

Supporting Information File

QUALITATIVE MULTI-RESIDUE SCREENING METHOD FOR 143 VETERINARY DRUGS AND PHARMACEUTICALS IN MILK AND FISH TISSUE USING LIQUID CHROMATOGRAPHY QUADRUPOLE-TIME-OF- FLIGHT MASS SPECTROMETRY

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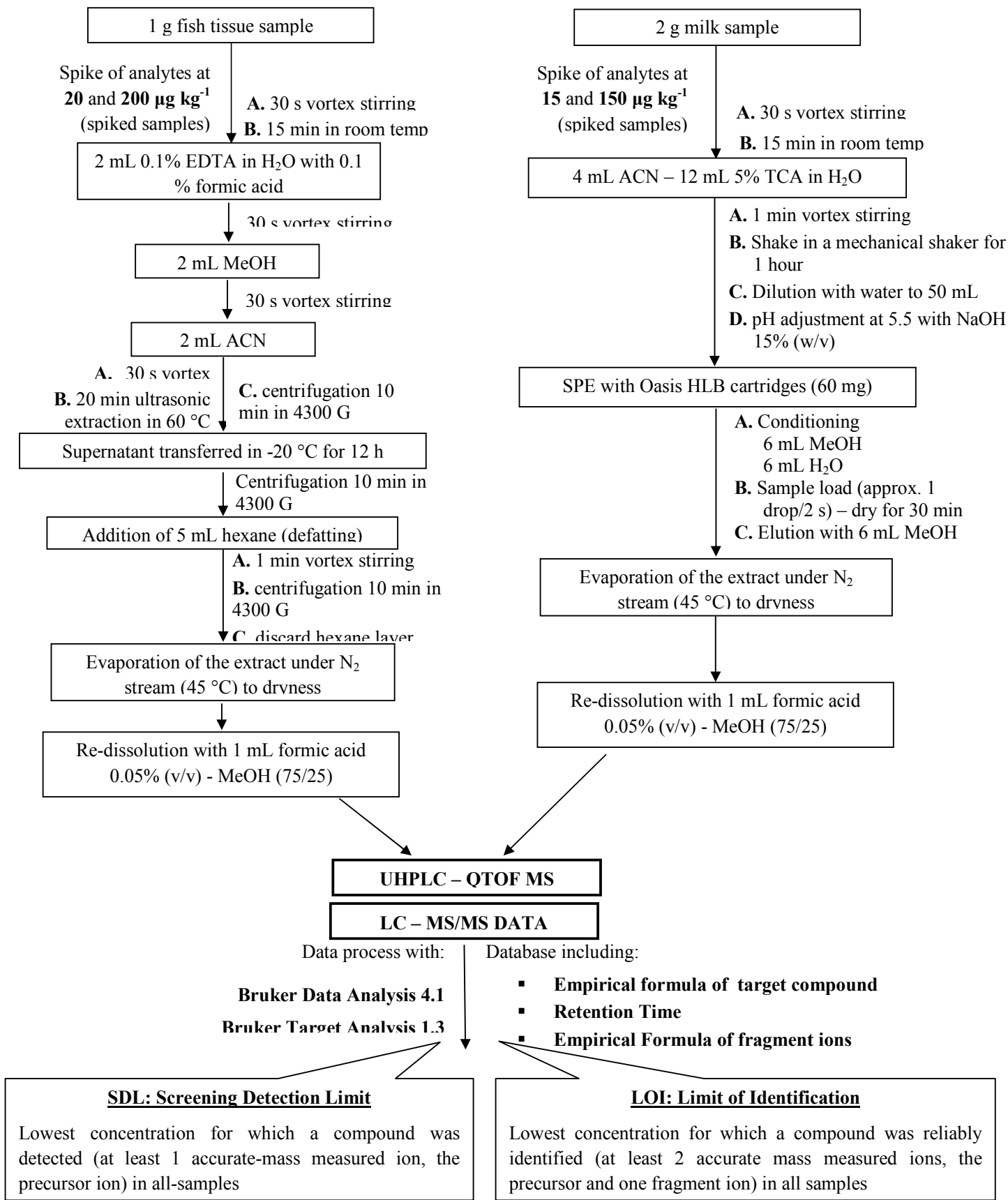


Figure S1: Overall scheme of the screening methodology.

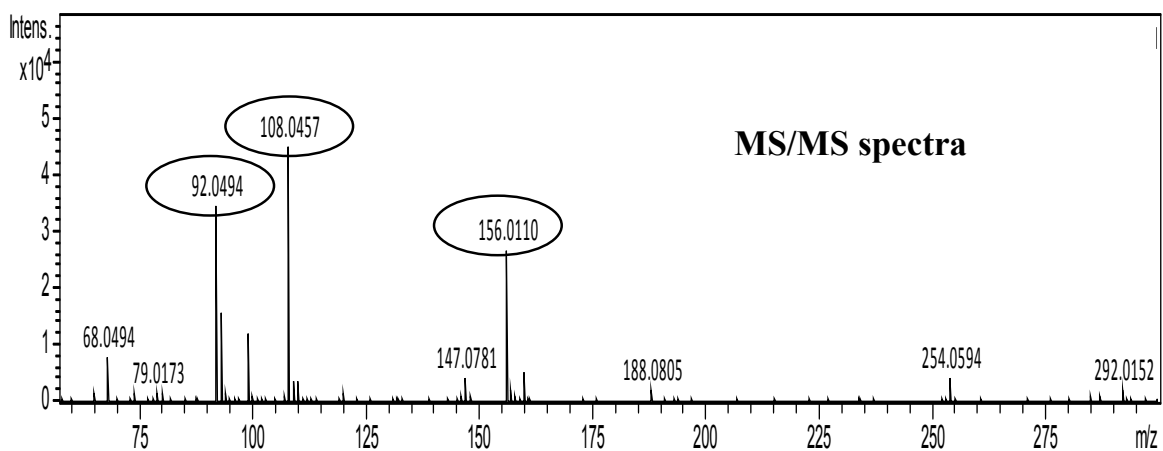
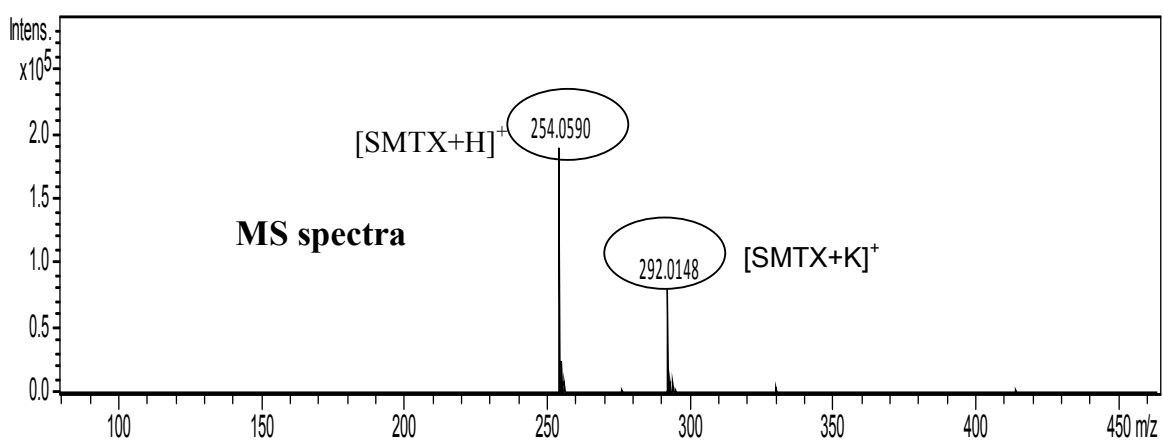
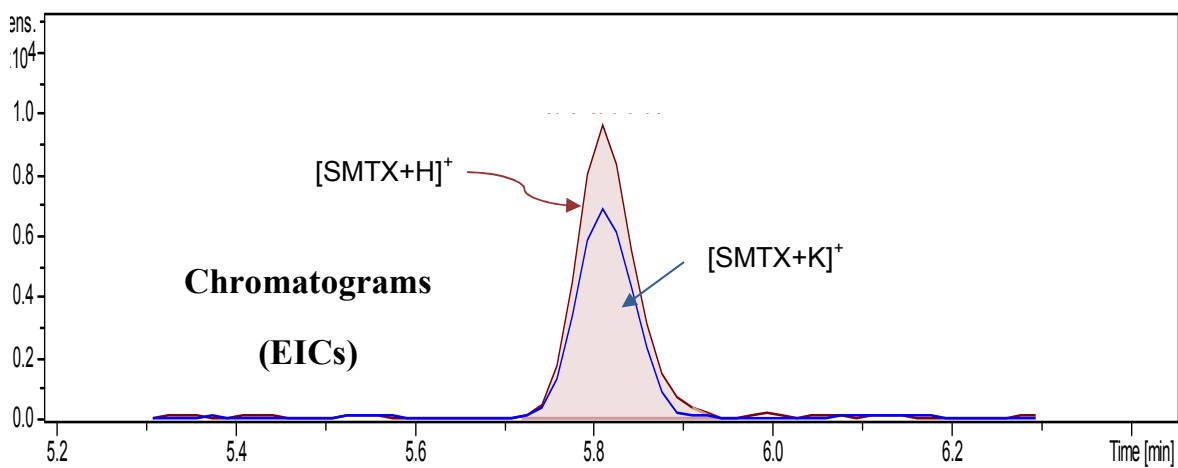


Figure S2: Chromatograms and MS and MS/MS spectra of sulfamethoxazole in a solvent standard solution at a concentration of $0.5 \mu\text{g mL}^{-1}$

Table S1. Retention time, elemental formulas and theoretical exact mass for precursor and fragment ions of veterinary drugs and pharmaceuticals.

Compounds	Elemental composition	Mr	Precursor ion	m/z (precur)	RT (min)	Fragment ion 1	m/z (fragm 1)	Fragment ion 2	m/z (fragm 2)	Fragment ion 3	m/z (fragm 3)
Quinolones											
Ciprofloxacin	C ₁₇ H ₁₈ FN ₃ O ₃	331.1332	[M+H] ⁺	332.1405	8.8	C ₁₇ H ₁₇ FN ₃ O ₂ ⁺	314.1299	C ₁₆ H ₁₉ FN ₃ O ⁺	288.1507		
Danofloxacin	C ₁₉ H ₂₀ FN ₃ O ₃	357.1489	[M+H] ⁺	358.1561	8.8	C ₁₉ H ₁₉ FN ₃ O ₂ ⁺	340.1456				
Difloxacin	C ₂₁ H ₁₉ F ₂ N ₃ O ₃	399.1394	[M+H] ⁺	400.1467	9.0	C ₂₁ H ₁₈ F ₂ N ₃ O ₂ ⁺	382.1362	C ₂₀ H ₂₀ F ₂ N ₃ O ⁺	356.1569	C ₁₇ H ₁₃ F ₂ N ₂ O ⁺	299.099
Enrofloxacin	C ₁₉ H ₂₂ FN ₃ O ₃	359.1645	[M+H] ⁺	360.1718	8.8	C ₁₈ H ₂₃ FN ₃ O ⁺	316.182	C ₁₉ H ₂₁ FN ₃ O ₂ ⁺	342.1612	C ₁₇ H ₁₉ FN ₃ O ₃ ⁺	332.1405
Flumequine	C ₁₄ H ₁₂ FNO ₃	261.0801	[M+H] ⁺	262.0874	10.6	C ₁₄ H ₁₁ FNO ₂ ⁺	244.0768				
Marbofloxacin	C ₁₇ H ₁₉ FN ₄ O ₄	362.1390	[M+H] ⁺	363.1463	8.2	C ₁₅ H ₁₅ FN ₃ O ₄ ⁺	320.1041	C ₁₇ H ₁₈ FN ₄ O ₃ ⁺	345.1353	C ₄ H ₁₀ N ⁺	72.0786
Norfloxacin	C ₁₆ H ₁₈ FN ₃ O ₃	319.1332	[M+H] ⁺	320.1405	8.7	C ₁₆ H ₁₇ FN ₃ O ₂ ⁺	302.1299	C ₁₅ H ₁₉ FN ₃ O ⁺	276.1507	C ₁₃ H ₁₄ FN ₂ O ⁺	233.1085
Ofloxacin	C ₁₈ H ₂₀ FN ₃ O ₄	361.1438	[M+H] ⁺	362.1511	8.5	C ₁₇ H ₂₁ FN ₃ O ₂ ⁺	318.1612	C ₁₄ H ₁₄ FN ₂ O ₂ ⁺	261.1034		
Oxolinic acid	C ₁₃ H ₁₁ NO ₅	261.0637	[M+H] ⁺	262.0710	10.1	C ₁₃ H ₁₀ NO ₄ ⁺	244.0604				
Sarafloxacin	C ₂₀ H ₁₇ F ₂ N ₃ O ₃	385.1238	[M+H] ⁺	386.1311	9.0	C ₂₀ H ₁₆ F ₂ N ₃ O ₂ ⁺	368.1205	C ₁₉ H ₁₈ F ₂ N ₃ O ⁺	342.1412		
Tetracyclines											
Chlortetracycline	C ₂₂ H ₂₃ ClN ₂ O ₈	478.1143	[M+H] ⁺	479.1216	9.8	C ₂₂ H ₁₉ ClNO ₇ ⁺	444.0845	C ₂₂ H ₂₁ ClNO ₈ ⁺	462.095		
Doxycycline	C ₂₂ H ₂₄ N ₂ O ₈	444.1533	[M+H] ⁺	445.1605	10.3	C ₂₂ H ₂₂ NO ₈ ⁺	428.1350	C ₁₆ H ₂₂ NO ₂ ⁺	260.1648		
Minocycline	C ₂₃ H ₂₇ N ₃ O ₇	457.1849	[M+H] ⁺	458.1922	9.4	C ₂₃ H ₂₅ N ₂ O ₇ ⁺	441.1662	C ₂₃ H ₂₃ N ₂ O ₆ ⁺	423.1551		
Oxytetracycline	C ₂₂ H ₂₄ N ₂ O ₉	460.1482	[M+H] ⁺	461.1555	9.0	C ₂₂ H ₂₀ NO ₈ ⁺	426.1183	C ₂₂ H ₂₂ NO ₉ ⁺	444.1289		
Tetracycline	C ₂₂ H ₂₄ N ₂ O ₈	444.1533	[M+H] ⁺	445.1605	9.0	C ₂₂ H ₂₀ NO ₇ ⁺	410.1234	C ₂₂ H ₂₀ NO ₈ ⁺	426.1183	C ₇ H ₈ NO ₃ ⁺	154.0499
Cefalosporines											
Cefaclor	C ₁₅ H ₁₄ C ₁₁ N ₃ O ₄ S	367.0394	[M+H] ⁺	368.0466	8.6	C ₇ H ₈ N ⁺	106.0651	C ₁₀ H ₈ NO ₂ ⁺	174.0550		
Cefadroxil	C ₁₆ H ₁₇ N ₃ O ₅ S	363.0889	[M+H] ⁺	364.0962	7.0	C ₄ H ₄ NOS ⁺	114.0008	C ₁₀ H ₁₁ O ₃ N ₂ ⁺	208.0842	C ₁₀ H ₈ NO ₃ ⁺	190.0499
Cefalexin	C ₁₆ H ₁₇ N ₃ O ₄ S	347.0940	[M+H] ⁺	348.1013	8.7	C ₇ H ₈ N ⁺	106.0651	C ₆ H ₈ NO ₂ S ⁺	158.027	C ₄ H ₄ NOS ⁺	114.0008
Cefapirin	C ₁₇ H ₁₇ N ₃ O ₆ S ₂	423.0553	[M+H] ⁺	424.0632	10.5	C ₁₃ H ₁₄ N ₃ OS ₂ ⁺	292.0573	C ₇ H ₆ NOS ⁺	152.0165		
Cefazolin	C ₁₄ H ₁₄ N ₈ O ₄ S ₃	454.0300	[M+H] ⁺	455.0373	11.3	C ₁₁ H ₁₁ N ₆ O ₄ S ⁺	353.0557				
Ceftiofur	C ₁₉ H ₁₇ N ₅ O ₇ S ₃	523.0290	[M+H] ⁺	524.0363	10.4	C ₁₆ H ₅ N ₂ O ⁺	241.0396				
Penicillins											

Amoxicillin	C ₁₆ H ₁₉ N ₃ O ₅ S	365.1045	[M+H] ⁺	366.1118	5.2	C ₉ H ₁₀ N ₃ ⁺	160.0869	C ₄ H ₄ NOS ⁺	114.0008	C ₁₆ H ₁₇ N ₂ O ₅ S ⁺	349.085
Ampicillin	C ₁₆ H ₁₉ N ₃ O ₄ S	349.1096	[M+H] ⁺	350.1169	7.2	C ₇ H ₈ N ⁺	106.0651	C ₆ H ₁₀ NO ₂ S ⁺	160.0427	C ₁₀ H ₈ NO ₂ ⁺	174.055
Cloxacillin	C ₁₉ H ₁₈ ClN ₃ O ₅ S	435.0656	[(MH ₂ -CO)+H] ⁺	410.0936	10.7	C ₇ H ₁₂ NO ₂ S ⁺	174.0583	C ₆ H ₁₀ NS ⁺	128.0528		
Dicloxacillin	C ₁₉ H ₁₇ C ₁₂ N ₃ O ₅ S	469.0266	[(MH ₂ -CO)+H] ⁺	444.0546	10.8	C ₆ H ₁₀ NO ₂ S ⁺	160.0427	C ₁₃ H ₉ C ₁₂ N ₂ O ₃ ⁺	310.9985		
Oxacillin	C ₁₉ H ₁₉ N ₃ O ₅ S	401.1045	[(MH ₂ -CO)+H] ⁺	376.1326	10.6	C ₆ H ₁₀ NO ₂ S ⁺	160.0427				
Penicillin G	C ₁₆ H ₁₈ N ₂ O ₄ S	334.0987	[(MH ₂ -CO)+H] ⁺	309.1267	10.3	C ₆ H ₁₀ NS ⁺	128.0522	C ₇ H ₁₂ NO ₂ S ⁺	174.0583	C ₇ H ₇ ⁺	91.0542
Penicillin V	C ₁₆ H ₁₈ N ₂ O ₅ S	350.0936	[(MH ₂ -CO)+H] ⁺	325.1217	10.5	C ₁₀ H ₁₃ N ₂ O ₂ ⁺	193.0972	C ₆ H ₁₀ NS ⁺	128.0528	C ₁₄ H ₁₉ N ₂ O ₂ S ⁺	279.1152
Macrolides											
Azithromycin	C ₃₈ H ₇₂ N ₂ O ₁₂	748.5085	[M+H] ⁺	749.5158	9.7	C ₈ H ₁₆ NO ₂ ⁺	158.1176	C ₆ H ₁₄ NO ⁺	116.107	C ₃₀ H ₅₉ N ₂ O ₉ ⁺	591.4215
Clarithromycin	C ₃₈ H ₆₉ NO ₁₃	747.4769	[M+H] ⁺	748.4842	10.8	C ₈ H ₁₆ NO ₂ ⁺	158.1176	C ₃₀ H ₅₆ NO ₁₀ ⁺	590.3899		
Erythromycin-H ₂ O	C ₃₇ H ₆₇ NO ₁₃	733.4612	[M-H ₂ O+H] ⁺	716.4579	10.6	C ₂₉ H ₅₂ NO ₉ ⁺	558.3637	C ₈ H ₁₆ NO ₂ ⁺	158.1174	C ₂₉ H ₅₀ NO ₈ ⁺	540.3538
Tiamulin	C ₂₈ H ₄₇ NO ₄ S	493.3226	[M+H] ⁺	494.3299	10.5	C ₈ H ₁₈ NO ₂ S ⁺	192.1053				
Tilmicosin	C ₄₆ H ₈₀ N ₂ O ₁₃	868.5660	[M+2H] ²⁺	435.2894	9.9	C ₃₈ H ₆₇ N ₂ O ₉ ⁺	695.4841	C ₈ H ₁₆ NO ₃ ⁺	174.1125	C ₅ H ₇ O ₂ ⁺	99.0441
Sulfonamides											
Dapsone	C ₁₂ H ₁₂ N ₂ O ₂ S	248.0619	[M+H] ⁺	249.0692	8.6	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfachloropyridazine	C ₁₀ H ₉ ClN ₄ O ₂ S	284.0135	[M+H] ⁺	285.0208	9.0	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfaclozine	C ₁₀ H ₉ ClN ₄ O ₂ S	284.0135	[M+H] ⁺	285.0208	9.8	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfadiazine	C ₁₀ H ₁₀ N ₄ O ₂ S	250.0524	[M+H] ⁺	251.0597	7.3	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfadimethoxine	C ₁₂ H ₁₄ N ₄ O ₄ S	310.0736	[M+H] ⁺	311.0809	9.9	C ₄ H ₄ N ₄ OS ⁺	156.0114	C ₆ H ₆ NO ⁺	108.0444		
Sulfadimidine	C ₁₂ H ₁₄ N ₄ O ₂ S	278.0837	[M+H] ⁺	279.091	8.8	C ₆ H ₁₀ N ₃ ⁺	124.0869	C ₆ H ₈ N ₃ O ₂ S ⁺	186.0332	C ₁₂ H ₄ N ₄ ⁺	204.043
Sulfadoxine	C ₁₂ H ₁₄ N ₄ O ₄ S	310.0736	[M+H] ⁺	311.0809	9.3	C ₄ H ₄ N ₄ OS ⁺	156.0114	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495
Sulfaguanidine	C ₇ H ₁₀ N ₄ O ₂ S	214.0524	[M+H] ⁺	215.0597	2.8	C ₆ H ₆ N ⁺	92.0495	C ₆ H ₆ NO ⁺	108.0444	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfamerazine	C ₁₁ H ₁₂ N ₄ O ₂ S	264.0681	[M+H] ⁺	265.0754	8.2	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfameter	C ₁₁ H ₁₂ N ₄ O ₃ S	280.0630	[M+H] ⁺	281.0703	8.6	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfamethizole	C ₉ H ₁₀ N ₄ O ₂ S ₂	270.0245	[M+H] ⁺	271.0318	8.7	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfamethoxazole	C ₁₀ H ₁₁ N ₃ O ₃ S	253.0521	[M+H] ⁺	254.0594	9.1	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfamethoxypridazine	C ₁₁ H ₁₂ N ₄ O ₃ S	280.0630	[M+H] ⁺	281.0703	8.9	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfamonomethoxine	C ₁₁ H ₁₂ N ₄ O ₃ S	280.0630	[M+H] ⁺	281.0703	9.2	C ₆ H ₆ NO ⁺	108.0444	C ₄ H ₄ N ₄ OS ⁺	156.0114	C ₆ H ₆ N ⁺	92.0495
Sulfamoxole	C ₁₁ H ₁₃ N ₃ O ₃ S	267.0678	[M+H] ⁺	268.075	9.3	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfapyridine	C ₁₁ H ₁₁ N ₃ O ₂ S	249.0572	[M+H] ⁺	250.0645	8.0	C ₆ H ₆ NO ⁺	108.0444	C ₄ H ₄ N ₄ OS ⁺	156.0114	C ₆ H ₆ N ⁺	92.0495

Sulfaquinoxaline	C ₁₄ H ₁₂ N ₄ O ₂ S	300.0681	[M+H] ⁺	301.0754	10.1	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Sulfathiazole	C ₉ H ₉ N ₃ O ₂ S ₂	255.0136	[M+H] ⁺	256.0209	7.8	C ₆ H ₆ NO ⁺	108.0444	C ₄ H ₄ N ₄ OS ⁺	156.0114	C ₆ H ₆ N ⁺	92.0495
Sulfisoxazole	C ₁₁ H ₁₃ N ₃ O ₃ S	267.0678	[M+H] ⁺	268.075	8.5	C ₆ H ₆ NO ⁺	108.0444	C ₆ H ₆ N ⁺	92.0495	C ₄ H ₄ N ₄ OS ⁺	156.0114
Quinoxalines											
Carbadox	C ₁₁ H ₁₀ N ₄ O ₄	262.0702	[M+H] ⁺	263.0775	9.2	C ₁₀ H ₇ N ₄ O ₃ ⁺	231.0513	C ₈ H ₅ N ₂ ⁺	129.0447		
Olaquinox	C ₁₂ H ₁₇ N ₃ O ₄	267.1219	[M+H] ⁺	268.1292	6.9	C ₁₂ H ₁₁ N ₃ O ₂ ⁺	229.0846	C ₁₀ H ₉ N ₂ O ₄ ⁺	221.0553	C ₉ H ₈ N ₂ O ⁺	160.0631
Amphenicols											
Florfenicol	C ₁₂ H ₁₄ C ₁₂ FNO ₄ S	357.0005	[M+NH ₄] ⁺	375.0343	9.3	C ₁₁ H ₉ Cl ₂ NO ⁺	241.0053				
Thiampenicol	C ₁₂ H ₁₅ C ₁₂ NO ₅ S	355.0048	[M+NH ₄] ⁺	373.0386	8.5	C ₁₁ H ₁₈ ClN ₂ O ₃ ⁺	261.1				
Diaminopyrimidines											
Baquiloprin	C ₁₇ H ₂₀ N ₆	308.1749	[M+H] ⁺	309.1822	6.2	C ₁₆ H ₁₈ N ₆ ⁺	294.1587	C ₁₁ H ₁₁ N ₂ ⁺	171.0917		
Trimethoprim	C ₁₄ H ₁₈ N ₄ O ₃	290.1379	[M+H] ⁺	291.1452	8.3	C ₅ H ₇ N ₄ ⁺	123.0665	C ₁₂ H ₁₄ N ₄ O ⁺	230.1176	C ₁₂ H ₁₂ N ₄ O ₃ ⁺	261.0957
Other antibiotics											
Lincomycin	C ₁₈ H ₃₄ N ₂ O ₆ S	406.2138	[M+H] ⁺	407.221	8.3	C ₈ H ₁₆ N ⁺	126.1277	C ₁₇ H ₃₁ N ₂ O ₆ ⁺	359.2177		
Novobiocin	C ₃₁ H ₃₆ N ₂ O ₁₁	612.2319	[M+H] ⁺	613.2392	11.7	C ₁₂ H ₁₃ O ₂ ⁺	189.091	C ₂₂ H ₂₂ NO ₆ ⁺	396.1442	C ₉ H ₁₆ NO ₅ ⁺	218.1023
Rifaximin	C ₄₃ H ₅₁ N ₃ O ₁₁	785.3524	[M+H] ⁺	786.3596	11.1	C ₄₂ H ₄₈ N ₃ O ₁₀ ⁺	754.3334				
Anthelmintics											
Albendazole	C ₁₂ H ₁₅ N ₃ O ₂ S	265.0885	[M+H] ⁺	266.0958	11.0	C ₁₁ H ₁₂ N ₃ OS ⁺	234.0696	C ₈ H ₅ N ₃ OS ⁺	191.0148	C ₈ H ₅ N ₃ O ⁺	159.0427
Albendazole oxide	C ₁₂ H ₁₅ N ₃ O ₃ S	281.0834	[M+H] ⁺	282.0907	9.9	C ₈ H ₆ N ₃ O ₂ S ⁺	208.0175	C ₉ H ₁₀ N ₃ O ₃ S ⁺	240.0437	C ₉ H ₉ N ₃ O ₂ ⁺	191.0689
Albendazole sulfone	C ₁₂ H ₁₅ N ₃ O ₄ S	297.0783	[M+H] ⁺	298.0856	11.5	C ₁₁ H ₁₂ N ₃ O ₃ S ⁺	266.0594	C ₈ H ₆ N ₃ O ₃ S ⁺	224.0124		
Dimetridazole	C ₅ H ₇ N ₃ O ₂	141.0538	[M+H] ⁺	142.0611	7.9	C ₅ H ₇ N ₂ ⁺	95.0604	C ₄ H ₅ N ₂ ⁺	81.0447		
Febantel	C ₂₀ H ₂₂ N ₄ O ₆ S	446.1260	[M+H] ⁺	447.1333	11.3	No fragments					
Fenbendazole	C ₁₅ H ₁₃ N ₃ O ₂ S	299.0728	[M+H] ⁺	300.0801	11.3	C ₁₄ H ₁₀ N ₃ OS ⁺	268.0539	C ₁₀ H ₇ O ₂ ⁺	159.0441		
Flubendazole	C ₁₆ H ₁₂ FN ₃ O ₃	313.0863	[M+H] ⁺	314.0935	10.8	C ₁₅ H ₉ FN ₃ O ₂ ⁺	282.0673	C ₇ H ₄ FO ⁺	123.0241		
Levamisole	C ₁₁ H ₁₂ N ₂ S	204.0721	[M+H] ⁺	205.0794	7.7	C ₁₀ H ₁₂ NS ⁺	178.0685	C ₁₀ H ₁₂ N ⁺	146.0964	C ₇ H ₇ S ⁺	123.0263
Mebendazole	C ₁₆ H ₁₃ N ₃ O ₃	295.0957	[M+H] ⁺	296.103	10.7	C ₁₅ H ₁₀ N ₃ O ₂ ⁺	264.0768				
Metronidazole	C ₆ H ₉ N ₃ O ₃	171.0644	[M+H] ⁺	172.0717	7.2	C ₄ H ₆ N ₃ O ₂ ⁺	128.0455	C ₄ N ₂ H ₅ ⁺	82.0525	C ₁₁ H ₁₁ O ⁺	
Morantel	C ₁₂ H ₁₆ N ₂ S	220.1034	[M+H] ⁺	221.1107	9.0	C ₆ H ₇ S ⁺	111.0263	C ₇ H ₇ S ⁺	123.0263		
Oxfendazole	C ₁₅ H ₁₃ N ₃ O ₃ S	315.0678	[M+H] ⁺	316.075	10.4	C ₁₁ H ₁₁ O ₃ ⁺	191.0703	C ₁₄ H ₁₀ N ₃ O ₂ S ⁺	284.0488		

Piperazine	C ₄ H ₁₀ N ₂	86.0844	[M+H] ⁺	87.0917	1.3	C ₄ H ₇ N ⁺	70.0651				
Ronidazole	C ₆ H ₈ N ₄ O ₄	200.0546	[M+H] ⁺	201.0618	7.2	C ₂ H ₄ N ₂ ⁺	56.0369				
Ternidazole	C ₇ H ₁₁ N ₃ O ₃	185.0800	[M+H] ⁺	186.0873	8.3	C ₄ H ₆ N ₃ O ₂ ⁺	128.0455	C ₄ H ₆ N ₂ ⁺	82.0525	C ₆ HN ₂ ⁺	101.0134
Thiabendazole	C ₁₀ H ₇ N ₃ S	201.0361	[M+H] ⁺	202.0433	9.1	C ₉ H ₇ N ₂ S ⁺	175.0324	C ₈ H ₇ N ₂ ⁺	131.0604		
Triclabendazole	C ₁₄ H ₉ Cl ₃ N ₂ OS	357.9501	[M+H] ⁺	358.9574	11.8	C ₁₃ H ₇ Cl ₃ N ₂ OS ⁺	343.9334	C ₁₃ H ₇ Cl ₃ N ₂ OS ⁺	345.931	C ₁₂ H ₁₁ Cl ₃ N ⁺	273.9952
Coccidiostats											
Arprinocid	C ₁₂ H ₉ ClFN ₅	277.0531	[M+H] ⁺	278.0603	10.3	C ₇ H ₅ ClF ⁺	143.0058				
Clopidol	C ₇ H ₇ Cl ₂ NO	190.9905	[M+H] ⁺	191.9977	8.3	C ₅ H ₆ Cl ⁺	101.0153	C ₄ H ₄ Cl ⁺	86.9996		
Decoquinatate	C ₂₄ H ₃₅ NO ₅	417.2515	[M+H] ⁺	418.2588	12.4	C ₂₂ H ₃₂ NO ₅ ⁺	390.2275	C ₂₂ H ₃₀ NO ₄ ⁺	372.2169		
Diaveridine	C ₁₃ H ₁₆ N ₄ O ₂	260.1273	[M+H] ⁺	261.1346	8.2	C ₁₂ H ₁₃ N ₄ O ₂ ⁺	245.1033	C ₅ H ₇ N ₄ ⁺	123.0665	C ₁₁ H ₁₃ N ₄ O ⁺	217.1084
Ethopabate	C ₁₂ H ₁₅ NO ₄	237.1001	[M+H] ⁺	238.1074	10.4	C ₇ H ₆ NO ₂ ⁺	136.0393	C ₉ H ₁₀ NO ₂ ⁺	164.0706	C ₁₁ H ₁₂ NO ₃ ⁺	206.0812
Halofuginone	C ₁₆ H ₁₇ BrClN ₃ O ₃	413.0142	[M+H] ⁺	414.0215	10.3	C ₅ H ₁₀ NO ⁺	100.0757	C ₈ H ₁₀ N ⁺	120.0808	C ₆ H ₁₄ NO ⁺	116.107
Imidocarb	C ₁₉ H ₂₀ N ₆ O	348.1699	[M+H] ⁺	349.1771	7.7	C ₁₀ H ₁₀ N ₃ O ⁺	188.0818	C ₉ H ₁₂ N ₃ ⁺	162.1026		
Lasalocid	C ₃₄ H ₅₄ O ₈	590.3819	[M+H] ⁺	591.3891	10.3	C ₂₃ H ₃₇ O ₄ ⁺	377.2686				
Monensin	C ₃₆ H ₆₂ O ₁₁	670.4291	[M+NH ₄] ⁺	688.4630	12.6	C ₂₅ H ₄₁ O ₅ ⁺	421.2949	C ₃₁ H ₄₃ NO ₂ ⁺	461.3288		
Narasin	C ₄₃ H ₇₂ O ₁₁	764.5074	[M+NH ₄] ⁺	782.5413	12.4	C ₂₃ H ₃₆ O ₆ NH ₄ ⁺	426.2850	[M+Na] ⁺	787.4967		
Nigericin	C ₄₀ H ₆₈ O ₁₁	724.4761	[M+NH ₄] ⁺	742.5100	12.9	[M+Na] ⁺	747.4654				
Robenidine	C ₁₅ H ₁₃ Cl ₂ N ₅	333.0548	[M+H] ⁺	334.0621	11.0	C ₇ H ₅ ClN ⁺	138.0105	C ₇ H ₈ ClN ₂ ⁺	155.0371	C ₈ H ₅ ClN ₃ ⁺	178.0167
Salinomycin	C ₄₂ H ₇₀ O ₁₁	750.4918	[M+NH ₄] ⁺	768.5256	12.3	C ₂₃ H ₃₆ O ₆ NH ₄ ⁺	426.2850				
NSAIDs											
5-Hydroxy-flunixin	C ₁₄ H ₁₁ F ₃ N ₂ O ₃	312.0722	[M+H] ⁺	313.0795	11.3	C ₁₄ H ₁₀ F ₃ N ₂ O ₂ ⁺	295.0689	C ₅ H ₈ F ₃ ⁺	125.0573		
Aceclofenac	C ₁₆ H ₁₃ Cl ₂ NO ₄	353.0222	[M+H] ⁺	354.0294	11.7	C ₇ H ₁₅ Cl ₂ NO ₂ ⁺	215.0474	C ₁₃ H ₁₀ Cl ₂ N ⁺	250.0185		
Diclofenac	C ₁₄ H ₁₁ Cl ₂ NO ₂	295.0167	[M+H] ⁺	296.024	11.5	C ₁₃ H ₁₀ ClN ⁺	215.0496	C ₁₃ H ₁₀ Cl ₂ N ⁺	250.0185		
Flunixin	C ₁₄ H ₁₁ F ₃ N ₂ O ₂	296.0773	[M+H] ⁺	297.0845	11.5	C ₁₄ H ₁₀ F ₃ N ₂ O ⁺	279.0748	C ₁₃ H ₈ F ₃ N ₂ O ⁺	265.0579		
Ketoprofen	C ₁₆ H ₁₄ O ₃	254.0943	[M+H] ⁺	255.1016	11.0	C ₇ H ₅ O ⁺	105.0335	C ₁₅ H ₁₃ O ⁺	209.0961	C ₁₀ H ₉ O ₃ ⁺	177.0546
Mefenamic acid	C ₁₅ H ₁₅ NO ₂	241.1103	[M+H] ⁺	242.1176	11.9	C ₁₅ H ₁₄ NO ⁺	224.107	C ₁₄ H ₁₁ NO ⁺	209.0827	C ₇ H ₁₃ O ₂ ⁺	129.091
Meloxicam	C ₁₄ H ₁₃ N ₃ O ₄ S ₂	351.0347	[M+H] ⁺	352.042	11.0	C ₄ H ₇ N ₂ S ⁺	115.0324	C ₅ H ₅ N ₂ OS ⁺	141.0117		
Naproxen	C ₁₄ H ₁₄ O ₃	230.0943	[M+H] ⁺	231.1016	11.1	C ₁₃ H ₁₃ O ⁺	185.0961	C ₁₀ H ₈ N ₃ ⁺	170.0713	C ₁₂ H ₉ ⁺	153.0699
Niflumic acid	C ₁₃ H ₉ F ₃ N ₂ O ₂	282.0616	[M+H] ⁺	283.0689	11.6	C ₁₃ H ₈ F ₃ N ₂ O ⁺	265.0583	C ₁₃ H ₇ F ₂ N ₂ O ⁺	245.0521		
Phenylbuntazone	C ₁₉ H ₂₀ N ₂ O ₂	308.1525	[M+H] ⁺	309.1598	11.3	C ₇ H ₆ NO ⁺	120.0444	C ₁₁ H ₁₄ N ⁺	160.1121	C ₁₃ H ₁₁ N ₂ O ⁺	211.0866

Tolfenamic acid	C ₁₄ H ₁₂ ClNO ₂	261.0556	[M+NH ₄] ⁺	279.0895	8.8	No fragments					
Vedaprofen	C ₁₉ H ₂₆ NO ₂	282.1620	[M+NH ₄] ⁺	300.1958	12.1	C ₁₂ H ₁₁ ⁺	155.0855	C ₁₈ H ₂₁ ⁺	237.1638		
beta-agonists											
Cimaterol	C ₁₂ H ₁₇ N ₃ O	219.1372	[M+H] ⁺	220.1444	6.8	C ₉ H ₁₀ N ₃ ⁺	160.0869	C ₉ H ₇ N ₂ ⁺	143.0604	C ₁₂ H ₁₆ N ₃ ⁺	202.1339
Clenbuterol	C ₁₂ H ₁₈ Cl ₂ N ₂ O	276.0796	[M+H] ⁺	277.0869	9.1	C ₈ H ₉ Cl ₂ N ₂ ⁺	203.0137	C ₁₂ H ₁₇ Cl ₂ N ₂ ⁺	259.0763	C ₁₁ H ₆ NO ⁺	168.0444
Clenpenterol	C ₁₃ H ₂₀ Cl ₂ N ₂ O	290.0953	[M+H] ⁺	291.1025	9.6	C ₈ H ₉ Cl ₂ N ₃ ⁺	203.0137				
Mabuterol	C ₁₃ H ₁₈ ClF ₃ N ₂ O	310.1060	[M+H] ⁺	311.1133	9.6	C ₉ H ₉ ClF ₃ N ₂ ⁺	237.0401	C ₉ H ₈ ClF ₂ N ₂ ⁺	217.0339		
Ractopamine	C ₁₈ H ₂₃ NO ₃	301.1678	[M+H] ⁺	302.1751	8.8	C ₈ H ₉ O ⁺	121.0648	C ₇ H ₇ O ⁺	107.0491	C ₁₀ H ₁₄ NO ⁺	164.1070
Salbutamol	C ₁₃ H ₂₁ NO ₃	239.1521	[M+H] ⁺	240.1594	7.2	C ₉ H ₁₀ NO ⁺	148.0757	C ₈ H ₉ O ⁺	121.0648		
Terbutaline	C ₁₂ H ₁₉ NO ₃	225.1365	[M+H] ⁺	226.1438	7.1	C ₈ H ₁₀ NO ₂ ⁺	152.0706	C ₇ H ₉ O ₂ ⁺	125.0597	C ₇ H ₇ O ⁺	107.0491
Steroids											
Betamethasone	C ₂₂ H ₂₉ FO ₅	392.1999	[M+H] ⁺	393.2072	10.8	C ₂₂ H ₂₇ O ₄ ⁺	355.1904	C ₂₂ H ₂₉ O ₅ ⁺	373.201	C ₂₂ H ₂₅ O ₃ ⁺	337.1798
Cortisol	C ₂₁ H ₃₀ O ₅	362.2093	[M+H] ⁺	363.2166	10.7	C ₈ H ₉ O ⁺	121.0648	C ₂₁ H ₂₇ O ₃ ⁺	327.1955	C ₂₁ H ₂₅ O ₂ ⁺	309.1849
Cortison	C ₂₁ H ₂₈ O ₅	360.1937	[M+H] ⁺	361.201	10.7	C ₁₁ H ₁₅ O ⁺	163.1117				
Dexamethazone	C ₂₂ H ₂₉ FO ₅	392.1999	[M+H] ⁺	393.2072	7.4	C ₂₂ H ₂₉ O ₅ ⁺	373.2009				
Methylprednisolone	C ₂₂ H ₃₀ O ₅	374.2093	[M+H] ⁺	375.2166	10.9	C ₂₂ H ₂₉ O ₄ ⁺	357.206	C ₂₂ H ₂₇ O ₃ ⁺	339.1955	C ₂₂ H ₂₅ O ₂ ⁺	321.1849
Progesteron	C ₂₁ H ₃₀ O ₂	314.2246	[M+H] ⁺	315.2319	11.5	C ₇ H ₉ O ⁺	109.0648	C ₆ H ₉ O ⁺	97.0648	C ₈ H ₁₁ O ⁺	123.0804
Thyreostats											
Methyl-thiouracil	C ₅ H ₆ N ₂ O ₂ S	158.0150	[M+H] ⁺	159.0223	3.9	C ₄ H ₆ NO ⁺	84.0444	C ₅ H ₄ NOS ⁺	126.0008		
Phenyl-thiouracil	C ₁₀ H ₈ N ₂ OS	204.0357	[M+H] ⁺	205.0430	9.8	C ₈ H ₇ ⁺	103.0542	C ₉ H ₈ NO ⁺	146.06	C ₁₀ H ₆ NOS ⁺	188.0165
Propyl-thiouracil	C ₇ H ₁₀ N ₂ OS	170.0514	[M+H] ⁺	171.0587	8.9	C ₆ H ₁₀ NO ⁺	112.0757	C ₇ H ₈ NOS ⁺	154.0321		
Pharmaceuticals											
Ambroxol	C ₁₃ H ₁₈ Br ₂ N ₂ O ₂	391.9735	[M+H] ⁺	392.9808	10.1	C ₆ H ₆ Br ₂ NO ⁺	263.8838	C ₆ H ₁₄ NO ⁺	116.1069		
Atenolol	C ₁₄ H ₂₂ N ₂ O ₃	266.1630	[M+H] ⁺	267.1703	7.1	C ₁₁ H ₁₂ NO ₂ ⁺	190.0863	C ₁₁ H ₁₇ N ₂ O ₃ ⁺	225.1234	C ₉ H ₁₀ NO ₂ ⁺	164.0706
Atorvastatin	C ₃₃ H ₃₅ FN ₂ O ₅	558.2530	[M+H] ⁺	559.2603	11.2	C ₂₆ H ₃₁ FNO ₄ ⁺	440.2232	C ₂₇ H ₂₉ FNO ₅ ⁺	466.2024		
Caffeine	C ₈ H ₁₀ N ₄ O ₂	194.0804	[M+H] ⁺	195.0877	8.7	C ₅ H ₇ N ₄ ⁺	123.0665	C ₆ H ₈ N ₃ O ⁺	138.0662	C ₅ H ₈ N ₃ ⁺	110.0713
Carbamazepine	C ₁₅ H ₁₂ N ₂ O	236.0950	[M+H] ⁺	237.1022	10.6	C ₁₄ H ₁₂ N ⁺	194.0964	C ₁₄ H ₁₁ N ⁺	193.0886		
Cimetidine	C ₁₀ H ₁₆ N ₆ S	252.1157	[M+H] ⁺	253.1230	7.4	C ₅ H ₇ N ₂ ⁺	95.0604	C ₅ H ₁₁ N ₄ S ⁺	159.0699	C ₄ H ₉ N ₂ S ⁺	117.0481
Gemfibrozil	C ₁₅ H ₂₂ O ₃	250.1569	[M+H] ⁺	251.1642	11.9	C ₇ H ₁₃ O ₂ ⁺	129.091				

Haloperidol	C ₂₁ H ₂₃ ClFNO ₂	375.1401	[M+H] ⁺	376.1474	10.4	C ₁₀ H ₁₀ FO ⁺	165.071	C ₂₁ H ₂₂ ClFNO ⁺	358.1368	C ₇ H ₄ FO ⁺	123.0241
Indapamide	C ₁₆ H ₁₆ ClN ₃ O ₃ S	365.0601	[M+H] ⁺	366.0674	10.4	C ₉ H ₁₀ N ⁺	132.0808				
Metformin	C ₄ H ₁₁ N ₅	129.1014	[M+H] ⁺	130.1087	3.1	C ₂ H ₅ N ₄ ⁺	85.0509	C ₃ H ₇ N ₂ ⁺	71.0604	CH ₆ N ₃ ⁺	60.0556
Metoprolol	C ₁₅ H ₂₅ NO ₃	267.1834	[M+H] ⁺	268.1907	9.3	C ₆ H ₁₂ N ⁺	98.0964	C ₆ H ₁₄ NO ⁺	116.107	C ₁₁ H ₁₁ O ⁺	159.0804
Paracetamol	C ₈ H ₉ NO ₂	151.0633	[M+H] ⁺	152.0706	7.0	C ₆ H ₈ NO ⁺	110.0600	C ₆ H ₅ O ⁺	93.0335		
Propranolol	C ₁₆ H ₂₁ NO ₂	259.1572	[M+H] ⁺	260.1645	10.3	C ₆ H ₁₄ NO ⁺	116.1070	C ₁₃ H ₁₁ O ⁺	183.0804	C ₁₂ H ₁₁ ⁺	155.0855
Ranitidine	C ₁₃ H ₂₂ N ₄ O ₃ S	314.1413	[M+H] ⁺	315.1485	7.1	C ₅ H ₁₀ N ₃ O ₂ S ⁺	176.0488	C ₁₁ H ₁₂ NO ₂ ⁺	190.0863		
Simvastatin	C ₂₅ H ₄₂ NO ₅	436.3063	[M+NH ₄] ⁺	436.3057	12.0	C ₁₅ H ₁₉ ⁺	199.1481	C ₁₉ H ₂₅ O ₂ ⁺	285.1850	C ₁₇ H ₂₁ ⁺	225.1638
Theophylline	C ₇ H ₈ N ₄ O ₂	180.0647	[M+H] ⁺	181.0720	8.1	C ₅ H ₆ N ₃ O ⁺	124.0505	C ₄ H ₆ N ₃ ⁺	96.0556	C ₃ H ₅ N ₂ ⁺	69.0447
Tramadol	C ₁₆ H ₂₅ NO ₂	263.1885	[M+H] ⁺	264.1958	9.2	C ₃ H ₈ N ⁺	58.0651				
Triamterene	C ₁₂ H ₁₁ N ₇	253.1076	[M+H] ⁺	254.1149	8.9	C ₁₂ H ₉ N ₆ ⁺	237.0883				
Valsartan	C ₂₄ H ₂₉ N ₅ O ₃	435.2270	[M+H] ⁺	436.2343	11.2	C ₁₄ H ₁₁ N ₄ ⁺	235.0978	C ₁₉ H ₁₉ N ₂ O ⁺	291.1492	C ₁₄ H ₁₁ N ₂ ⁺	207.0917
Others											
Bromhexine	C ₁₄ H ₂₀ Br ₂ N ₂	373.9993	[M+H] ⁺	375.0066	10.6	C ₇ H ₆ Br ₂ N ⁺	261.8861	C ₇ NH ₁₆ ⁺	114.1277		
Chlorpromazine	C ₁₇ H ₁₉ ClN ₂ S	318.0957	[M+H] ⁺	319.1030	10.8	C ₅ H ₁₂ N ⁺	86.0964	C ₁₃ H ₉ ClNS ⁺	246.0139		
Colchicine	C ₂₂ H ₂₅ NO ₆	399.1682	[M+H] ⁺	400.1755	10.3	C ₂₀ H ₂₄ NO ₅ ⁺	358.1649	C ₂₀ H ₂₁ O ₅ ⁺	341.1384	C ₂₂ H ₂₄ NO ₅ ⁺	382.1649
Coumaphos	C ₁₄ H ₁₆ ClO ₅ PS	362.0145	[M+H] ⁺	363.0217	11.5	C ₁₀ H ₉ ClO ₅ PS ⁺	306.9591	C ₁₂ H ₁₃ ClO ₅ PS ⁺	334.9904	C ₁₀ H ₇ ClO ₂ S ⁺	226.9923
Melamine	C ₃ H ₆ N ₆	126.0654	[M+H] ⁺	127.0727	2.9	C ₂ H ₅ N ₄ ⁺	85.0509	C ₂ H ₂ N ₃ ⁺	68.0219		