramadol	Positive	5.2	264.1957	$C_{16}H_{26}NO_2$	264.1958	0.3	3.4	4.5
Trimebutine	Positive	7.5	388.2125	$C_{22}H_{30}NO_5$	388.2118	-1.6	12.1	8.5
Venlafaxine	Positive	6.4	278.2113	$C_{17}H_{28}NO_2$	278.2115	0.4	0.8	4.5
Zuclopenthixol	Positive	10.1	401.1451	$C_{22}H_{26}ClN_2OS$	401.1449	-0.4	4.2	10.5

Where: * mSigma: indicates the error in relation to the isotopic profile

** RDB: ring double bonds

Section S7. Process of confirmation of the presence of pharmaceuticals

This Section explains in more detail the process of confirming the presence of pharmaceuticals in the screening analysis.

The pharmaceuticals screening was performed after the samples were analyzed by UHPLC-QTOF MS as described in Section 2.2. Firstly, using the TargetAnalysis software, the databases were loaded to a pharmaceuticals screening method based on the following acceptance parameters: exact mass of the molecular ion with an error less than 5 ppm, mSigma (isotopic profile) with an error less than 50, retention time with a tolerance of 0.2 min and presence of at least characteristic fragments with an error below 5 ppm.

(A)

Score	Cmpd.Name	Reg.No.	Formula	PMI	deltaRT [min]	Err [mDa]	Err [ppm]	mSigma	RT meas. [min]	RT exp.[min]	m/z meas.	m/z calc.
++++	Acetaminophen		C 8 H 9 N 1 O 2	[M+H]+	0.0	0.2	1.0	4.9	2.3	2.3	152.0708	152.0706
++++	Atenolol		C 14 H 22 N 2 O 3	[M+H]+	0.1	-0.2	-0.6	0.9	2.0	2.1	267.1705	267.1703
++++	Caffeine		C 8 H 10 N 4 O 2	[M+H]+	0.1	0.3	1.5	9.7	4.1	4.2	195.0879	195.0877
++++	Carisoprodol		C 12 H 24 N 2 O 4	[M+H]+	0.0	0.5	1.8	7.0	8.0	8.0	261.1804	261.1809
++++	Desvenlafaxine		C 16 H 25 N 1 O 2	[M+H]+	0.0	-0.1	-0.5	3.9	5.1	5.1	264.1957	264.1958
++++	Diazepam		C 16 H 13 Cl 1 N 2 O 1	[M+H]+	0.0	-0.1	-0.2	18.7	8.9	8.9	285.0789	285.0789
++++	Diclofenac		C 14 H 11 Cl 2 N 1 O 2	[M+H]+	0.1	0.3	0.9	11.2	9.5	9.6	296.0237	296.0240
++++	Dipyrone		C 12 H 15 N 3 O 1	[M+H]+	0.0	-0.2	-0.8	8.3	4.2	4.2	218.1286	218.1288
++++	Divalproate		C 8 H 16 O 2	[M+H]+	-0.1	-0.1	-0.4	6.0	9.1	9.0	145.1223	145.1223
++++	Ketoprofen		C 16 H 14 O 3	[M+H]+	0.1	0.6	2.4	2.3	8.3	8.4	255.1010	255.1016
++++	Lamotrigine		C 9 H 7 Cl 2 N 5	[M+H]+	0.0	0.0	0.0	15.7	5.6	5.6	256.0151	256.0151
++++	Losartan		C 22 H 23 Cl 1 N 6 O 1	[M+H]+	0.1	-0.7	-1.5	9.7	8.2	8.3	423.1688	423.1695
++++	Mesalazine		C 7 H 7 N 1 O 3	[M+H]+	-0.2	0.6	3.8	5.3	1.4	1.2	154.0505	154.0499
++++	Metformin		C 4 H 11 N 5	[M+H]+	0.0	0.2	1.8	9.4	1.1	1.1	130.1090	130.1087
++++	Naproxen		C 14 H 14 O 3	[M+H]+	0.3	-0.4	-1.6	11.3	8.5	8.8	231.1012	231.1016
++++	Omeprazole		C 17 H 19 N 3 O 3 S 1	[M+H]+	0.6	0.3	0.8	14.2	7.0	7.6	346.1217	346.1220
++++	Pseudoephedrine		C 10 H 15 N 1 O 1	[M+H]+	0.1	0.1	0.6	4.9	3.0	3.1	166.1227	166.1226
++++	Rosuvastatin		C 22 H 28 F 1 N 3 O ...	[M+H]+	0.1	0.6	1.2	18.8	8.1	8.2	482.1750	482.1756
++++	Topiramate		C 12 H 21 N 1 O 8 S 1	[M+H]+	0.0	0.2	0.6	10.9	6.2	6.2	340.1058	340.1061
++++	Tramadol		C 16 H 25 N 1 O 2	[M+H]+	0.1	-0.1	-0.5	3.9	5.1	5.2	264.1957	264.1958

(B)

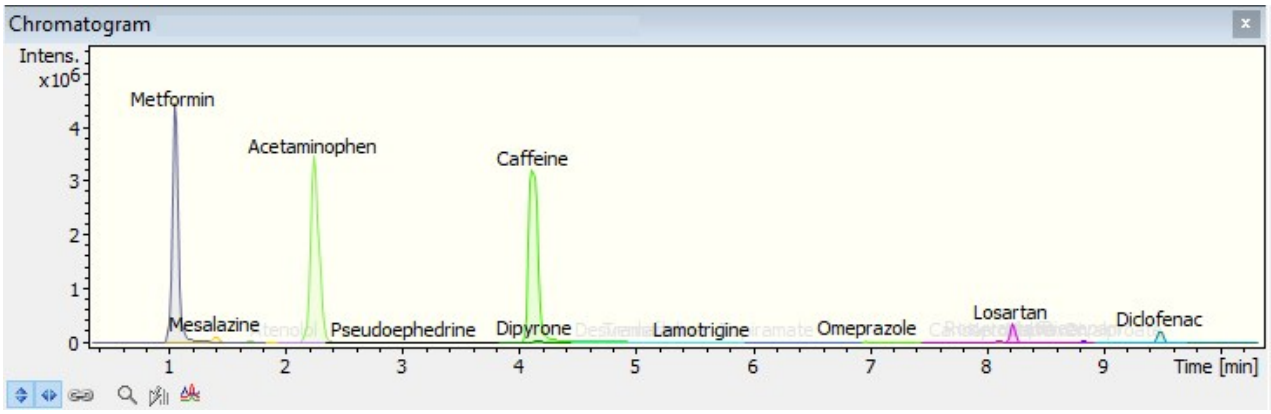


Figure S4. Data provided by softwares during data processing analysis in one sample on positive ionization mode: (A) TargetAnalysis software; (B) DataAnalysis software.

Figure S4(A) illustrates the results of screening for a sample (September 2017). The TagetAnalysis software indicates, from a score indicating with the positive symbol (+), how

many acceptance parameters were recognized for the identified pharmaceuticals. Figure S4(A) indicates, for the pharmaceuticals listed, that all acceptance parameters were established in the analyzed sample.

However, in order to confirm the establishment of all identified parameters and, consequently, the presence of pharmaceuticals, using the DataAnalysis software (Figure S4(B), where all molecular ion and fragments were verified.

As an example, Figure S5 illustrates the validation of acceptance parameters for the diclofenac identified in the positive ionization mode (sample September 2017).The chromatographic peak corresponding, possibly, to diclofenac (Figure S4(B)) was observed in 9.5 min. The low collision energy (LE) mass spectrum (Figure S5) showed a signal with *m/z* 296.0236 Da, which corresponded to the protonated diclofenac $[C_{14}H_{12}Cl_2NO_2]^+$.In addition to the molecular ion, the sodium adduct $[C_{14}H_{11}Cl_2NNaO_2]^+$ was also identified in the low collision energy (LE) mass spectrum. The high collision energy (HE) mass spectrum identified several characteristic fragments compatible with the fragmentation profile of diclofenac, presenting the same retention time as the active ingredient. The active ingredient, the sodium adduct and all the fragments identified showed a mass error of less than 5 ppm and an isotopic profile with an error of less than 50. In addition, the retention time variance was less than, 2 min.

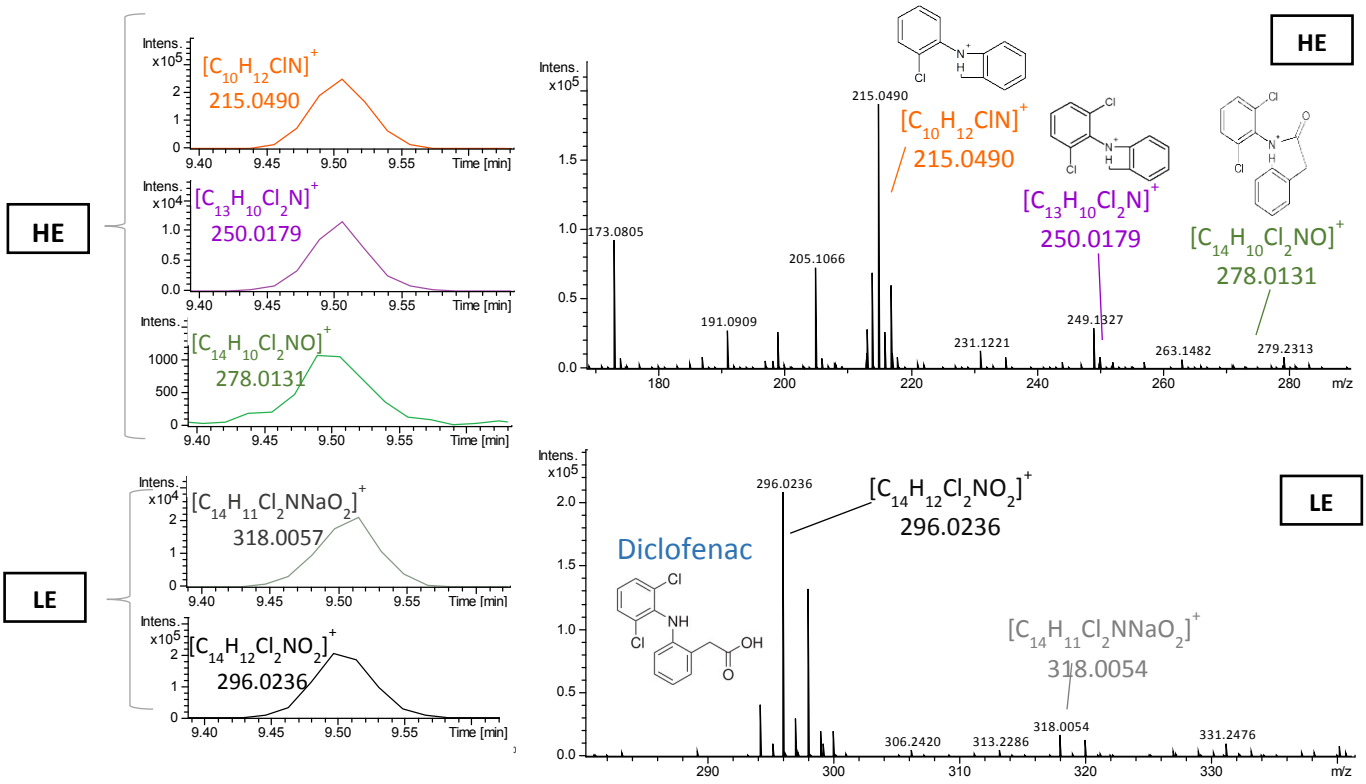


Figure S5. Confirmation process of diclofenac in sample analyzed in positive ionization mode. WhereHE = High collision energy/MS spectra and LE = Low collision energy/bbCID spectra.

Section S8.Pharmaceuticals screening results

Table S3. Detailed information on the confirmed pharmaceuticals identified.

Sample	Compound	Ionization mode	rt (min)	Measured *m/z*	Ion formula	Calculated *m/z*	Error (ppm)	mSigma*	RDB**
Aug. 17	Acetaminophen	Positive	2.2	152.0708	$C_8H_{10}NO_2$	152.0706	-1.1	3.3	4.5
		Negative	2.2	150.0560	$C_8H_8NO_2$	150.0561	0.1	15.4	5.5
	Atenolol	Positive	2.0	267.1709	$C_{14}H_{23}N_2O_3$	267.1703	-2.3	0.7	4.5
	Caffeine	Positive	4.1	195.0884	$C_8H_{11}N_4O_2$	195.0877	-3.7	14.4	5.5
	Desvenlafaxine	Positive	5.0	264.1963	$C_{16}H_{26}NO_2$	264.1958	-1.7	6.9	4.5
	Diazepam	Positive	8.9	285.0787	$C_{16}H_{14}ClN_2O$	285.0789	0.7	19.7	10.5
	Diclofenac	Positive	9.5	296.0238	$C_{14}H_{12}Cl_2NO_2$	296.0240	0.7	15.7	8.5
		Negative	8.3	294.0092	$C_{14}H_{10}Cl_2NO_2$	294.0094	0.5	5.7	9.5
	Dipyrone	Positive	4.2	218.1290	$C_{12}H_{16}N_3O$	218.1288	-0.8	9.1	6.5
	Fexofenadine	Positive	7.8	502.2932	$C_{32}H_{40}NO_4$	502.2952	3.9	38.3	13.5
	Hydrochlorothiazide	Negative	2.1	295.9570	$C_7H_7ClN_3O_4S_2$	295.9572	0.7	34.5	5.5
	Ibuprofen	Negative	8.5	205.1236	$C_{13}H_{17}O_2$	205.1234	-1.1	49.8	5.5
	Lamotrigine	Positive	5.6	256.0156	$C_9H_8Cl_2N_5$	256.0151	-1.7	6.8	7.5
	Losartan	Positive	8.2	423.1691	$C_{22}H_{24}ClN_6O$	423.1695	0.9	22.9	13.5
	Mesalazine	Positive	1.4	154.0501	$C_7H_8NO_3$	154.0499	-1.7	5.6	4.5
	Metformin	Positive	1.1	130.1088	$C_4H_{12}N_5$	130.1087	-0.8	9.5	1.5
	Naproxen	Positive	8.6	231.1017	$C_{14}H_{15}O_3$	231.1016	-0.7	4.7	7.5
		Negative	6.7	229.0867	$C_{14}H_{13}O_3$	229.0870	1.4	18.3	8.5
	Nimesulide	Negative	7.8	307.0394	$C_{13}H_{11}N_2O_5S$	307.0394	-0.0	15.1	9.5
	Ondansetron	Positive	5.6	294.1600	$C_{18}H_{20}N_3O$	294.1601	0.1	14.1	10.5
	Pseudoephedrine	Positive	3.0	166.1230	$C_{10}H_{16}NO$	166.1226	-2.1	8.8	3.5
	Pyridoxine	Positive	1.2	170.0813	$C_8H_{12}NO_3$	170.0812	-0.5	5.9	3.5
	Rosuvastatin	Positive	8.1	482.1749	$C_{22}H_{29}FN_3O_6S$	482.1756	1.4	16.6	9.5
		Negative	7.5	480.1609	$C_{22}H_{27}FN_3O_6S$	480.1610	0.3	19.7	10.5
	Thiamine	Positive	1.0	265.1119	$C_{12}H_{17}N_4OS$	265.1118	-0.7	30.5	6.5
	Topiramate	Negative	6.1	338.0913	$C_{12}H_{20}NO_8S$	338.0915	0.5	21.4	3.5
	Tramadol	Positive	5.0	264.1960	$C_{16}H_{26}NO_2$	264.1958	-0.6	8.8	4.5
Sep. 17	Acetaminophen	Positive	2.3	152.0706	$C_8H_{10}NO_2$	152.0706	-0.2	4.4	4.5
		Negative	2.3	150.0560	$C_8H_8NO_2$	150.0561	0.5	10.7	5.5
	Atenolol	Positive	2.0	267.1705	$C_{14}H_{23}N_2O_3$	267.1703	-0.8	7.1	4.5
	Caffeine	Positive	4.1	195.0882	$C_8H_{11}N_4O_2$	195.0877	-3	23.6	5.5
	Carisoprodol	Positive	8.0	261.1804	$C_{12}H_{25}N_2O_4$	261.1809	1.7	12.6	1.5
	Celecoxib	Negative	9.4	380.0678	$C_{17}H_{13}F_3N_3O_2S$	380.0686	2	26.4	12
	Desvenlafaxine	Positive	5.1	264.1958	$C_{16}H_{26}NO_2$	264.1958	0.1	2.9	4.5
	Diazepam	Positive	8.9	285.0790	$C_{16}H_{14}ClN_2O$	285.0789	-0.3	20.9	10.5
	Diclofenac	Positive	9.5	296.0236	$C_{14}H_{12}Cl_2NO_2$	296.0240	1.3	12	8.5

		Negative	8.3	294.0093	$C_{14}H_{10}Cl_2NO_2$	294.0094	0.5	4.3	9.5
	Divalproate	Positive	9.1	145.1220	$C_8H_{17}O_2$	145.1223	1.8	50	0.5
	Ibuprofen	Negative	8.5	205.1231	$C_{13}H_{17}O_2$	205.1234	1.3	26.3	5.5
	Ketoprofen	Positive	8.3	255.1010	$C_{16}H_{15}O_3$	255.1016	2.2	2.3	9.5
	Losartan	Positive	8.2	423.1685	$C_{22}H_{24}ClN_6O$	423.1695	2.2	7.9	13.5
	Mesalazine	Positive	1.4	154.0501	$C_7H_8NO_3$	154.0499	-1.7	7.3	4.5
	Metformin	Positive	1.1	130.1088	$C_4H_{12}N_5$	130.1087	-0.9	9.1	1.5
	Naproxen	Positive	8.6	231.1014	$C_{14}H_{15}O_3$	231.1016	0.8	15	7.5
	Nimesulide	Negative	7.8	307.0394	$C_{13}H_{11}N_2O_5S$	307.0394	0.1	34.9	9.5
	Pseudoephedrine	Positive	3.0	166.1226	$C_{10}H_{16}NO$	166.1226	0.1	3.6	3.5
	Rosuvastatin	Positive	8.2	482.1752	$C_{22}H_{29}FN_3O_6S$	482.1756	0.8	16.8	9.5
	Rosuvastatin	Negative	7.5	480.1601	$C_{22}H_{27}FN_3O_6S$	480.1610	1.9	14.5	10.5
	Topiramate	Positive	6.1	340.1053	$C_{12}H_{22}NO_8S$	340.1061	2.2	10.2	2.5
		Negative	6.2	338.0915	$C_{12}H_{20}NO_8S$	338.0915	-0.1	8.4	3.5
	Acetaminophen	Positive	2.2	152.0705	$C_8H_{10}NO_2$	152.0706	0.4	1.8	4.5
		Negative	2.2	150.0563	$C_8H_8NO_2$	150.0561	-1.4	4.6	5.5
	Atenolol	Positive	2.0	267.1700	$C_{14}H_{23}N_2O_3$	267.1703	1.1	6.3	4.5
	Caffeine	Positive	4.1	195.0878	$C_8H_{11}N_4O_2$	195.0877	-0.5	8	5.5
	Codeine	Positive	2.7	300.1595	$C_{18}H_{22}NO_3$	300.1594	-0.4	3.3	8.5
	Desvenlafaxine	Positive	5.0	264.1958	$C_{16}H_{26}NO_2$	264.1958	-0.1	21.7	4.5
	Diazepam	Positive	8.8	285.0789	$C_{16}H_{14}ClN_2O$	285.0789	0	23.1	10.5
	Diclofenac	Positive	9.5	296.0241	$C_{14}H_{12}Cl_2NO_2$	296.0240	-0.6	34.5	8.5
		Negative	8.3	294.0087	$C_{14}H_{10}Cl_2NO_2$	294.0094	2.3	32.5	9.5
	Dipyrone	Positive	4.1	218.1292	$C_{12}H_{16}N_3O$	218.1288	-1.9	32.1	6.5
	Escitalopram	Positive	6.9	325.1712	$C_{20}H_{22}FN_2O$	325.1711	-0.5	21.9	10.5
	Etodolac	Positive	9.4	288.1606	$C_{17}H_{22}NO_3$	288.1594	-4	111.4	7.5
		Negative	8.7	286.1446	$C_{17}H_{20}NO_3$	286.1449	1.1	36.8	8.5
	Fexofenadine	Positive	7.8	502.2938	$C_{32}H_{40}NO_4$	502.2952	2.8	24.2	13.5
	Furosemide	Positive	6.3	331.0156	$C_{12}H_{12}ClN_2O_5S$	331.0150	-1.9	49.4	7.5
Oct. 17		Negative	5.4	329.0002	$C_{12}H_{10}ClN_2O_5S$	329.0004	0.9	48.7	8.5
	Hydrochlorothiazide	Negative	2.2	295.9574	$C_7H_7ClN_3O_4S_2$	295.9572	-0.8	39	5.5
	Ibuprofen	Positive	9.8	207.1379	$C_{13}H_{19}O_2$	207.1380	0	10.3	4.5
		Negative	8.5	205.1232	$C_{13}H_{17}O_2$	205.1234	0.8	4.6	5.5
	Mesalazine	Positive	1.4	154.0501	$C_7H_8NO_3$	154.0499	-1.4	6.6	4.5
	Metformin	Positive	1.0	130.1087	$C_4H_{12}N_5$	130.1087	0.4	4.9	1.5
	Naproxen	Positive	8.6	231.1017	$C_{14}H_{15}O_3$	231.1016	-0.8	1.8	7.5
		Negative	6.7	229.0869	$C_{14}H_{13}O_3$	229.0870	0.6	7.9	8.5
	Nimesulide	Positive	8.3	309.0545	$C_{13}H_{13}N_2O_5S$	309.0540	-1.8	50.4	8.5
		Negative	7.9	307.0394	$C_{13}H_{11}N_2O_5S$	307.0394	0.1	9.2	9.5
	Omeprazole	Positive	7.5	346.1218	$C_{17}H_{20}N_3O_3S$	346.1220	0.6	11	9.5
	Ondansetron	Positive	5.5	294.1600	$C_{18}H_{20}N_3O$	294.1601	0.5	0.9	10.5
	Propranolol	Positive	6.8	260.1647	$C_{16}H_{22}NO_2$	260.1645	-0.8	18.1	6.5
	Pseudoephedrine	Positive	2.9	166.1227	$C_{10}H_{16}NO$	166.1226	-0.4	1.8	3.5
	Thiamine	Positive	1.0	265.1119	$C_{12}H_{17}N_4OS$	265.1118	-0.4	50	6.5
	Tramadol	Positive	5.0	278.2117	$C_{17}H_{28}NO_2$	278.2115	-0.8	3.2	4.5

	Venlafaxine	Positive	6.4	278.2115	$C_{17}H_{28}NO_2$	278.2115	-0.3	3.2	4.5
Nov. 17	Acetaminophen	Positive	2.2	152.0706	$C_8H_{10}NO_2$	152.0706	0.1	3.3	4.5
		Negative	2.2	150.0562	$C_8H_8NO_2$	150.0561	-0.8	2.3	5.5
	Atenolol	Positive	2.0	267.1700	$C_{14}H_{23}N_2O_3$	267.1703	1.1	5.4	4.5
	Caffeine	Positive	4.1	195.0880	$C_8H_{11}N_4O_2$	195.0877	-1.8	14.2	5.5
	Celecoxib	Negative	9.4	380.0689	$C_{17}H_{13}F_3N_3O_2S$	380.0686	-0.8	45.1	12
	Desvenlafaxine	Positive	4.9	264.1961	$C_{16}H_{26}NO_2$	264.1958	-1.2	13.2	4.5
	Diazepam	Positive	8.8	285.0793	$C_{16}H_{14}ClN_2O$	285.0789	-1.2	17.2	10.5
	Diclofenac	Positive	9.5	296.0241	$C_{14}H_{12}Cl_2NO_2$	296.0240	-0.5	17.6	8.5
		Negative	8.3	294.0088	$C_{14}H_{10}Cl_2NO_2$	294.0094	2.1	39.8	9.5
	Dimenhydrinate	Positive	4.7	215.0330	$C_7H_8ClN_4O_2$	215.0330	0.3	50	5.5
	Dipyrone	Positive	4.1	218.1289	$C_{12}H_{16}N_3O$	218.1288	-0.5	7.1	6.5
	Enalapril	Positive	7.0	377.2071	$C_{20}H_{29}N_2O_5$	377.2071	0.1	22.6	7.5
	Fexofenadine	Positive	7.8	502.2952	$C_{32}H_{40}NO_4$	502.2952	0	5.2	13.5
		Negative	7.6	500.2807	$C_{32}H_{38}NO_4$	500.2806	-0.1	16.8	15
	Furosemide	Positive	6.3	331.0148	$C_{12}H_{12}ClN_2O_5S$	331.0150	0.7	67.9	7.5
		Negative	5.4	329.0001	$C_{12}H_{10}ClN_2O_5S$	329.0004	1	50.9	8.5
	Ibuprofeno	Positive	10.0	207.1384	$C_{13}H_{19}O_2$	207.1380	-2.1	8	4.5
		Negative	8.5	205.1234	$C_{13}H_{17}O_2$	205.1234	0.2	6.5	5.5
	Mesalazine	Positive	1.4	154.0499	$C_7H_8NO_3$	154.0499	-0.3	6.3	4.5
	Metformin	Positive	1.1	130.1087	$C_4H_{12}N_5$	130.1087	0	10.9	1.5
	Metronidazole	Positive	2.5	172.0717	$C_6H_{10}N_3O_3$	172.0717	-0.1	10.9	3.5
	Naproxen	Positive	8.6	231.1017	$C_{14}H_{15}O_3$	231.1016	-0.4	3.4	7.5
	Nimesulide	Negative	7.8	307.0392	$C_{13}H_{11}N_2O_5S$	307.0394	0.7	5.3	9.5
	Pseudoephedrine	Positive	3.0	166.1228	$C_{10}H_{16}NO$	166.1226	-1.2	5.5	3.5
	Tramadol	Positive	5.0	264.1962	$C_{16}H_{26}NO_2$	264.1958	-1.5	13.2	4.5
Dec. 17	Acetaminophen	Positive	2.3	152.0708	$C_8H_{10}NO_2$	152.0706	-1.2	4	4.5
		Negative	2.2	150.0561	$C_8H_8NO_2$	150.0561	-0.1	1.1	5.5
	Atenolol	Positive	2.0	267.1702	$C_{14}H_{23}N_2O_3$	267.1703	0.3	9.7	4.5
	Caffeine	Positive	4.1	195.0878	$C_8H_{11}N_4O_2$	195.0877	-0.9	6.9	5.5
	Codeine	Positive	2.7	300.1596	$C_{18}H_{22}NO_3$	300.1594	-0.8	5.2	8.5
	Diazepam	Positive	8.9	285.0791	$C_{16}H_{14}ClN_2O$	285.0789	-0.5	17.2	10.5
	Diclofenac	Positive	9.5	296.0242	$C_{14}H_{12}Cl_2NO_2$	296.0240	-1	50	8.5
		Negative	8.3	294.0090	$C_{14}H_{10}Cl_2NO_2$	294.0094	1.4	49.8	9.5
	Dimenhydrinate	Positive	4.7	215.0333	$C_7H_8ClN_4O_2$	215.0330	-1.0	28.4	5.5
	Dipyrone	Positive	4.2	218.1291	$C_{12}H_{16}N_3O$	218.1288	-1.3	5.7	6.5
	Enalapril	Positive	7.0	377.2079	$C_{20}H_{29}N_2O_5$	377.2071	-2	3.4	7.5
	Fexofenadine	Positive	7.8	502.2956	$C_{32}H_{40}NO_4$	502.2952	-0.8	15	13.5
	Furosemide	Positive	6.3	331.0153	$C_{12}H_{12}ClN_2O_5S$	331.0150	-1	29.2	7.5
		Negative	5.5	329.0000	$C_{12}H_{10}ClN_2O_5S$	329.0004	1.3	10	8.5
	Hydrochlorothiazide	Negative	2.1	295.9572	$C_7H_7ClN_3O_4S_2$	295.9572	0.1	9.1	5.5
	Losartan	Positive	8.2	423.1696	$C_{22}H_{24}ClN_6O$	423.1695	-0.3	19.7	13.5
	Metformin	Positive	1.1	130.1088	$C_4H_{12}N_5$	130.1087	-0.8	17.2	1.5
	Nimesulide	Negative	7.9	307.0392	$C_{13}H_{11}N_2O_5S$	307.0394	0.7	11.3	9.5

	Pyridoxine	Positive	1.2	170.0813	$C_8H_{12}NO_3$	170.0812	-0.6	4.1	3.5
	Rosuvastatin	Positive	8.1	482.1765	$C_{22}H_{29}FN_3O_6S$	482.1756	-1.9	14.3	9.5
	Sotalol	Positive	1.7	273.1269	$C_{12}H_{21}N_2O_3S$	273.1267	-0.6	48.9	3.5
	Tramadol	Positive	5.0	264.1960	$C_{16}H_{26}NO_2$	264.1958	-0.6	11.8	4.5
Jan. 18	Acetaminophen	Positive	2.3	152.0704	$C_8H_{10}NO_2$	152.0706	1.1	2.4	4.5
		Negative	2.3	150.0563	$C_8H_8NO_2$	150.0561	-1.5	5.1	5.5
	Atenolol	Positive	2.0	267.1701	$C_{14}H_{23}N_2O_3$	267.1703	0.6	1.8	4.5
	Caffeine	Positive	4.1	195.0875	$C_8H_{11}N_4O_2$	195.0877	0.9	7.6	5.5
	Codeine	Positive	2.7	300.1593	$C_{18}H_{22}NO_3$	300.1594	0.6	6.9	8.5
	Desvenlafaxine	Positive	4.9	264.1959	$C_{16}H_{26}NO_2$	264.1958	-0.2	6.3	4.5
	Diclofenac	Positive	9.5	296.0239	$C_{14}H_{12}Cl_2NO_2$	296.0240	0.3	19.2	8.5
		Negative	8.3	294.0083	$C_{14}H_{10}Cl_2NO_2$	294.0094	3.8	50	9.5
	Dipyrone	Positive	4.1	218.1293	$C_{12}H_{16}N_3O$	218.1288	-2.5	49.7	6.5
	Fexofenadine	Positive	7.8	502.2944	$C_{32}H_{40}NO_4$	502.2952	1.6	7.2	13.5
		Negative	7.7	500.2804	$C_{32}H_{38}NO_4$	500.2806	0.5	8.3	15
	Furosemide	Negative	5.4	329.0004	$C_{12}H_{10}ClN_2O_5S$	329.0004	0.1	26.3	8.5
	Hydrochlorothiazide	Negative	2.2	295.9571	$C_7H_7ClN_3O_4S_2$	295.9572	0.4	35.8	5.5
	Mesalazine	Positive	1.4	154.0500	$C_7H_8NO_3$	154.0499	-1.1	6.4	4.5
	Metformin	Positive	1.1	130.1088	$C_4H_{12}N_5$	130.1087	-0.6	43.6	1.5
	Nimesulide	Negative	7.8	307.0390	$C_{13}H_{11}N_2O_5S$	307.0394	1.5	9.7	9.5
	Ondansetron	Positive	5.5	294.1599	$C_{18}H_{20}N_3O$	294.1601	0.5	18.7	10.5
	Rosuvastatin	Negative	7.5	480.1625	$C_{22}H_{27}FN_3O_6S$	480.1610	-3.1	33.7	11
	Tramadol	Positive	5.2	264.1956	$C_{16}H_{26}NO_2$	264.1958	0.8	12.9	4.5

Where: * mSigma: indicates the error in relation to the isotopic profile

** RDB: ring double bonds

Notes and References

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