Supplementary Materials

Critical Evaluation of Two Qualitative Analytical Approaches for Multiclass Determination of Veterinary Drugs in Bovine Muscle Using UHPLC-Q-Orbitrap: The Wind of Change in Brazilian Monitoring

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Table S1. Concentration of the standard solution, maximum residue limit (MRL), minimum required performance level (MRPL) in bovine muscle.

Group/Class - Pharmacologically active Substance	Solvent used	Stock standard concentration (µg mL^{-1})	MRL in bovine muscle (µg Kg^{-1})	Reference
Antimicrobials/Aminoglycosides				
Amikacin	Water	512.6	500[a]	
Apramycin	Water	486.8	1000	[101]
Dihydrostreptomycin	Water	499.2	600	[101]
Spectinomycin	Water	511.3	500	[101]
Streptomycin	Water	504.1	500	[101]
Gentamicin	Water	510.8	100	[101]
Hygromycin B	Water	489.8	500[a]	
Kanamycin A	Water	505.4	100	[101]
Neomycin B	Water	494.2	500	[101]
Tobramycin	Water	200.0	500[a]	
Antimicrobials/Amphenicols				
Chloramphenicol	Methanol	100.2	0.30	[94]
Florfenicol	Methanol	100.0	200	[101]
Thiamphenicol	Methanol	100.3	50	[96]
Antimicrobials/Betalactams				
Amoxicillin	Water	195.3	50	[101]
Ampicillin	Water	194.7	50	[101]
Cephalexin	Water	297.8	200	[101]
Cefalonium	DMSO (sonicated)	194.8	10	[103]
Cephapirin	Acetonitrile/Water 75:25 (v/v)	199.8	50	[101]
Cefazolin	Water	200.7	50	[103]
Cefoperazone	Acetonitrile/Water 75:25 (v/v)	79.7	50[a]	
Cefquinome	12.5% DMSO/ methanol	167.1	50	[101]
Cloxacillin	Water	320.9	300	[101]
Dicloxacillin	Water	338.3	300	[101]
Nafcillin	Water	347.9	300	[101]
Oxacillin	Water	516.4	300	[96]
Benzylpenicillin	Water	196.9	50	[101]
Phenoxymethyl penicillin	Water	203.5	25[b,c]	[101]
Antimicrobials/Lincosamides				
Clindamycin	Methanol	474.2	50[a]	
Lincomycin	Methanol	491.0	100	[101]
Antimicrobials/Macrolides				
Azithromycin	Water	101.2	50	[94]

Group/Class - Pharmacologically active Substance	Solvent used	Stock standard concentration (µg mL^{-1})	MRL in bovine muscle (µg Kg^{-1})	Reference
Erythromycin A	Methanol	472.8	200	[101]
Spiramycin I	Methanol	497.7	200	[101]
Tilmicosin	Methanol	500.4	100	[101]
Tylosin A	Methanol	496.8	100	[101]
Antimicrobials/Quinolones-Fluoroquinolones				
Nalidixic acid	NaOH 1 mol L^{-1}/Methanol	1001.8	20	[94]
Oxolinic acid	NaOH 1 mol L^{-1}/Methanol	125.0	100	[101]
Ciprofloxacin	NaOH 1 mol L^{-1}/Methanol	300.9	100	[101]
Danofloxacin	Acetone/Methanol	995.0	200	[101]
Difloxacin	Acetone/Methanol	999.0	400	[101]
Enrofloxacin	Acetone/Methanol	1004.9	100	[101]
Flumequine	NaOH 1 mol L^{-1}/Methanol	204.0	500	[101]
Norfloxacin	Acetone/Methanol	1005.0	20	[94]
Sarafloxacin	Acetone/Methanol	220.1	10[d]	[101]
Antimicrobials/Sulphonamides				
Sulfachlorpyridazine	Methanol	1000.0	100	[101]
Sulfadiazine	Methanol	500.0	100	[101]
Sulfadimethoxine	Methanol	250.0	100	[101]
Sulfadoxine	Methanol	250.0	100	[101]
Sulfisoxazole/Sulfafurazole	Methanol	1000.0	100	[101]
Sulfamerazine	Methanol	1000.0	100	[101]
Sulfamethazine/Sulfadimidine	Methanol	250.0	100	[101]
Sulfathiazole	Methanol	1000.0	100	[101]
Sulfamethoxazole	Methanol	1000.0	100	[101]
Sulfaquinoxaline	Acetone/Methanol	1000.0	100	[101]
Antimicrobials/Tetracyclines				
Chlortetracycline	Methanol	511.7	200	[101]
Doxycycline	Methanol	463.0	100	[101]
Oxytetracycline	Methanol	498.7	200	[101]
Tetracycline	Methanol	515.8	200	[101]
Antimicrobials/Others				
Bromhexine	Methanol	490.3	10	
Dapsone	Methanol	393.6	10	
Rifampicin	Methanol	367.7	10	
Tiamulin	Methanol	171.3	100[c,d]	[101]
Antimicrobials Prospect/Quinolones-Fluoroquinolones				
Marbofloxacin	NaOH 1 mol L^{-1}/Methanol	100.0	150	[101]
Antimicrobials Prospect/Macrolides				

Group/Class - Pharmacologically active Substance	Solvent used	Stock standard concentration (µg mL^{-1})	MRL in bovine muscle (µg Kg^{-1})	Reference
Josamycin/Leucomycin A_3	Methanol	202.3	100[a]	
Leucomycin/Leucomycin A_5	Methanol	100.3	100[a]	
Tildipirosin	Methanol	446.3	400	[101]
Tulathromycin A	Methanol	270.6	300	[101]
Antimicrobials Prospect/ Sulfonamides				
Phthalylsulfathiazole	Methanol	251.0	100	[101]
Sulfacetamide/*N*-Sulfanilylacetamide	Methanol	250.2	100	[101]
Sulfamethoxypyridazine	Methanol	250.0	100	[101]
Antimicrobials Prospect/Others				
Diminazene	Methanol	218.5	500	[101]
Fosfomycin	Water	184.3	500	[103]
Isoniazid	6% DMSO in methanol	640.6	10	
Novobiocin	Methanol	287.1	1000	[102]
Rifaximin	Methanol/Water 50:50 (v/v)	282.9	10	
Antibiotic Growth Promoters				
Dichloroisoeverninic acid	Methanol	1000.0	800	[103]
Halquinol/Chlorhydroxyquinoline	12.5% DMSO in methanol	102.6	40[c]	[101]
Virginiamycin M_1	Methanol	100.9	100	[103]
Anticoccidials				
Amprolium	Methanol	1000.0	500	[102]
Clopidol	Methanol	1000.0	200	[103]
Diaveridine	Methanol	1000.0	50[b]	[103]
Decoquinate	Methanol	1000.0	1000	[103]
Diclazuril	DMSO	1000.0	50	[103]
Ethopabate	Methanol	1000.0	500[b]	[102]
Lasalocid A	Acetonitrile	1000.0	10	[101]
Maduramicin	Methanol	100.6	30[b]	[101]
Monensin A	Methanol	101.9	10	[101]
Narasin A	Methanol	1000.0	15	[101]
4,4′-Dinitrocarbanilide – DNC	DMSO	1000.0	4000[d]	[101]
Robenidine	Methanol	1000.0	200[d]	[101]
Salinomycin	DMSO	1000.0	20	[103]
Toltrazuril	DMSO	1000.0	100	[101]
Trimethoprim	Methanol	1000.0	50	[101]
Anti-inflammatories/Steroidal				
Prednisolone	Methanol	270.2	4	[101]
Prednisone	Methanol	276.4	4	
Anti-inflammatories Prospect/Steroidal				

Group/Class - Pharmacologically active Substance	Solvent used	Stock standard concentration (µg mL^{-1})	MRL in bovine muscle (µg Kg^{-1})	Reference
Isoflupredone acetate/9-Fluoroprednisolone acetate	Methanol	169.3	10	
Flumetasone	Methanol	352.8	10	
Anti-Inflammatory/Non-Steroidal				
Mefenamic acid	Methanol	203.3	20	[94]
Tolfenamic acid	Acetonitrile	184.5	50	[101]
Carprofen	6% DMSO in methanol	201.6	500	[101]
Ketoprofen	Acetonitrile	180.5	50	[103]
Diclofenac	6% DMSO in methanol	204.0	5	[101]
Flunixin	Methanol	99.2	20	[101]
Indomethacin	Methanol	177.5	20	[94]
Meloxicam	12.5% DMSO in methanol	192.0	20	[101]
Naproxen	6% DMSO in methanol	162.2	20	[94]
Nimesulide	Methanol	205.0	20	[94]
Piroxycam	DMSO	100.8	20	[94]
Propyphenazone	Methanol	193.4	20	[94]
Antiparasitic/Avermectins				
Avermectin B_{1a}/Abamectin B_{1a}	Methanol	113.1	20	[103]
Doramectin	Methanol	109.4	10	[101]
Emamectin B_{1a}	Methanol	151.1	2	[103]
Eprinomectin B_{1a}	Methanol	89.8	100	[101]
Ivermectin B_{1a}/22,23-Dihydroavermectin B_1	Methanol	93.2	30	[101]
Moxidectin	Methanol	88.6	20	[101]
Antiparasitic/Benzimidazoles				
Albendazole	12.5% DMSO in acetonitrile	205.5	100	[101]
Albendazole sulfone	12.5% DMSO in methanol	216.4	100	[101]
Albendazole sulfoxide	12.5% DMSO in methanol	147.6	100	[101]
Closantel	Acetonitrile	210.1	1000	[101]
Febantel	Acetonitrile	254.4	100	[101]
Fenbendazole	12.5% DMSO in acetonitrile	221.0	100	[101]
Fenbendazole sulfone	12.5% DMSO in acetonitrile	181.4	100	[101]
Flubendazole	12.5% DMSO in acetonitrile	213.7	20	[103]
2-Aminoflubendazole	12.5% DMSO in acetonitrile	134.7	20	[103]
Levamisole	Acetonitrile/ DMSO/Methanol	217.0	10	[101]
Mebendazole	Acetonitrile	204.3	20	[104]

Group/Class - Pharmacologically active Substance	Solvent used	Stock standard concentration (µg mL^{-1})	MRL in bovine muscle (µg Kg^{-1})	Reference
Oxibendazole	Methanol	103.2	100	[101]
Oxfendazole	Acetonitrile/ DMSO	211.1	100	[101]
Thiabendazole	Acetonitrile	164.8	100	[101]
Triclabendazole	Acetonitrile	404.5	250	[101]
Antiparasitic/Phenylpyrazoles				
Fipronil	Methanol	134.9	500	[103]
Fipronil sulfone	Methanol	87.2	500	[103]
Antiparasitic/Nitroimidazoles				
Dimetridazole	Acetonitrile/ DMSO	225.6	10	
Hydroxydimetridazole/HMMNI	Acetonitrile	203.3	10	
Ipronidazole	Acetonitrile	203.3	3	[94]
Hydroxy Ipronidazole	Acetonitrile	94.1	3	[94]
Metronidazole	Acetonitrile/ DMSO	246.5	10	
Hydroxymetronidazole	Acetonitrile/ DMSO	220.7	10	
Ronidazole/1-Methyl-2-carbamoyloxymethyl-5-nitroimidazole	Acetonitrile/ DMSO	203.8	10	
Antiparasitic/Isoquinoline-pyrazines				
Praziquantel	Methanol	240.5	300	[103]
Beta-Agonists				
Cimaterol	Methanol	100.2	10	
Clenbuterol	Methanol	1000.0	0.2	[101]
Ractopamine	Methanol	100.1	10	[101]
Salbutamol	Methanol	1000.0	10	
Zilpaterol	Methanol	100.8	0.5	[101]
Sedatives				
Acepromazine	Methanol	101.1	10	
Azaperol	Methanol	101.4	60[c]	[101]
Azaperone	Methanol	102.7	60[c]	[101]
Carazolol	Methanol	101.2	5	[101]
Chlorpromazine	Methanol	211.5	10	
Prospecting sedatives				
Xylazine	Methanol	100.2	20	[103]
Corants				
Gentian violet/Crystal violet	Acetonitrile	98.9	10	
Leucocrystal Violet	Acetonitrile	290.8	10	
Malachite green	Acetonitrile	140.7	10	
Leucomalachite green	Acetonitrile	113.9	10	

[a]Class - Pharmacologically active substance; [b]Chicken, muscle; [c]Pig, muscle; [d]Broiler chicken, muscle. Abbreviations: µg/mL: microgram per milliliter; µg Kg^{-1}: micrograms per kilogram; DMSO: dimethyl sulfoxide.

Table S2. Chromatographic conditions of the different methods evaluated for the Accela 1,250 Pump UHPLC system.

Parameter	**Condition**		
	Method A	**Method B**	
		Aqueous extract	**Organic extract (ACN)**
Column and Pre-column	Acquity UHPLC® BEH C18 (50 mm x 2.1 mm d.i x 1.7 μm). Waters VanGuardAcquity UPLC® BEH C18 (5 mm x 2.1 mm d.i x 1.7 μm). Waters		
Column and inlet temperature	30 ± 5°C and 15 °C	35 ± 5°C and 15°C	30 ± 5°C and 15°C
Injection volume	5 μL	10 μL	
Mobile phase	MPA: 0.01% formic acid in water MPB: MeOH	MPA: Amonium formate 5 mmol L^{-1} + 0.1% formic acid in water MPB: H_2O/ACN 5:95 + 0.1% formic acid	MPA: Amonium formate 0.2 mol L^{-1}+ 0.1% formic acid MPB: H_2O/ACN 5:95 + 0.1% formic acid
Gradient	0.0 min: 95% MPA. 5% MPB → 7.0 min: 0% MPA. 100% MPB → 10.0 min: 0% MPA. 100% MPB → 10.1 min: 95% MPA. 5% MPB → 17 min: 95% MPA. 5% MPB	0.0 min: 100% MPA. 0% MPB →2.0 min: 80% MPA. 20% MPB → 3.5 min: 5% MPA. 95% MPB → 4.5 min: 5% MPA. 95% MPB → 5.0 min: 100% MPA. 0% MPB	0.0 min: 100% MPA. 0% MPB → 1.5 min: 100% MPA. 0% MPB → 2.5 min: 2% MPA. 98% MPB → 3.5 min: 2% MPA. 98% MPB → 4.0 min: 100% MPA. 0% MPB
Flow	0.1 mL min^{-1}	0.4 mL min^{-1}	
Run time	17.0 min	20.0 min	

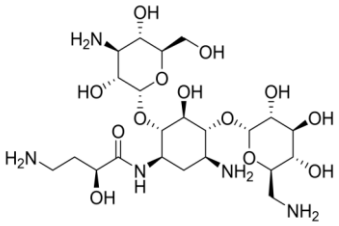
Abbreviations: μL: microliter; min: minute; mL min^{-1}: milliliter per minute; ACN: acetonitrile; H_2O: water; MeOH: methanol; MPA: mobile phase A; MPB: mobile phase B.

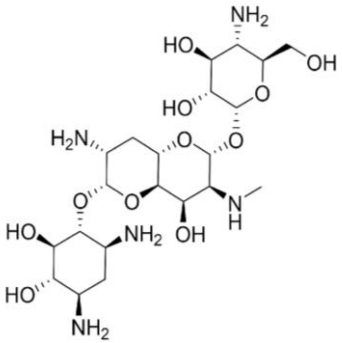
Table S3. Mass spectrometer conditions of different methods evaluated for the Q-Exactive Orbitrap HRMS system.

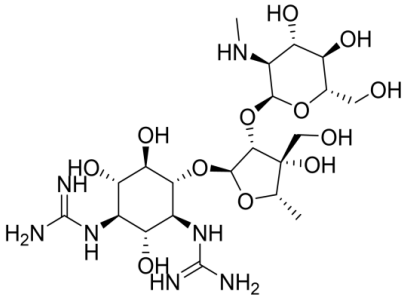
Parameter ($HESI^+$), ($HESI^-$)	
Ion source	
Spray voltage	3.9 kV ($HESI^+$); 2.9 kV ($HESI^-$)
Capillary temperature	350°C
Sheath gas	40 arb
Auxiliary gas	15 arb
S-Lens RF	50 arb
Full-MS	
Microscans	1
Resolution	35,000 FWHM
Target automatic gain control (AGC targed)	3.0×10^6
Maximum injection time (IT)	100 ms
Scan range	65-975 *m/z*
AIF	
Microscans	1
Resolution	17,500 FWHM
AGC targed	3.0×10^6
Maximum injection time	100 ms
Normalized collision energy (NCE)	10, 35 and 80 eV
Scan range	65-975 *m/z*

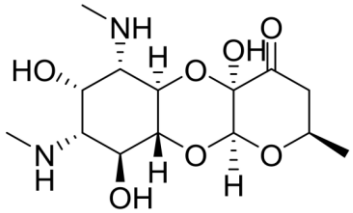
Abbreviations: Arb: arbitrary units; FWHM: full width at half maximum; ms: milli seconds; *m/z*: mass to charge.

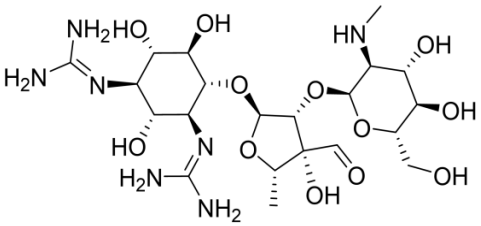
Table S4. Physicochemical properties of veterinary drugs and the main conditions determined by Q-Exactive Orbitrap HRMS.

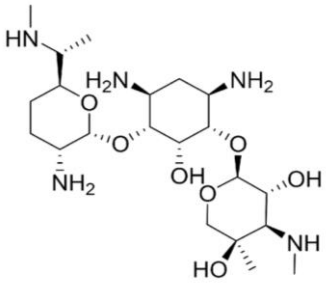
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Aminoglycosides						
Amikacin CAS registration number: 37517-28-5 ChemSpider ID: 34635 PubChem CID: 37768 	Molecular formula: $C_{22}H_{43}N_5O_{13}$ Monoisotopic mass (Da): 585.2852 pKa (strongest acidic): 12.16 pKa (strongest basic): 9.61 Partition coefficient (Log P): -8.584 Intrinsic solubility (mg mL^{-1}): 0.406 (High)	$[M+H]^+$; $[M-H]^-$	586.2930; 584.2785	425.2242; 264.1554; 163.1077; 324.1765; 467.2348	405.1993; 423.2099; 287.1238; 270.0986; 244.1305	

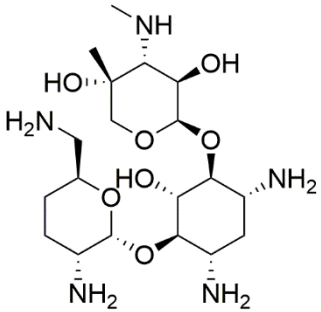
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Apramycin CAS registration number: 37321-09-8 ChemSpider ID: 2339128 PubChem CID: 3081545 	Molecular formula: $C_{21}H_{41}N_5O_{11}$ Monoisotopic mass (Da): 539.2797 pKa (strongest acidic): 12.23 pKa (strongest basic): 9.05 Partition coefficient (Log P): -6.508 Intrinsic solubility (mg mL^{-1}): 1.526 (High)	$[M+H]^+$	540.2875; 270.6474	378.1841; 344.1816; 217.1183; 523.2610; 163.1077		$[M+2H]^{2+}$ 217.1183; 163.1077

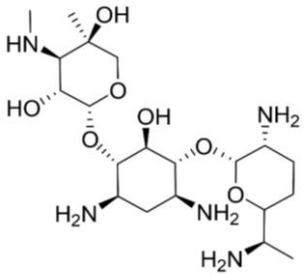
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Dihydrostreptomycin CAS registration number: 128-46-1 ChemSpider ID: 388489 PubChem CID: 439369 	Molecular formula: $C_{21}H_{41}N_7O_{12}$ Monoisotopic mass (Da): 583.2808 pKa (strongest acidic): 11.91 pKa (strongest basic): 10.91 Partition coefficient (Log P): -7.35 Intrinsic solubility (mg mL^{-1}): -0.185(High)	$[M+H]^+$; $[M-H]^-$; $[M+2H]^{2+}$	584.2886; 582.2740; 292.6479	263.1462; 221.1244; 176.0917; 186.0873; 409.2041	407.1898; 261.1319; 234.0986; 243.1214; 219.1101	$[M+2H]^{2+}$ 263.1462; 176.0917; 158.0812; 110.0600; 409.2041

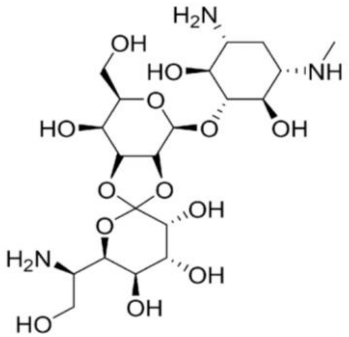
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Spectinomycin CAS registration number: 1695-77-8 ChemSpider ID: - PubChem CID: 15541 	Molecular formula: $C_{14}H_{24}N_2O_7$ Monoisotopic mass (Da): 332.1578 pKa (strongest acidic): 8.98 pKa (strongest basic): 8.38 Partition coefficient (Log P): -2.076 Intrinsic solubility (mg mL^{-1}): -0.846 (High)	$[M+H]^+$; $[M+H_3O]^+$	333.1656; 352.1840	98.0600; 94.0651; 207.1339 140.0706; 110.0600		$[M+H_3O]^+$ 351.1762; 207.1339; 140.0706; 189.1234; 116.0706

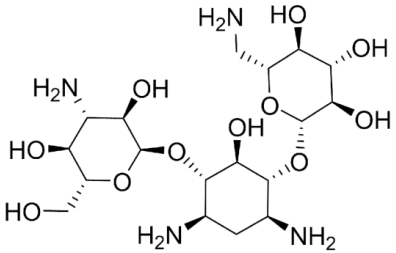
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Streptomycin CAS registration number: 57-92-1 ChemSpider ID: 18508 PubChem CID: 19649 	Molecular formula: $C_{21}H_{39}N_7O_{12}$ Monoisotopic mass (Da): 581.2651 pKa (strongest acidic): 11.16 pKa (strongest basic): 10.73 Partition coefficient (Log P): -7.192 Intrinsic solubility (mg mL^{-1}): -0.378 (High)	$[M+H]^+$; $[M-H]^-$; $[M+2H]^{2+}$; $[M+H_2O+H]^+$; $[M+H_2O+2H]^{2+}$	582.2730; 580.2584; 291.6401; 600.2835; 300.6454	263.1462; 407.1885; 540.2511; 176.0917; 246.1197	261.1319; 381.1742; 318.1197; 219.1101; 119.0352	$[M+2H]^{2+}$ 263.1462; 176.0917; 158.0812; 110.0600 $[M+H_2O+H]^+$ 101.0597; 263.1462; 176.0917 $[M+H_2O+2H]^{2+}$ 101.0597; 263.1462; 176.0917

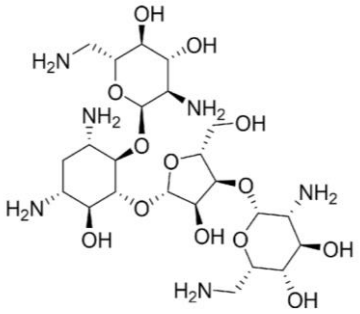
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Gentamicin (Gentamicin C_1) CAS registration number: 25876-10-2 ChemSpider ID: 65328 PubChem CID: 72395 	Molecular formula: $C_{21}H_{43}N_5O_7$ Monoisotopic mass (Da): 477.3157 pKa (strongest acidic): 12.55 pKa (strongest basic): 10.03 Partition coefficient (Log P): -3.137 Intrinsic solubility (mg mL^{-1}): -0.419 (High)	$[M+H]^+$; $[M+2H]^{2+}$	478.3235; 239.6654	160.0968; 322.1973; 157.1335		$[M+2H]^{2+}$ 160.0968; 322.1973

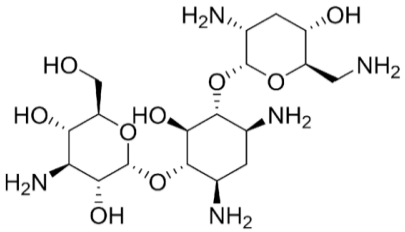
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Gentamicin (Gentamicin C_{1a}) CAS registration number: 26098-04-4 ChemSpider ID: 65329 PubChem CID: 72396 	Molecular formula: $C_{19}H_{39}N_5O_7$ Monoisotopic mass (Da): 449.2844 pKa (strongest acidic): 12.55 pKa (strongest basic): 9.66 Partition coefficient (Log P): -3.986 Intrinsic solubility (mg mL^{-1}): -0.335 (High)	$[M+2H]^{2+}$	225.6498			$[M+2H]^{2+}$ 129.1022; 322.1973

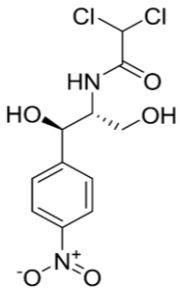
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Gentamicin (Gentamicin C_2-C_{2a}) CAS registration number: 25876-11-3 ChemSpider ID: 65330 PubChem CID: 72397 	Molecular formula: $C_{20}H_{41}N_5O_7$ Monoisotopic mass (Da): 463.3001 pKa (strongest acidic): 12.55 pKa (strongest basic): 9.87 Partition coefficient (Log P): -3.57 Intrinsic solubility (mg mL^{-1}): -0.638 (High)	$[M+H]^+$; $[M+2H]^{2+}$	464.3079; 232.6576	160.0968; 163.1077; 322.1973		$[M+2H]^{2+}$ 160.0968; 163.1077

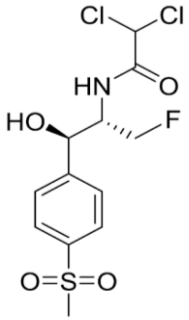
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Hygromycin (Hygromycin B) CAS registration number: 31282-04-9 ChemSpider ID: 28634700 PubChem CID: 56928061 	Molecular formula: $C_{20}H_{37}N_3O_{13}$ Monoisotopic mass (Da): 527.2321 pKa (strongest acidic): 11.4 pKa (strongest basic): 9.4 Partition coefficient (Log P): -6.372 Intrinsic solubility (mg mL^{-1}): -0.323 (High)	$[M+H]^+$; $[M-H]^-$; $[M+2H]^{2+}$	528.2399; 526.2254; 264.6236	352.1238; 177.1234; 257.0656; 150.0761; 303.1551	206.0659; 319.1500; 188.0553; 368.1187	$[M+2H]^{2+}$ 177.1234; 159.1128; 132.0655; 190.0710

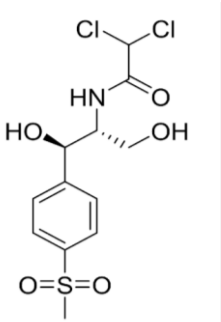
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Kanamycin (Kanamycin A) CAS registration number: 59-01-8 ChemSpider ID: 388665 PubChem CID: 6032 	Molecular formula: $C_{18}H_{36}N_4O_{11}$ Monoisotopic mass (Da): 484.2375 pKa (strongest acidic): 12.05 pKa (strongest basic): 9.34 Partition coefficient (Log P): -7.061 Intrinsic solubility (mg mL^{-1}): 0.24 (High)	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$	485.2453; 483.2308; 507.2273	163.1077; 84.0444; 68.0495; 102.0550; 324.1756	322.1622; 354.0694	$[M+Na]^+$ 346.1582; 163.1077; 249.0921; 263.2345

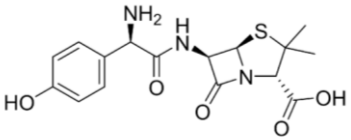
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Neomycin (Neomycin B) CAS registration number: 119-04-0 ChemSpider ID: 8075 PubChem CID: 8378 	Molecular formula: $C_{23}H_{46}N_6O_{13}$ Monoisotopic mass (Da): 614.3117 pKa (strongest acidic): 12.15 pKa (strongest basic): 9.3 Partition coefficient (Log P): Index -1 out of bounds for length 42 Intrinsic solubility (mg mL^{-1}): 0.525 (High)	$[M+H]^+$; $[M+2H]^{2+}$	615.3196; 308.1634	455.2348; 323.1925; 161.0921; 203.1026		$[M+2H]^{2+}$ 161.0921; 114.0550; 163.1077; 125.0709; 455.2348

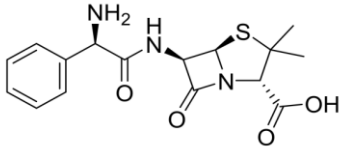
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Tobramycin CAS registration number: 32986-56-4 ChemSpider ID: 33377 PubChem CID: 36294 	Molecular formula: $C_{18}H_{37}N_5O_9$ Monoisotopic mass (Da): 467.2586 pKa (strongest acidic): 12.53 pKa (strongest basic): 9.42 Partition coefficient (Log P): -6.478 Intrinsic solubility (mg mL^{-1}): -0.023 (High)	$[M+H]^+$; $[M-H]^-$	468.2664; 466.2519	324.1765; 163.1077; 145.0972; 205.1182	305.1833; 234.0986; 304.1517; 178.0723; 287.1238	

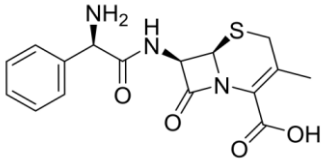
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Amphenicols						
Chloramphenicol CAS registration number: 56-75-7 ChemSpider ID: 5744 PubChem CID: 5959 	Molecular formula: $C_{11}H_{12}Cl_2N_2O_5$ Monoisotopic mass (Da): 322.0118 pKa (strongest acidic): 10.79 pKa (strongest basic): - Partition coefficient (Log P): 0.879 Intrinsic solubility (mg mL^{-1}): -2.903 (High)	$[M+H]^+$; $[M-H]^-$	323.0196; 321.0051	274.9985; 165.0659; 82.9450; 151.0628; 305.0090	152.0353; 321.0051; 121.0293; 151.0274; 257.0335	

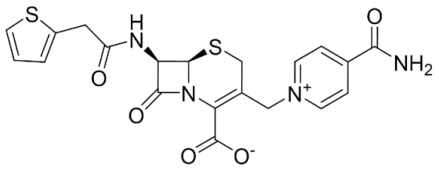
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Florfenicol CAS registration number: 73231-34-2 ChemSpider ID: 102776 PubChem CID: 114811 	Molecular formula: $C_{12}H_{14}Cl_2FNO_4S$ Monoisotopic mass (Da): 356.9999 pKa (strongest acidic): 10.68 pKa (strongest basic): - Partition coefficient (Log P): 0.67 Intrinsic solubility (mg mL^{-1}): -2.955 (High)	$[M+H]^+$; $[M-H]^-$	358.0077; 355.9932	103.0542; 319.9907; 241.0053; 210.0582; 206.0366	185.0278; 335.9870; 119.0499; 78.9854; 121.0286	

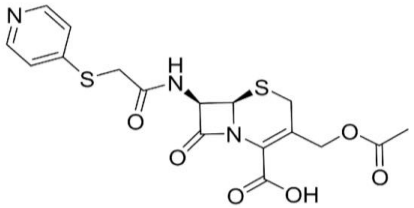
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Thiamphenicol CAS registration number: 15318-45-3 ChemSpider ID: 25315 PubChem CID: 27200 	Molecular formula: $C_{12}H_{15}Cl_2NO_5S$ Monoisotopic mass (Da): 355.0043 pKa (strongest acidic): 10.95 pKa (strongest basic): - Partition coefficient (Log P): -0.221 Intrinsic solubility (mg mL^{-1}): -2.266 (High)	$[M+H]^+$; $[M-H]^-$	356.0121; 353.9975	307.9909; 241.0056; 229.0056; 119.0729; 82.9450	353.9975; 185.0278; 78.9859; 121.0296; 119.0504	

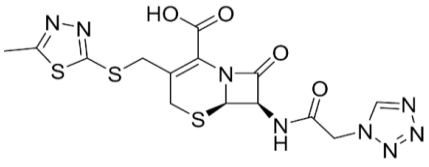
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Betalactams						
Amoxicillin CAS registration number: 26787-78-0 ChemSpider ID: 31006 PubChem CID: 33613 	Molecular formula: $C_{16}H_{19}N_3O_5S$ Monoisotopic mass (Da): 365.1040 pKa (strongest acidic): 3.23 pKa (strongest basic): 7.22 Partition coefficient (Log P): -2.308 Intrinsic solubility (mg mL^{-1}): -4.35 (Moderate)	$[M+H]^+$; $[M-H]^-$	366.1118; 364.0973	349.0853; 211.0711; 86.0059; 107.0491; 114.0007	223.0547; 206.0281; 83.0251; 133.0295; 123.0451	

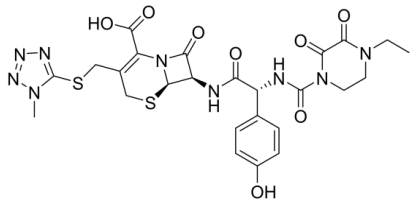
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Ampicillin CAS registration number: 69-53-4 ChemSpider ID: 6013 PubChem CID: 6249 	Molecular formula: $C_{16}H_{19}N_3O_4S$ Monoisotopic mass (Da): 349.1091 pKa (strongest acidic): 3.24 pKa (strongest basic): 7.23 Partition coefficient (Log P): -2.005 Intrinsic solubility (mg mL^{-1}): -4.789 (Low)	$[M+H]^+$; $[M-H]^-$	350.1169; 348.1024	106.0651; 160.0427; 89.0389; 79.0542; 95.0491	207.0598; 348.1023; 74.0070; 99.9863; 304.1125	

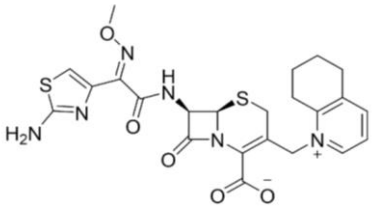
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Cephalexin CAS registration number: 15686-71-2 ChemSpider ID: 25541 PubChem CID: 27447 	Molecular formula: $C_{16}H_{17}N_3O_4S$ Monoisotopic mass (Da): 347.0934 pKa (strongest acidic): 3.45 pKa (strongest basic): 7.23 Partition coefficient (Log P): -2.141 Intrinsic solubility (mg mL^{-1}): -3.959 (Moderate)	$[M+H]^+$; $[M-H]^-$; $[(M+H_2-CO)+H]^+$; $[M+H+CH_3OH]^+$	348.1013; 346.0867; 322.1220; 380.1275	68.0495; 160.0426; 158.0270; 106.0651	233.0390; 70.9835; 268.1092; 173.0720; 107.0615	$[(M+H_2-CO)+H]^+$ 191.0815; 184.9777; 106.0651; 220.0791; 209.0743 $[M+H+CH_3OH]^+$ 106.0651; 174.0550; 151.0866; 198.0219

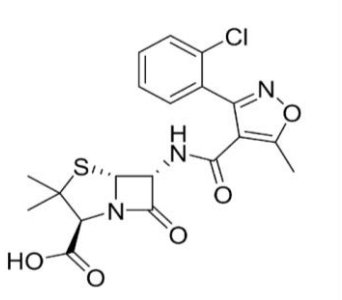
Group/Class - Pharmacologically active Substance	**Physicochemical properties**	**Monitored ion**	**Theoretical exact mass MS (*m/z*)**	**Fragment ions (*m/z*) MS^2**		
				$[M+H]^+$	$[M-H]^-$	Others
Cefalonium CAS registration number: 5575-21-3 ChemSpider ID: 20438 PubChem CID: 21743 	Molecular formula: $C_{20}H_{18}N_4O_5S_2$ Monoisotopic mass (Da): 458.0713 pKa (strongest acidic): 3.09 pKa (strongest basic): -0.86 Partition coefficient (Log P): -4.243 Intrinsic solubility (mg mL^{-1}): The molecule cannot be neutralized and the calculation is not defined for molecules with non-zero charge	$[M+H]^+$; $[(M+H_2CO)+H]^+$	459.0791; 433.0999	337.0311; 152.0165; 97.0106; 80.0495; 108.0682		$[(M+H_2-CO)+H]^+$ 119.0855; 337.0311; 311.0512; 228.0325; 209.0379

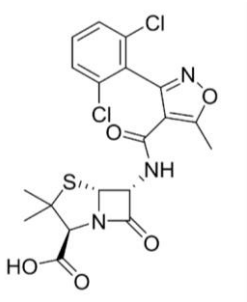
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Cephapirin CAS registration number: 21593-23-7 ChemSpider ID: - PubChem CID: 30699 	Molecular formula: $C_{17}H_{17}N_3O_6S_2$ Monoisotopic mass (Da): 423.0553 pKa (strongest acidic): 3.54 pKa (strongest basic): 5 Partition coefficient (Log P): -2.001 Intrinsic solubility (mg mL^{-1}): -3.723 (High)	$[M+H]^+$	424.0632	292.0573; 181.0431; 152.0166; 141.0482; 112.0216		

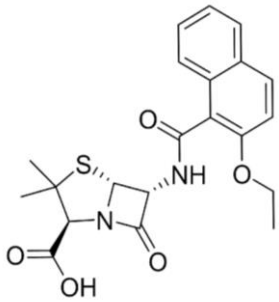
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Cefazolin CAS registration number: 25953-19-9 ChemSpider ID: 30723 PubChem CID: 33255 	Molecular formula: $C_{14}H_{14}N_8O_4S_3$ Monoisotopic mass (Da): 454.0295 pKa (strongest acidic): 3.03 pKa (strongest basic): 0.26 Partition coefficient (Log P): -1.519 Intrinsic solubility (mg mL^{-1}): -4.131 (Moderate)	$[M+H]^+$; $[M-H]^-$	455.0373; 453.0227	156.0112; 80.0495; 323.0557; 112.0215; 97.0106	167.0285; 69.0207; 251.0131; 130.9743; 207.0233	

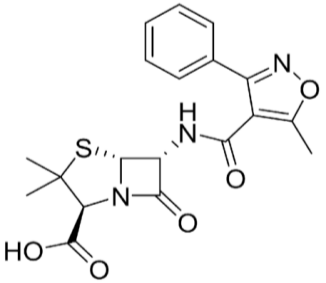
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Cefoperazone CAS registration number: 62893-19-0 ChemSpider ID: 40206 PubChem CID: 44187 	Molecular formula: $C_{25}H_{27}N_9O_8S_2$ Monoisotopic mass (Da): 645.1419 pKa (strongest acidic): 3.38 pKa (strongest basic): -1.98 Partition coefficient (Log P): -0.9 Intrinsic solubility (mg mL^{-1}): -5.213 (Low)	$[M+H]^+$; $[M-H]^-$	646.1497; 644.1351	530.1340; 115.0502; 186.0874; 156.0114; 143.0815	115.0083; 117.0345; 71.9788; 144.0454; 89.0397	

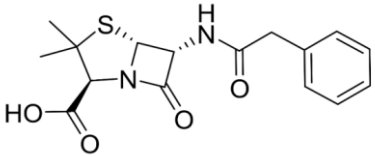
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Cefquinome CAS registration number: 84957-30-2 ChemSpider ID: 16736863 PubChem CID: 5464355 	Molecular formula: $C_{23}H_{24}N_6O_5S_2$ Monoisotopic mass (Da): 528.1244 pKa (strongest acidic): 2.85 pKa (strongest basic): 3.61 Partition coefficient (Log P): -3.531 Intrinsic solubility (mg mL^{-1}): The molecule cannot be neutralized and the calculation is not defined for molecules with non-zero charge	$[M+H]^+$; $[M+2H]^{2+}$; $[(M+H_2CO)+H]^+$	529.1322; 265.0698; 503.1530	125.0056; 324.0579; 167.0272; 156.0224; 134.0964		$[M+2H]^{2+}$ 134.0964; 199.1230; 167.0274; 125.0056 $[(M+H_2-CO)+H]^+$ 201.0441; 134.0964; 241.0390; 370.0631; 126.0120

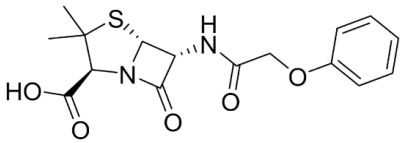
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Cloxacillin CAS registration number: 61-72-3 ChemSpider ID: 5873 PubChem CID: 6098 	Molecular formula: $C_{19}H_{18}ClN_3O_5S$ Monoisotopic mass (Da): 435.0650 pKa (strongest acidic): 3.75 pKa (strongest basic): -0.42 Partition coefficient (Log P): 2.302 Intrinsic solubility (mg mL^{-1}): -6.259 (Low)	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[(M+H_2-CO)+H]^+$; $[M+H+CH_3OH]^+$	436.0729; 434.0583; 458.0548; 410.0936; 468.0991	122.9996; 87.0263; 178.0052; 160.0425; 114.0371	293.0157; 74.9910; 65.9986; 83.0139; 257.0391	$[M+Na]^+$ 182.0241; 299.0189; 282.0397; 278.0448; 271.0240 $[(M+H_2-CO)+H]^+$ 174.0583; 128.0528; 364.0881; 100.0393; 220.0160 $[M+H+CH_3OH]^+$ 160.0427; 309.0632; 436.0728; 232.0636

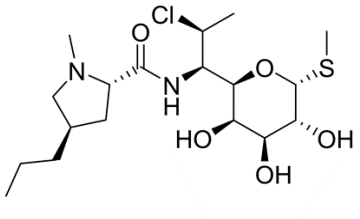
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Dicloxacillin CAS registration number: 3116-76-5 ChemSpider ID: 17358 PubChem CID: 18381 	Molecular formula: $C_{19}H_{17}Cl_2N_3O_5S$ Monoisotopic mass (Da): 469.0261 pKa (strongest acidic): 3.75 pKa (strongest basic): -0.71 Partition coefficient (Log P): 2.906 Intrinsic solubility (mg mL^{-1}): -6.893 (Low)	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[(M+H_2-CO)+H]^+$; $[M+H+CH_3OH]^+$	470.0339; 468.0193; 492.0158 444.0546; 502.0601	160.0427; 114.0372; 87.0263; 156.9606; 108.9840	326.9767; 291.0000; 83.0140; 65.9986; 72.9992	$[M+Na]^+$ 332.9794; 182.0243; 316.0007; 312.0058 $[(M+H_2-CO)+H]^+$ 174.0583; 128.0528; 312.0301; 398.0491; 271.0031 $[M+H+CH_3OH]^+$ 160.0427; 470.0339; 343.0242; 232.0636

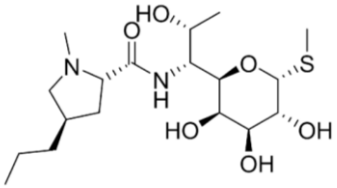
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Nafcillin CAS registration number: 147-52-4 ChemSpider ID: 8634 PubChem CID: 8982 	Molecular formula: $C_{21}H_{22}N_2O_5S$ Monoisotopic mass (Da): 414.1244 pKa (strongest acidic): 3.31 pKa (strongest basic): -1.88 Partition coefficient (Log P): 2.289 Intrinsic solubility (mg mL^{-1}): -7.052 (Low)	$[M+H]^+$; $[M-H]^-$; $[(M+H_2CO)+H]^+$	415.1322; 413.1177; 389.1530	199.0754; 115.0542; 171.0441; 143.0491; 89.0386	272.0751; 243.0359; 72.9992; 115.0553; 70.9835	$[(M+H_2-CO)+H]^+$ 199.0754; 372.1264; 343.1475; 115.0542; 143.0491

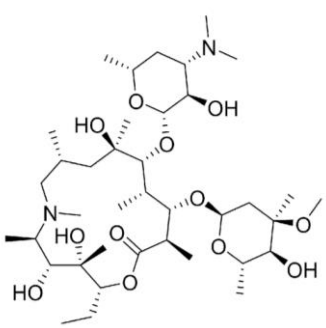
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Oxacillin CAS registration number: 66-79-5 ChemSpider ID: 5961 PubChem CID: 6196 	Molecular formula: $C_{19}H_{19}N_3O_5S$ Monoisotopic mass (Da): 401.1040 pKa (strongest acidic): 3.75 pKa (strongest basic): -0.12 Partition coefficient (Log P): 1.698 Intrinsic solubility (mg mL^{-1}): -5.606 (Low)	$[M+H]^+$; $[M-H]^-$; $[(M+H_2-CO)+H]^+$	402.1118; 400.0973; 376.1326	160.0427; 114.0372; 95.0490; 243.0764; 87.0263	259.0547; 74.9910; 65.9985; 83.0139; 70.9835	$[(M+H_2-CO)+H]^+$ 174.0583; 128.0528; 330.1271; 186.0548; 144.0444

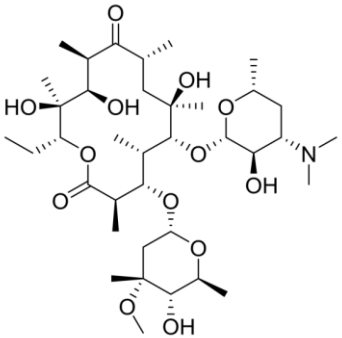
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Benzylpenicillin CAS registration number: 61-33-6 ChemSpider ID: 5693 PubChem CID: 5904 	Molecular formula: $C_{16}H_{18}N_2O_4S$ Monoisotopic mass (Da): 334.0982 pKa (strongest acidic): 3.53 pKa (strongest basic): - Partition coefficient (Log P): 1.081 Intrinsic solubility (mg mL^{-1}): -4.555 (Low)	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$	335.1060; 333.0915; 357.0880	189.0692; 176.0706; 160.0427; 114.0372; 91.05417	192.0489; 255.1128; 171.0598; 289.1017	$[M+Na]^+$ 181.0733; 182.0246; 198.0525; 239.0791; 313.0981

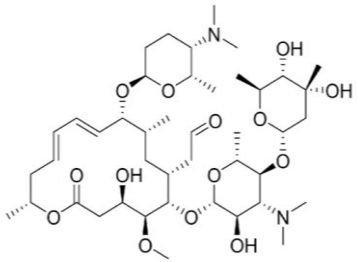
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Phenoxymethylpenicillin/Phenoxymethyl V penicillin CAS registration number: 87-08-1 ChemSpider ID: 6607 PubChem CID: 6869 	Molecular formula: $C_{16}H_{18}N_2O_5S$ Monoisotopic mass (Da): 350.0931 pKa (strongest acidic): 3.39 pKa (strongest basic): - Partition coefficient (Log P): 0.763 Intrinsic solubility (mg mL^{-1}): -4.957 (Low)	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[(M+H_2CO)+H]^+$	351.1009; 349.0864; 373.0829; 325.1217	87.0263; 160.0425; 114.0371; 70.0651; 105.0447	93.0346; 208.0438; 114.0019; 65.0397; 211.0547	$[M+Na]^+$ 214.0475; 182.0243; 269.1260; 245.0879; 303.0563 $[(M+H_2-CO)+H]^+$ 279.1162; 193.0972; 174.0583; 128.0528; 100.0393

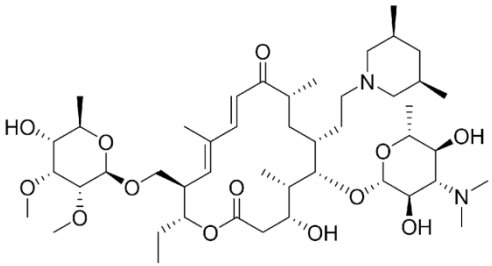
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Lincosamides						
Clindamycin CAS registration number: 13441-63-9 ChemSpider ID: 393915 PubChem CID: 446598 	Molecular formula: $C_{18}H_{33}ClN_2O_5S$ Monoisotopic mass (Da): 424.1793 pKa (strongest acidic): 12.41 pKa (strongest basic): 7.55 Partition coefficient (Log P): 1.038 Intrinsic solubility (mg mL^{-1}): -3.463 (High)	$[M+H]^+$; $[M-H]^-$	425.1872; 423.1726	126.1277; 377.1838; 389.2105; 407.1766; 299.1965	387.1948; 279.1703; 251.1772; 223.1805; 263.1772	

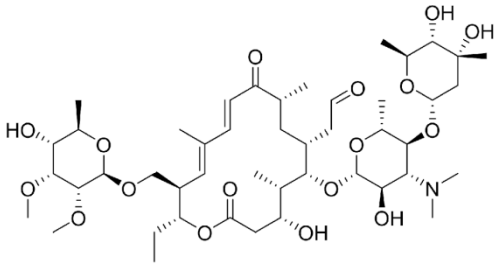
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Lincomycin CAS registration number: 154-21-2 ChemSpider ID: 2272112 PubChem CID: 3000540 	Molecular formula: $C_{18}H_{34}N_2O_6S$ Monoisotopic mass (Da): 406.2132 pKa (strongest acidic): 12.37 pKa (strongest basic): 7.97 Partition coefficient (Log P): -0.317 Intrinsic solubility (mg mL^{-1}): -2.386 (High)	$[M+H]^+$; $[M-H]^-$	407.2210; 405.2065	389.2101; 359.2173; 126.1277; 70.0651; 82.0651	405.2065; 169.1346; 127.0401; 71.0139; 85.0295	

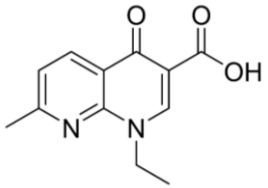
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Macrolides						
Azithromycin CAS registration number: 83905-01-5 ChemSpider ID: 10482163 PubChem CID: 447043 	Molecular formula: $C_{38}H_{72}N_2O_{12}$ Monoisotopic mass (Da): 748.5080 pKa (strongest acidic): 12.46 pKa (strongest basic): 11.16 Partition coefficient (Log P): 2.183 Intrinsic solubility (mg mL^{-1}): -1.617 (High)	$[M+H]^+$; $[M+2H]^{2+}$	749.5158; 375.2615	591.4215; 158.1176; 116.1070; 83.0491; 72.0808		$[M+2H]^{2+}$ 158.1176; 591.4215; 83.0491; 116.1070

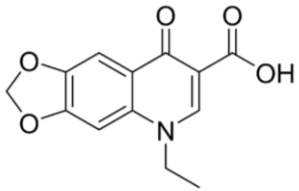
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Erythromycin (Erythromycin A) CAS registration number: 114-07-8 ChemSpider ID: 12041 PubChem CID: 12560 	Molecular formula: $C_{37}H_{67}NO_{13}$ Monoisotopic mass (Da): 733.4607 pKa (strongest acidic): 12.45 pKa (strongest basic): 9 Partition coefficient (Log P): 2.596 Intrinsic solubility (mg mL^{-1}): -2.273 (High)	$[M+H]^+$; $[M-H_2O+H]^+$	734.4685; 716.4580	158.1176; 127.0754; 116.0706; 83.0491; 72.0808		$[M-H_2O+H]^+$ 558.3637; 158.1176; 540.3525; 522.3425; 98.0966

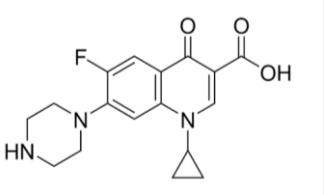
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Spiramycin (Spiramycin I) CAS registration number: 8025-81-8 ChemSpider ID: 4451378 PubChem CID: 5356392 	Molecular formula: $C_{43}H_{74}N_2O_{14}$ Monoisotopic mass (Da): 842.5135 pKa (strongest acidic): 12.53 pKa (strongest basic): 9.33 Partition coefficient (Log P): 2.496 Intrinsic solubility (mg mL^{-1}): -0.929 (High)	$[M+H]^+$; $[M-H]^-$; $[M+2H]^{2+}$; $[M+H+CH_3OH]^+$	843.5213; 841.5067; 422.2643; 875.5475	174.1125; 83.0491; 73.0522; 101.0597; 88.0757	823.4951; 488.3007; 506.3112; 474.2580; 334.1860	$[M+2H]^{2+}$ 101.0597; 145.0859; 174.1125; 142.1226 $[M+H+CH_3OH]^+$ 145.0859; 174.1125; 232.1543; 318.1911; 142.1226

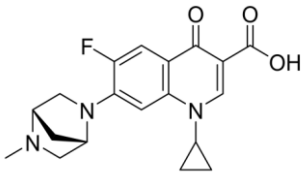
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Tilmicosin CAS registration number: 108050-54-0 ChemSpider ID: 4445656 PubChem CID: 5282521 	Molecular formula: $C_{46}H_{80}N_2O_{13}$ Monoisotopic mass (Da): 868.5655 pKa (strongest acidic): 12.55 pKa (strongest basic): 10.16 Partition coefficient (Log P): 4.19 Intrinsic solubility (mg mL^{-1}): -2.653 (High)	$[M+H]^+$; $[M-H]^-$; $[M+2H]^{2+}$	869.5733; 867.5588; 435.2903	73.0522; 174.1123; 132.1017; 116.0704; 88.07553	116.0717; 675.4591; 676.4625; 222.1863; 116.0353	$[M+2H]^{2+}$ 99.0441; 143.0703; 340.2482; 174.1125

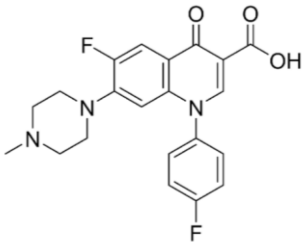
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Tylosin (Tylosin A) CAS registration number: 1401-69-0 ChemSpider ID: 4444097 PubChem CID: 5280440 	Molecular formula: $C_{46}H_{77}NO_{17}$ Monoisotopic mass (Da): 915.5186 pKa (strongest acidic): 12.45 pKa (strongest basic): 8.43 Partition coefficient (Log P): 2.316 Intrinsic solubility (mg mL^{-1}): -1.206 (High)	$[M+H]^+$	916.5264	174.1123; 145.0858; 132.1018; 101.0596; 83.0491		

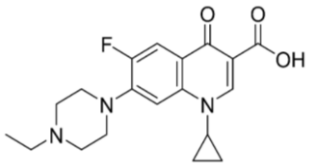
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Quinolones-Fluoroquinolones						
Nalidixic acid CAS registration number: 389-08-2 ChemSpider ID: 4268 PubChem CID: 4421 	Molecular formula: $C_{12}H_{12}N_2O_3$ Monoisotopic mass (Da): 232.0842 pKa (strongest acidic): 5.95 pKa (strongest basic): 4.68 Partition coefficient (Log P): 0.873 Intrinsic solubility (mg mL^{-1}): -2.016 (High)	$[M+H]^+$	233.0921	205.0608; 104.0495; 159.0553; 131.0604; 187.0502		

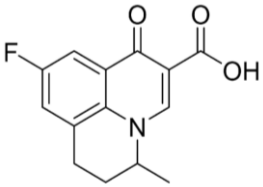
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Oxolinic acid CAS registration number: 14698-29-4 ChemSpider ID: 4467 PubChem CID: 4628 	Molecular formula: $C_{13}H_{11}NO_5$ Monoisotopic mass (Da): 261.0632 pKa (strongest acidic): 5.58 pKa (strongest basic): - Partition coefficient (Log P): 1.36 Intrinsic solubility (mg mL^{-1}): -2.338 (High)	$[M+H]^+$	262.0710	244.0602; 234.0397; 130.0651; 160.0393; 172.0393		

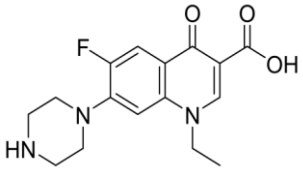
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Ciprofloxacin CAS registration number: 85721-33-1 ChemSpider ID: 2662 PubChem CID: 2764 	Molecular formula: $C_{17}H_{18}FN_3O_3$ Monoisotopic mass (Da): 331.1327 pKa (strongest acidic): 5.33 pKa (strongest basic): 8.77 Partition coefficient (Log P): -0.88 Intrinsic solubility (mg mL^{-1}): -2.314 (High)	$[M+H]^+$	332.1405	203.0615; 288.1503; 231.0558; 148.0554; 188.0376		

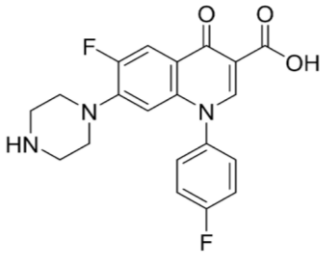
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Danofloxacin CAS registration number: 112398-08-0 ChemSpider ID: 64439 PubChem CID: 71335 	Molecular formula: $C_{19}H_{20}FN_3O_3$ Monoisotopic mass (Da): 357.1483 pKa (strongest acidic): 5.26 pKa (strongest basic): 7.72 Partition coefficient (Log P): -0.386 Intrinsic solubility (mg mL^{-1}): -2.639 (High)	$[M+H]^+$	358.1562	82.0651; 314.1659; 283.1241; 255.0564; 96.0808		

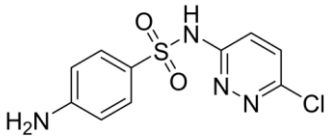
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Difloxacin CAS registration number: 98106-17-3 ChemSpider ID: 50725 PubChem CID: 56206 	Molecular formula: $C_{21}H_{19}F_2N_3O_3$ Monoisotopic mass (Da): 399.1389 pKa (strongest acidic): 5.7 pKa (strongest basic): 8.44 Partition coefficient (Log P): 0.709 Intrinsic solubility (mg mL^{-1}): -3.668 (High)	$[M+H]^+$	400.1467	356.1565; 299.0987; 227.0538; 209.0634; 75.0228		

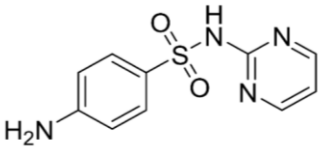
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Enrofloxacin CAS registration number: 93106-60-6 ChemSpider ID: 64326 PubChem CID: 71188 	Molecular formula: $C_{19}H_{22}FN_3O_3$ Monoisotopic mass (Da): 359.1640 pKa (strongest acidic): 5.32 pKa (strongest basic): 8.72 Partition coefficient (Log P): -0.359 Intrinsic solubility (mg mL^{-1}): -2.415 (High)	$[M+H]^+$; $[M-H]^-$	360.1718; 358.1572	316.1816; 245.1082; 189.0459; 203.0613; 148.0556	189.0472; 314.1674; 274.1362; 182.0614; 220.0779	

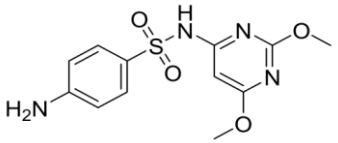
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Flumequine CAS registration number: 42835-25-6 ChemSpider ID: 3257 PubChem CID: 3374 	Molecular formula: $C_{14}H_{12}FNO_3$ Monoisotopic mass (Da): 261.0796 pKa (strongest acidic): 5.6 pKa (strongest basic): - Partition coefficient (Log P): 2.424 Intrinsic solubility (mg mL^{-1}): -2.583 (High)	$[M+H]^+$	262.0874	238.0499; 98.0152; 220.0404; 262.0874; 99.0077		

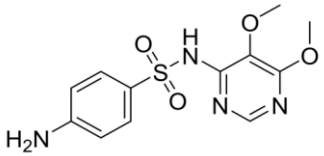
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Norfloxacin CAS registration number: 70458-96-7 ChemSpider ID: 4380 PubChem CID: 4539 	Molecular formula: $C_{16}H_{18}FN_3O_3$ Monoisotopic mass (Da): 319.1327 pKa (strongest acidic): 5.34 pKa (strongest basic): 8.77 Partition coefficient (Log P): -0.988 Intrinsic solubility (mg mL^{-1}): -2.087 (High)	$[M+H]^+$	320.1405	276.1503; 256.1440; 233.1082; 219.0926; 205.0770		

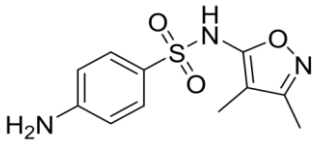
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sarafloxacin CAS registration number: 98105-99-8 ChemSpider ID: 50727 PubChem CID: 56208 	Molecular formula: $C_{20}H_{17}F_2N_3O_3$ Monoisotopic mass (Da): 385.1233 pKa (strongest acidic): 5.7 pKa (strongest basic): 8.76 Partition coefficient (Log P): 0.396 Intrinsic solubility (mg mL^{-1}): -3.891 (Moderate)	$[M+H]^+$	386.1311	342.1411; 299.0989; 285.0832; 255.0726; 227.0539		

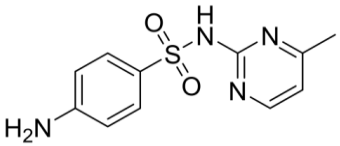
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Sulphonamides						
Sulfachlorpyridazine CAS registration number: 80-32-0 ChemSpider ID: 6382 PubChem CID: 6634 	Molecular formula: $C_{20}H_{17}F_2N_3O_3$ Monoisotopic mass (Da): 385.1233 pKa (strongest acidic): 6.6 pKa (strongest basic): 2.02 Partition coefficient (Log P): 0.853 Intrinsic solubility (mg mL^{-1}): -3.786 (Moderate)	$[M+H]^+$	386.1311	342.1411; 299.0989; 285.0832; 255.0726; 227.0539		

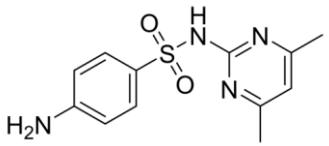
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfadiazine CAS registration number: 68-35-9 ChemSpider ID: 5026 PubChem CID: 5215 	Molecular formula: $C_{10}H_{10}N_4O_2S$ Monoisotopic mass (Da): 250.0519 pKa (strongest acidic): 6.99 pKa (strongest basic): 2.01 Partition coefficient (Log P): 0.387 Intrinsic solubility (mg mL^{-1}): -2.499 (High)	$[M+H]^+$; $[M-H]^-$	251.0597; 249.0452	156.0114; 108.0444; 96.0556; 92.0495; 65.0386	185.0822; 94.0413; 93.0335; 92.0257; 222.0332	

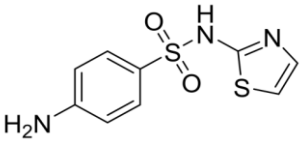
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfadimethoxine CAS registration number: 122-11-2 ChemSpider ID: 5132 PubChem CID: 5323 	Molecular formula: $C_{12}H_{14}N_4O_4S$ Monoisotopic mass (Da): 310.0730 pKa (strongest acidic): 6.91 pKa (strongest basic): 1.95 Partition coefficient (Log P): 1.261 Intrinsic solubility (mg mL^{-1}): -3.599 (High)	$[M+H]^+$; $[M-H]^-$	311.0809; 309.0663	245.1032; 236.0334; 156.0768; 108.0443; 92.0495	309.0652; 66.0097; 65.0144; 122.0359; 154.0621	

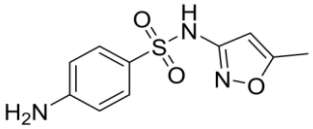
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfadoxine CAS registration number: 2447-57-6 ChemSpider ID: 16218 PubChem CID: 17134 	Molecular formula: $C_{12}H_{14}N_4O_4S$ Monoisotopic mass (Da): 310.0730 pKa (strongest acidic): 6.12 pKa (strongest basic): 2.41 Partition coefficient (Log P): 0.582 Intrinsic solubility (mg mL^{-1}): -3.115 (High)	$[M+H]^+$; $[M-H]^-$	311.0809; 309.0663	156.0113; 108.0443; 92.0495; 65.0380; 140.0448	309.0661; 156.0127; 294.0428; 279.0193; 215.0576	

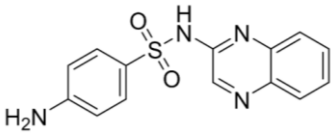
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfisoxazole/Sulfafurazole CAS registration number: 127-69-5 ChemSpider ID: 5151 PubChem CID: 5344 	Molecular formula: $C_{11}H_{13}N_3O_3S$ Monoisotopic mass (Da): 267.0672 pKa (strongest acidic): 4.81 pKa (strongest basic): 2.17 Partition coefficient (Log P): 0.731 Intrinsic solubility (mg mL^{-1}): -2.392 (High)	$[M+H]^+$; $[M-H]^-$	268.0750; 266.0605	268.0748; 156.0113; 113.0712; 108.0447; 92.0495	266.0605; 171.0233; 63.9223; 239.0496; 79.9811	

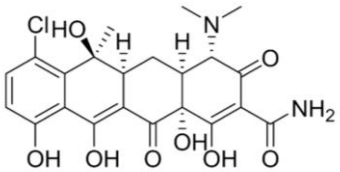
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfamerazine CAS registration number: 127-79-7 ChemSpider ID: 5134 PubChem CID: 5325 	Molecular formula: $C_{11}H_{12}N_4O_2S$ Monoisotopic mass (Da): 264.0676 pKa (strongest acidic): 6.99 pKa (strongest basic): 2 Partition coefficient (Log P): 0.519 Intrinsic solubility (mg mL^{-1}): -2.66 (High)	$[M+H]^+$; $[M-H]^-$	265.0754; 263.0608	190.0281; 156.0113; 110.0712; 108.0443; 92.0495	199.0978; 108.0570; 92.0257; 132.0570; 106.0413	

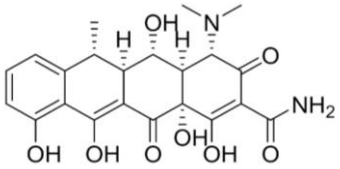
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfamethazine/Sulfadimidine CAS registration number: 57-68-1 ChemSpider ID: - PubChem CID: 5327 	Molecular formula: $C_{12}H_{14}N_4O_2S$ Monoisotopic mass (Da): 278.0832 pKa (strongest acidic): 6.99 pKa (strongest basic): 2 Partition coefficient (Log P): 0.65 Intrinsic solubility (mg mL^{-1}): -2.818 (High)	$[M+H]^+$; $[M-H]^-$	279.0910; 277.0765	124.0869; 92.0495; 108.0444; 186.0332; 156.0114	106.0413; 196.0175; 122.0726; 132.0570; 236.0488	

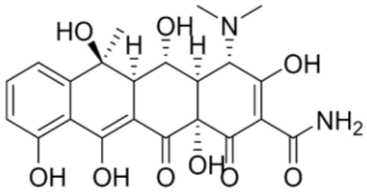
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfathiazole CAS registration number: 72-14-0 ChemSpider ID: 5148 PubChem CID: 5340 	Molecular formula: $C_9H_9N_3O_2S_2$ Monoisotopic mass (Da): 255.0131 pKa (strongest acidic): 5.73 pKa (strongest basic): 2.04 Partition coefficient (Log P): 0.975 Intrinsic solubility (mg mL^{-1}): -2.669 (High)	$[M+H]^+$; $[M-H]^-$	256.0209; 254.0063	156.0114; 108.0444; 101.0168; 92.0495; 68.0495	156.0125; 254.0063; 97.9944; 63.9624; 65.0145	

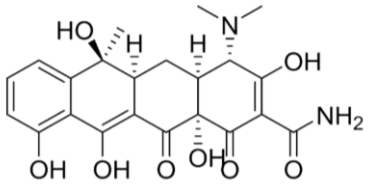
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfamethoxazole CAS registration number: 723-46-6 ChemSpider ID: 5138 PubChem CID: 5329 	Molecular formula: $C_{10}H_{11}N_3O_3S$ Monoisotopic mass (Da): 253.0516 pKa (strongest acidic): 5.86 pKa (strongest basic): 1.97 Partition coefficient (Log P): 0.791 Intrinsic solubility (mg mL^{-1}): -2.202 (High)	$[M+H]^+$; $[M-H]^-$	254.0594; 252.0448	156.0113; 147.0791; 108.0443; 99.0553; 93.0573	156.0124; 252.0449; 79.9574; 92.0505; 108.0454	

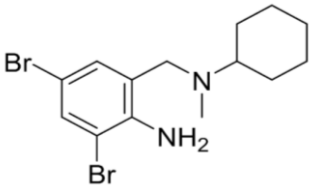
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfaquinoxaline CAS registration number: 59-40-5 ChemSpider ID: 5147 PubChem CID: 5338 	Molecular formula: $C_{14}H_{12}N_4O_2S$ Monoisotopic mass (Da): 300.0676 pKa (strongest acidic): 6.79 pKa (strongest basic): 2.13 Partition coefficient (Log P): 1.552 Intrinsic solubility (mg mL^{-1}): -2.917 (High)	$[M+H]^+$; $[M-H]^-$	301.0754; 299.0608	156.0112; 146.0712; 108.0443; 80.0495; 92.0495	299.0595; 144.0565; 142.0409; 117.0458; 115.0300	

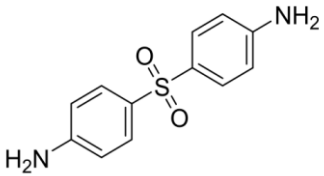
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Tetracyclines						
Chlortetracycline CAS registration number: 57-62-5 ChemSpider ID: 10469370 PubChem CID: 54675777 	Molecular formula: $C_{22}H_{23}ClN_2O_8$ Monoisotopic mass (Da): 478.1137 pKa (strongest acidic): 2.98 pKa (strongest basic): 8.88 Partition coefficient (Log P): -2.9 Intrinsic solubility (mg mL^{-1}): -2.958 (High)	$[M+H]^+$; $[M-H]^-$	479.1216; 477.1070	462.0936; 444.0832; 154.0495; 98.0603; 260.0230	392.0905; 477.1070; 169.0062; 65.9986; 194.9854	

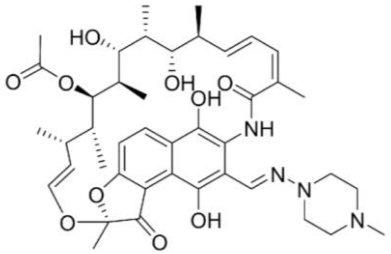
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Doxycycline CAS registration number: 564-25-0 ChemSpider ID: 10469369 PubChem CID: 54671203 	Molecular formula: $C_{22}H_{24}N_2O_8$ Monoisotopic mass (Da): 444.1527 pKa (strongest acidic): 7.45 pKa (strongest basic): 6 Partition coefficient (Log P): -0.611 Intrinsic solubility (mg mL^{-1}): -2.746 (High)	$[M+H]^+$; $[M-H]^-$	445.1605; 443.1460	428.1340; 410.1233; 98.0600; 168.0570; 154.0498	443.1460; 240.0428; 358.1296; 255.0663; 211.0411	

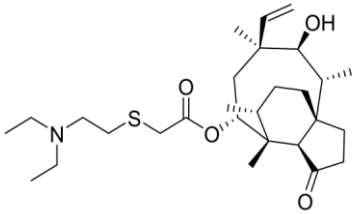
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Oxytetracycline CAS registration number: 79-57-2 ChemSpider ID: 10482174 PubChem CID: 54675779 	Molecular formula: $C_{22}H_{24}N_2O_9$ Monoisotopic mass (Da): 460.1476 pKa (strongest acidic): 3.18 pKa (strongest basic): 8.65 Partition coefficient (Log P): -4.569 Intrinsic solubility (mg mL^{-1}): -1.93 (High)	$[M+H]^+$; $[M-H]^-$	461.1555; 459.1409	426.1183; 201.0546; 212.0648; 184.0519; 145.0648	459.1409; 374.1245; 135.0452; 171.0452; 65.9985	

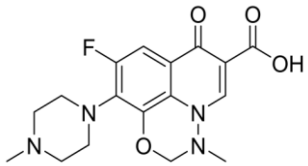
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Tetracycline CAS registration number: 60-54-8 ChemSpider ID: 10257122 PubChem CID: 54675776 	Molecular formula: $C_{22}H_{24}N_2O_8$ Monoisotopic mass (Da): 444.1527 pKa (strongest acidic): 3.25 pKa (strongest basic): 8.96 Partition coefficient (Log P): -3.499 Intrinsic solubility (mg mL^{-1}): -2.329 (High)	$[M+H]^+$; $[M-H]^-$	445.1605; 443.1460	428.1336; 410.1229; 154.0497; 445.1605; 98.0600	135.0452; 161.0244; 142.0146; 187.0765; 125.0720	

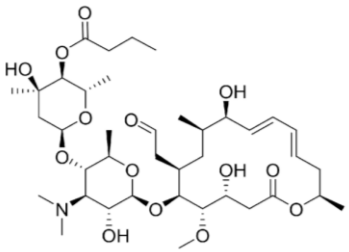
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials/Others						
Bromhexine CAS registration number: 3572-43-8 ChemSpider ID: 2348 PubChem CID: 2442 	Molecular formula: $C_{14}H_{20}Br_2N_2$ Monoisotopic mass (Da): 373.9988 pKa (strongest acidic): - pKa (strongest basic): 9.23 Partition coefficient (Log P): 4.422 Intrinsic solubility (mg mL^{-1}): -4.685 (Low)	$[M+H]^+$	375.0066	375.0066; 261.8862; 114.1277; 104.0495; 95.0491		

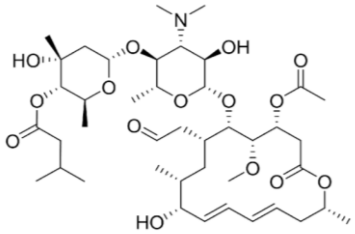
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Dapsone CAS registration number: 80-08-0 ChemSpider ID: 2849 PubChem CID: 2955 	Molecular formula: $C_{12}H_{12}N_2O_2S$ Monoisotopic mass (Da): 248.0614 pKa (strongest acidic): - pKa (strongest basic): 2.39 Partition coefficient (Log P): 1.27 Intrinsic solubility (mg mL^{-1}): -2.91 (High)	$[M+H]^+$; $[M-H]^-$	249.0692 247.0547	156.0114; 108.0444; 65.0386; 92.0495; 80.0495	79.9574; 97.0659; 107.0377; 121.0295; 95.0502	

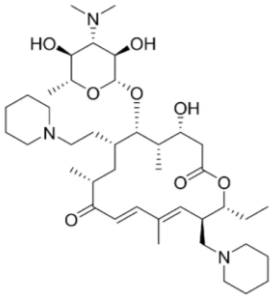
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Rifampicin CAS registration number: 13292-46-1 ChemSpider ID: 10468813 PubChem CID: 135900090 	Molecular formula: $C_{43}H_{58}N_4O_{12}$ Monoisotopic mass (Da): 822.4046 pKa (strongest acidic): 6.94 pKa (strongest basic): 7.53 Partition coefficient (Log P): 2.833 Intrinsic solubility (mg mL^{-1}): -5.484 (Low)	$[M+H]^+$; $[M-H]^-$	823.4124; 821.3979	91.0542; 95.0855; 791.3862; 151.0754; 105.0699	297.0517; 270.0408; 397.1514; 65.9985; 298.0595	

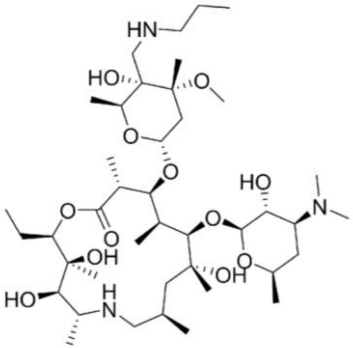
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Tiamulin CAS registration number: 55297-95-5 ChemSpider ID: 571196 PubChem CID: 656958 	Molecular formula: $C_{28}H_{47}NO_4S$ Monoisotopic mass (Da): 493.3220 pKa (strongest acidic): 14.43 pKa (strongest basic): 9.51 Partition coefficient (Log P): 4.501 Intrinsic solubility (mg mL^{-1}): -4.309 (Moderate)	$[M+H]^+$	494.3299	192.1053; 119.0161; 95.0491; 91.0542; 73.0106		

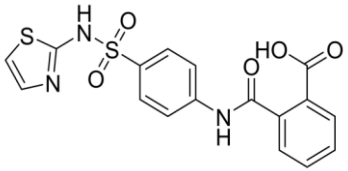
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials Prospect/Quinolones-Fluoroquinolones						
Marbofloxacin CAS registration number: 115550-35-1 ChemSpider ID: 54663 PubChem CID: 60651 	Molecular formula: $C_{17}H_{19}FN_4O_4$ Monoisotopic mass (Da): 362.1385 pKa (strongest acidic): 5.1 pKa (strongest basic): 8.38 Partition coefficient (Log P): -1.887 Intrinsic solubility (mg mL^{-1}): -2.06 (High)	$[M+H]^+$	363.1463	320.1036; 277.0615; 205.0404; 72.0807; 70.0651		

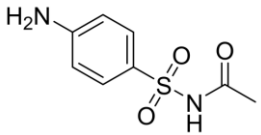
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials Prospect/Macrolides						
Leucomycin/Leucomycin A_5 CAS registration number: 18361-45-0 ChemSpider ID: 21250867 PubChem CID: 5282324 	Molecular formula: $C_{39}H_{65}NO_{14}$ Monoisotopic mass (Da): 771.4400 pKa (strongest acidic): 12.68 pKa (strongest basic): 8.51 Partition coefficient (Log P): 2.488 Intrinsic solubility (mg mL^{-1}): -2.201 (High)	$[M+H]^+$	772.4478	174.1125; 109.0648; 558.3273; 215.1278; 132.1019		

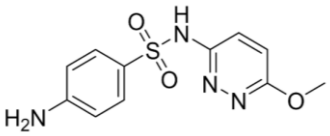
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Josamycin/Leucomycin A_3 CAS registration number: 16846-24-5 ChemSpider ID: 4445361 PubChem CID: 5282165 	Molecular formula: $C_{42}H_{69}NO_{15}$ Monoisotopic mass (Da): 827.4662 pKa (strongest acidic): 12.71 pKa (strongest basic): 8.51 Partition coefficient (Log P): 3.216 Intrinsic solubility (mg mL^{-1}): -2.608 (High)	$[M+H]^+$	828.4740	174.1125; 109.0648; 83.0491; 79.0543; 81.0699		

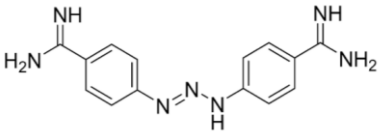
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Tildipirosin CAS registration number: 328898-40-4 ChemSpider ID: 30790722 PubChem CID: 24860548 	Molecular formula: $C_{41}H_{71}N_3O_8$ Monoisotopic mass (Da): 733.5236 pKa (strongest acidic): 12.68 pKa (strongest basic): 10.05 Partition coefficient (Log P): 4.457 Intrinsic solubility (mg mL^{-1}): -2.731 (High)	$[M+H]^+$; $[M+3H]^{3+}$	734.5314; 245.5153	561.4262; 98.0964; 73.0522; 70.0651; 116.0706		$[M+3H]^{3+}$ 281.2138; 174.1125; 98.0964; 88.0757

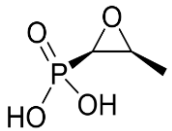
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Tulathromycin (Tulathromycin A) CAS registration number: 217500-96-4 ChemSpider ID: 8008030 PubChem CID: 9832301 	Molecular formula: $C_{41}H_{79}N_3O_{12}$ Monoisotopic mass (Da): 805.5658 pKa (strongest acidic): 12.2 pKa (strongest basic): 10.21 Partition coefficient (Log P): 2.5 Intrinsic solubility (mg mL^{-1}): -1.691 (High)	$[M+H]^+$; $[M+2H]^{2+}$; $[M+3H]^{3+}$	806.5737; 403.7905; 269.5294	577.4059; 72.0808; 158.1176; 116.1073; 98.0964		$[M+2H]^{2+}$ 230.1751; 158.1176; 116.1070; 72.0808 $[M+3H]^{3+}$ 158.1176; 72.0808; 116.0706

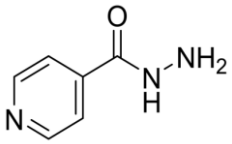
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials Prospect/ Sulfonamides						
Phthalylsulfathiazole CAS registration number: 85-73-4 ChemSpider ID: 4641 PubChem CID: 4806 	Molecular formula: $C_{17}H_{13}N_3O_5S_2$ Monoisotopic mass (Da): 403.0291 pKa (strongest acidic): 4.38 pKa (strongest basic): 0.59 Partition coefficient (Log P): 2.553 Intrinsic solubility (mg mL^{-1}): -4.801 (Low)	$[M+H]^+$; $[M-H]^-$	404.0369; 402.0224	149.0233; 256.0209; 156.0113; 108.0443; 92.0493	358.0315; 254.0066; 196.0767; 190.0447; 260.0376	

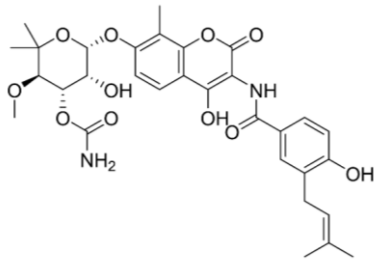
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfacetamide/N-Sulfanilylacetamide CAS registration number: 144-80-9 ChemSpider ID: 5129 PubChem CID: 5320 	Molecular formula: $C_8H_{10}N_2O_3S$ Monoisotopic mass (Da): 214.0407 pKa (strongest acidic): 5.6 pKa (strongest basic): 2.14 Partition coefficient (Log P): -0.261 Intrinsic solubility (mg mL^{-1}): -1.51 (High)	$[M+H]^+$; $[M-H]^-$	215.0485; 213.0339	215.1252; 156.0112; 108.0443; 92.0493; 68.0495	195.0223; 171.0223	

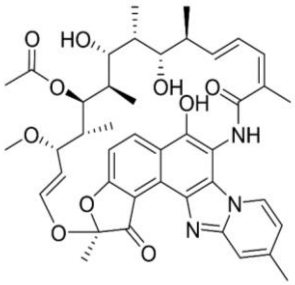
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Sulfamethoxypyridazine CAS registration number: 80-35-3 ChemSpider ID: 5139 PubChem CID: 5330 	Molecular formula: $C_{11}H_{12}N_4O_3S$ Monoisotopic mass (Da): 280.0625 pKa (strongest acidic): 6.84 pKa (strongest basic): 2.02 Partition coefficient (Log P): 0.466 Intrinsic solubility (mg mL^{-1}): -2.908 (High)	$[M+H]^+$; $[M-H]^-$	281.0703; 279.0557	156.0113; 126.0662; 108.0443; 92.0495; 126.0662	156.0123; 279.0551; 79.9574; 92.0505; 264.0322	

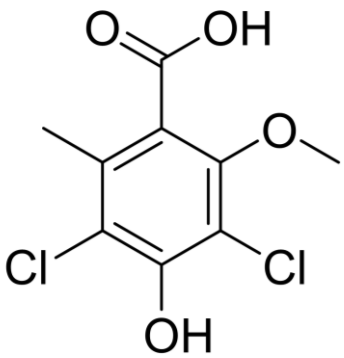
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antimicrobials Prospect/Others						
Diminazene CAS registration number: 536-71-0 ChemSpider ID: 2264 PubChem CID: 2354 	Molecular formula: $C_{14}H_{15}N_7$ Monoisotopic mass (Da): 281.1384 pKa (strongest acidic): - pKa (strongest basic): 12.07 Partition coefficient (Log P): 1.763 Intrinsic solubility (mg mL^{-1}): -4.181 (Moderate)	$[M+H]^+$; $[M-H]^-$	282.1462; 280.1316	119.0604; 237.1135	252.1244; 235.0978; 193.0760; 210.1026; 218.0713	

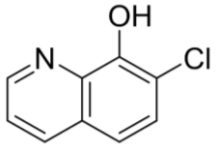
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Fosfomycin CAS registration number: 23155-02-4 ChemSpider ID: 394204 PubChem CID: 446987 	Molecular formula: $C_3H_7O_4P$ Monoisotopic mass (Da): 138.0077 pKa (strongest acidic): 1.25 pKa (strongest basic): - Partition coefficient (Log P): -0.738 Intrinsic solubility (mg mL^{-1}): 1.629 (High)	$[M+H]^+$; $[M+Ca]^+$	139.0155; 178.9781	98.9842; 121.0049; 82.9893; 109.0049		$[M+Ca]^+$ 98.9842; 121.0049; 82.9893; 109.0049

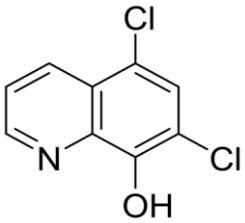
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Isoniazid CAS registration number: 54-85-3 ChemSpider ID: 3635 PubChem CID: 3767 	Molecular formula: $C_6H_7N_3O$ Monoisotopic mass (Da): 137.0584 pKa (strongest acidic): 13.61 pKa (strongest basic): 3.26 Partition coefficient (Log P): -0.69 Intrinsic solubility (mg mL^{-1}): -0.41 (High)	$[M+H]^+$	138.0662	121.0397; 109.0524; 138.0662; 79.0417; 78.0338		

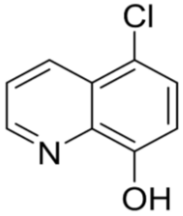
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Novobiocin CAS registration number: 303-81-1 ChemSpider ID: 10226117 PubChem CID: 54675769 	Molecular formula: $C_{31}H_{36}N_2O_{11}$ Monoisotopic mass (Da): 612.2314 pKa (strongest acidic): 5.51 pKa (strongest basic): - Partition coefficient (Log P): 3.409 Intrinsic solubility (mg mL^{-1}): -5.919 (Low)	$[M+H]^+$	613.2392	189.0910; 218.1023; 77.0386; 151.0390; 133.0284		

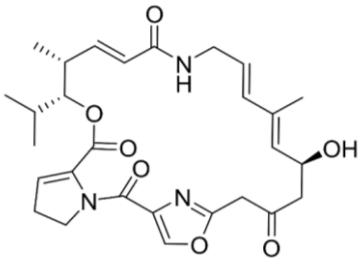
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Rifaximin CAS registration number: 80621-81-4 ChemSpider ID: 10482302 PubChem CID: 6436173 	Molecular formula: $C_{43}H_{51}N_3O_{11}$ Monoisotopic mass (Da): 785.3518 pKa (strongest acidic): 6.72 pKa (strongest basic): 5.89 Partition coefficient (Log P): 4.599 Intrinsic solubility (mg mL^{-1}): -7.704 (Low)	$[M+H]^+$; $[M-H]^-$	786.3596; 784.3451	91.0542; 95.0855; 151.0754; 754.3334; 65.0386	784.3451; 360.0987; 482.1718; 156.0567; 65.9985	

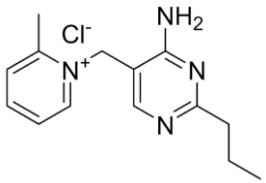
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
Antibiotic Growth Promoters						
Avilamycin (Dichloroisoeverninic acid) CAS registration number: 4101-80-8 ChemSpider ID: 10311534 PubChem CID: 21724963 	Molecular formula: $C_9H_8Cl_2O_4$ Monoisotopic mass (Da): 249.9794 pKa (strongest acidic): 3.4 pKa (strongest basic): - Partition coefficient (Log P): 2.891 Intrinsic solubility (mg mL^{-1}): -2.95 (High)	$[M+H]^-$	248.9727		204.9818; 189.9583; 174.9712; 169.0051; 233.9481	
Halquinol/Chlorhydroxyquinoline (7-Chloro-8-quinolinol) CAS registration number: 876-86-8	Molecular formula: C_9H_6ClNO Monoisotopic mass (Da): 179.0132	$[M+H]^+$	180.0211	145.0522; 162.0105; 117.0573; 127.0417; 116.0495		

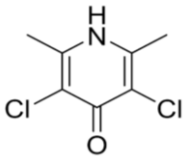
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
ChemSpider ID: 23089 PubChem CID: 24691  	pKa (strongest acidic): 8.33 pKa (strongest basic): 4.16 Partition coefficient (Log P): 2.431 Intrinsic solubility (mg mL^{-1}): -2.367 (High)					
Halquinol/Chlorhydroxyquinoline (5,7-Dichloro-8-quinolinol/Chloroxine) CAS registration number: 773-76-2	Molecular formula: $C_9H_5Cl_2NO$ Monoisotopic mass (Da): 212.9743	$[M+H]^+$	213.9821	179.0132; 164.9976; 150.0105; 122.9996; 151.0183		

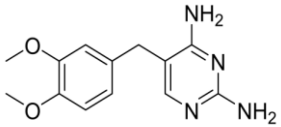
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
ChemSpider ID: 2621 PubChem CID: 2722  	pKa (strongest acidic): 7.85 pKa (strongest basic): 3.4 Partition coefficient (Log P): 3.035 Intrinsic solubility (mg mL^{-1}): -3.139 (High)					
Halquinol/Chlorhydroxyquinoline (5-Chloro-8-hydroxyquinoline) CAS registration number: 130-16-5 ChemSpider ID:	Molecular formula: C_9H_6ClNO Monoisotopic mass (Da): 179.0132	$[M+H]^+$	180.0211	145.0522; 117.0573; 162.0105; 116.0495; 127.0417		

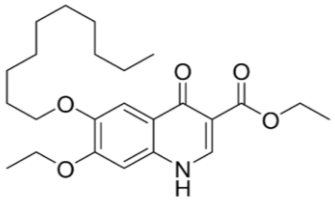
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
2715 PubChem CID: 2817  	pKa (strongest acidic): 8.77 pKa (strongest basic): 4.01 Partition coefficient (Log P): 2.431 Intrinsic solubility (mg mL^{-1}): -2.367 (High)					
Virginiamycin (Virginiamycin M_1) CAS registration number: 21411-53-0 ChemSpider ID: 10222381	Molecular formula: $C_{28}H_{35}N_3O_7$ Monoisotopic mass (Da): 525.2470	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$	526.2548; 524.2402; 548.2367	109.1016; 355.1281; 508.2439; 337.1185	245.0557; 219.0764; 420.2180; 263.0662; 206.1185	$[M+Na]^+$ 287.0638; 243.0737; 109.1012; 284.1618; 114.0550

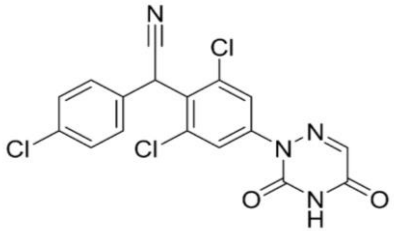
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 5459319 	pKa (strongest acidic): 13.17 pKa (strongest basic): -0.62 Partition coefficient (Log P): 2.376 Intrinsic solubility (mg mL^{-1}): -4.097 (Moderate)					
Anticoccidials						
Amprolium CAS registration number: 121-25-5	Molecular formula: $C_{14}H_{19}N_4$ Monoisotopic mass (Da): 243.1604	$[M]^+$; $[M+Na]^+$; $[M+NH_4]^+$	243.1604; 266.1502; 261.1948			$[M]^+$ 150.1026; 122.0713; 94.0651; 174.1026;

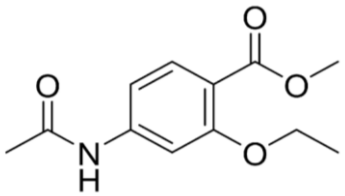
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
ChemSpider ID: 66070 PubChem CID: 73341  	pKa (strongest acidic): - pKa (strongest basic): 5.33 Partition coefficient (Log P): -2.308 Intrinsic solubility (mg mL^{-1}): The molecule cannot be neutralized and the calculation is not defined for molecules with non-zero charge					108.0556 $[M+Na]^+$ 150.1026; 122.0713; 94.0651; 174.1026; 108.0556 $[M+NH_4]^+$ 150.1026; 122.0713; 94.0651; 174.1026; 108.0556
Clopidol CAS registration number: 2971-90-6 ChemSpider ID:	Molecular formula: $C_7H_7Cl_2NO$ Monoisotopic mass (Da): 190.9899	$[M+H]^+$; $[M+Na]^+$	191.9978; 213.9797	101.0153; 86.9996; 65.0386; 72.9840; 128.0262		$[M+Na]^+$ 84.9606; 170.9613; 120.9815; 101.0153; 86.9996

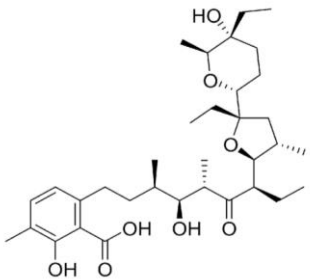
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
17084 PubChem CID: 18087 	No ionizable atoms found. pKa (strongest acidic): - pKa (strongest basic): - Partition coefficient (Log P): 1.144 Intrinsic solubility (mg mL^{-1}): -2.335 (High)					
Diaveridine CAS registration number: 5355-16-8 ChemSpider ID:	Molecular formula: $C_{13}H_{16}N_4O_2$ Monoisotopic mass (Da): 260.1268	$[M+H]^+$; $[M+Na]^+$	261.1346; 283.1166	245.1033; 123.0665; 95.0491; 81.0447; 245.1033		$[M+Na]^+$ 74.0964; 152.1182

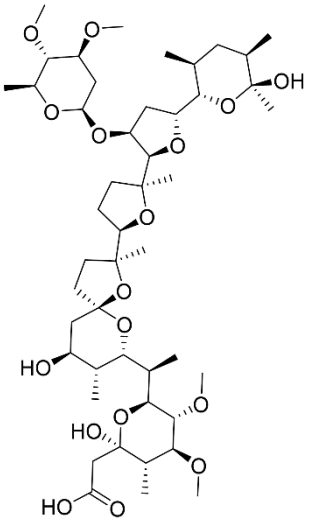
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
20162 PubChem CID: 21453  	pKa (strongest acidic): - pKa (strongest basic): 7.16 Partition coefficient (Log P): 1.442 Intrinsic solubility (mg mL^{-1}): -2.803 (High)					
Decoquinate CAS registration number: 18507-89-6 ChemSpider ID:	Molecular formula: $C_{24}H_{35}NO_5$ Monoisotopic mass (Da): 417.2510	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$	418.2588; 416.2443; 440.2407	390.2275; 222.0397; 148.0393; 121.0284; 250.0710	118.0298; 275.0799; 65.9985; 218.0095; 246.0408	$[M+Na]^+$ 321.1571; 236.0596; 130.1590; 167.9927; 261.1335

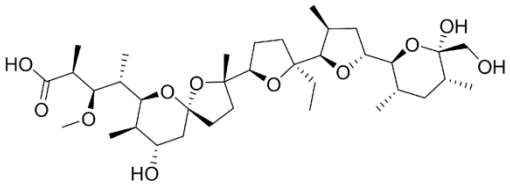
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
27081 PubChem CID: 29112 	pKa (strongest acidic): 5.82 pKa (strongest basic): - Partition coefficient (Log P): 6.164 Intrinsic solubility (mg mL^{-1}): -7.341 (Low)					
Diclazuril CAS registration number: 101831-37-2 ChemSpider ID:	Molecular formula: $C_{17}H_9Cl_3N_4O_2$ Monoisotopic mass (Da): 405.9786	$[M-H]^-$	404.9718		337.9711; 298.9783; 186.9943; 404.9718; 235.0070	

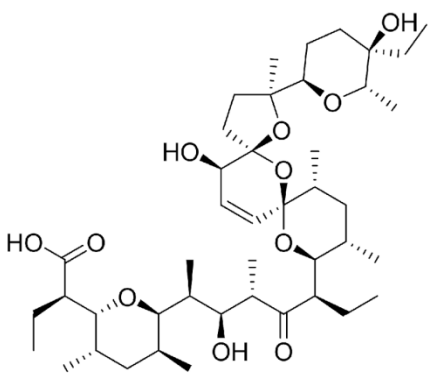
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
401855 PubChem CID: 456389 	pKa (strongest acidic): 6.5 pKa (strongest basic): - Partition coefficient (Log P): 4.234 Intrinsic solubility (mg mL^{-1}): 5.448 (Low)					
Ethopabate CAS registration number: 59-06-3 ChemSpider ID:	Molecular formula: $C_{12}H_{15}NO_4$ Monoisotopic mass (Da): 237.0996	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$	238.1074; 236.0928; 260.0893	238.1074; 136.0393; 164.0706; 206.0812	208.0604; 206.0448; 192.0291; 207.0526	$[M+Na]^+$ 147.1168; 101.0597; 182.0448; 168.0655; 196.0968

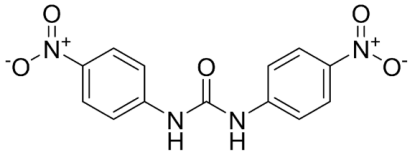
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
5812 PubChem CID: 6034 	pKa (strongest acidic): 13.31 pKa (strongest basic): - Partition coefficient (Log P): 1.414 Intrinsic solubility (mg mL^{-1}): -2.243 (High)					
Lasalocid (Lasalocid A) CAS registration number: 25999-31-9 ChemSpider ID:	Molecular formula: $C_{34}H_{54}O_8$ Monoisotopic mass (Da): 590.3813	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[M+NH_4]^+$	591.3892; 589.3746; 613.3711; 608.4157	237.1849; 337.2737; 95.0855; 133.1012; 91.0542	235.0976; 173.0972; 121.0659; 157.0659; 191.1078	$[M+Na]^+$ 377.2662; 559.3394; 557.3500; 359.2557; 481.2561

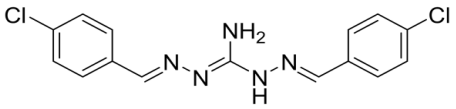
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
4514598 PubChem CID: 5360807 	pKa (strongest acidic): 2.64 pKa (strongest basic): - Partition coefficient (Log P): 7.665 Intrinsic solubility (mg mL^{-1}): -5.983 (Low)					$[M+NH_4]^+$ 237.1849; 573.3786; 91.0542; 133.1012; 95.0855
Maduramicin CAS registration number: 79356-08-4 ChemSpider ID:	Molecular formula: $C_{47}H_{80}O_{17}$ Monoisotopic mass (Da): 916.5390	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[M+NH_4]^+$	917.5468; 915.5323; 939.5288; 934.5734	877.5284; 633.4337; 451.2666; 473.2878; 433.2562	112.0530; 84.0217; 613.3593; 99.0452; 839.5162	$[M+Na]^+$ 877.5284; 451.2666; 473.2878; 433.2562; 397.1833

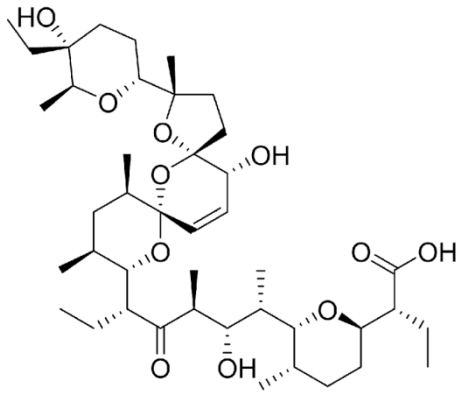
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
169976 PubChem CID: 196129 	pKa (strongest acidic): 4.01 pKa (strongest basic): - Partition coefficient (Log P): 4.774 Intrinsic solubility (mg mL^{-1}): -3.941 (High)					$[M+NH_4]^+$ 629.4047; 375.2530; 109.1012; 67.0542; 91.0542
Monensin (Monensin A) CAS registration number: 17090-79-8 ChemSpider ID:	Molecular formula: $C_{36}H_{62}O_{11}$ Monoisotopic mass (Da): 670.4287	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[M+NH_4]^+$	671.4365; 669.4219; 693.4184; 688.4630	461.2874; 479.2979; 443.2768; 501.3187; 461.2000	87.0452; 101.0608; 137.0972; 71.0502; 85.0295	$[M+Na]^+$ 675.4079; 461.2874; 581.3806; 479.2979; 443.2768

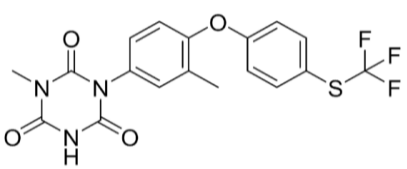
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
389937 PubChem CID: 441145 	pKa (strongest acidic): 4.24 pKa (strongest basic): - Partition coefficient (Log P): 4.816 Intrinsic solubility (mg mL^{-1}): -5.073 (Low)					$[M+NH_4]^+$ 635.4154; 461.3264; 125.0961; 149.0961; 91.0542
Narasin (Narasin A) CAS registration number: 55134-13-9 ChemSpider ID:	Molecular formula: $C_{43}H_{72}O_{11}$ Monoisotopic mass (Da): 764.5069	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[M+NH_4]^+$	765.5147; 763.5002; 787.4967; 782.5413	431.2404; 403.2455; 207.1356; 531.3316; 279.1567	255.1602; 87.0452; 69.0346; 83.0502; 99.0815	$[M+Na]^+$ 431.2424; 403.2455; 207.1356; 531.3316; 279.1567

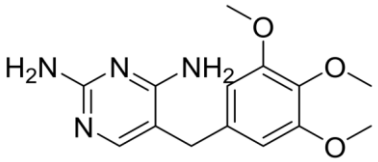
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
58911 PubChem CID: 65452 	pKa (strongest acidic): 4.5 pKa (strongest basic): - Partition coefficient (Log P): 7.877 Intrinsic solubility (mg mL^{-1}): -7.343 (Low)					$[M+NH_4]^+$ 373.2373; 91.0542; 95.0855; 165.1274; 81.0699
Nicarbazin (4,4'-Dinitrocarbanilide - DNC) CAS registration number: 587-90-6 ChemSpider ID:	Molecular formula: $C_{13}H_{10}N_4O_5$ Monoisotopic mass (Da): 302.0646	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$	303.0724; 301.0578; 325.0543	93.0573; 139.0502; 66.0464; 65.0386; 74.0151	137.0357; 107.0376; 91.0427; 65.9985; 90.0348	$[M+Na]^+$ 248.9781; 245.0067; 125.0709; 169.0346; 219.0012

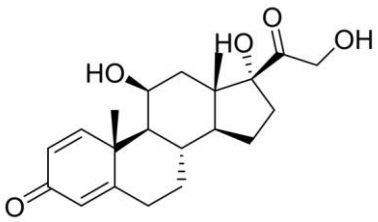
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
9137 PubChem CID: 9509 	pKa (strongest acidic): 10.99 pKa (strongest basic): - Partition coefficient (Log P): 2.999 Intrinsic solubility (mg mL^{-1}): -4.256 (Moderate)					
Robenidine CAS registration number: 25875-51-8 ChemSpider ID:	Molecular formula: $C_{15}H_{13}Cl_2N_5$ Monoisotopic mass (Da): 333.0543	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$	334.0621; 332.0475; 356.0440	138.0105; 139.0058; 155.0371; 75.0229; 140.0262	195.0443; 153.0225; 115.0302; 125.0161; 89.0397	$[M+Na]^+$ 107.0328; 133.0760; 125.0153; 218.0330

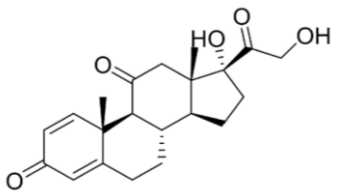
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
30671 PubChem CID: 33196  	pKa (strongest acidic): - pKa (strongest basic): 2.01 Partition coefficient (Log P): 3.985 Intrinsic solubility (mg mL^{-1}): -5.533 (Low)					
Salinomycin CAS registration number: 53003-10-4 ChemSpider ID: 2342058	Molecular formula: $C_{42}H_{70}O_{11}$ Monoisotopic mass (Da): 750.4913	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[M+NH_4]^+$	751.4991; 749.4845; 773.4810; 768.5256	431.2474; 265.1410; 207.1356; 91.0542; 67.0542	241.1434; 407.2428; 337.2010; 221.1172; 259.1540	$[M+Na]^+$ 431.2474; 265.1410; 207.1356; 91.0542; 530.3155

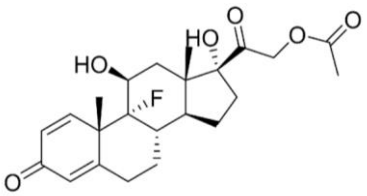
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 3085092 	pKa (strongest acidic): 4.45 pKa (strongest basic): - Partition coefficient (Log P): 7.512 Intrinsic solubility (mg mL^{-1}): -6.995 (Low)					$[M+NH_4]^+$ 225.1485; 91.0542; 67.0542; 81.0699; 165.1274
Toltrazuril CAS registration number: 69004-03-1 ChemSpider ID:	Molecular formula: $C_{18}H_{14}F_3N_3O_4S$ Monoisotopic mass (Da): 425.0652	$[M+H]^+$; $[M-H]^-$	426.0730; 424.0584	192.9929; 348.0700 325.1057; 283.0399; 148.0393	316.9813; 404.9767; 213.0919; 138.0274; 424.4000	

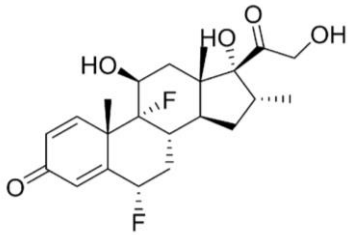
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
61859 PubChem CID: 68591  	pKa (strongest acidic): 7.42 pKa (strongest basic): - Partition coefficient (Log P): 5.053 Intrinsic solubility (mg mL^{-1}): -6.816 (Low)					
Trimethoprim CAS registration number: 738-70-5 ChemSpider ID:	Molecular formula: $C_{14}H_{18}N_4O_3$ Massa monoisotópica (Da): 290.1373	$[M+H]^+$	291.1452	275.1137; 261.0982; 245.1033; 81.0447; 123.0665		

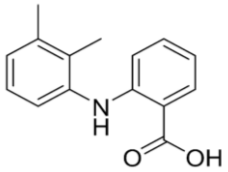
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
5376 PubChem CID: 5578 	pKa (strongest acidic): - pKa (strongest basic): 7.16 Partition coefficient (Log P): 1.284 Intrinsic solubility (mg mL^{-1}): -2.801 (High)					
Anti-inflammatories/Steroidal						
Prednisolone CAS registration number: 50-24-8	Molecular formula: $C_{21}H_{28}O_5$ Monoisotopic mass (Da): 360.1931	$[M+H]^+$	361.2010	343.1901; 147.0804; 121.0648; 91.0542; 325.1798		

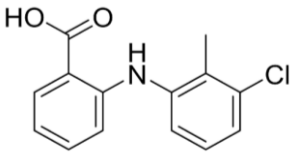
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
ChemSpider ID: 5552 PubChem CID: 5755 	pKa (strongest acidic): 12.59 pKa (strongest basic): - Partition coefficient (Log P): 1.273 Intrinsic solubility (mg mL^{-1}): -3.46 (High)					
Prednisone CAS registration number: 53-03-2 ChemSpider ID: 5656	Molecular formula: $C_{21}H_{26}O_5$ Monoisotopic mass (Da): 358.1775	$[M+H]^+$; $[M-H]^-$	359.1853; 357.1708	147.0804; 91.0542; 359.1853; 341.1747; 237.1271	327.1602; 123.0452; 149.0608; 122.0373; 121.0659	

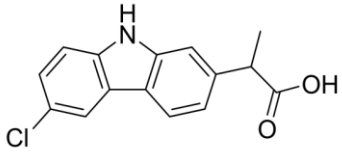
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 5865 	pKa (strongest acidic): 12.58 pKa (strongest basic): - Partition coefficient (Log P): 1.659 Intrinsic solubility (mg mL^{-1}): -3.379 (High)					
Anti-inflammatories Prospect/Steroidal						
Isoflupredone acetate/9-Fluoroprednisolone acetate CAS registration number:	Molecular formula: $C_{23}H_{29}FO_6$ Monoisotopic mass (Da): 420.1943	$[M+H]^+$	421.2021	341.1747; 91.0542; 147.0804; 265.1587; 121.0648		

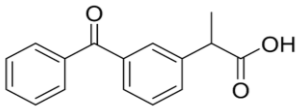
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
338-98-7 ChemSpider ID: 194836 PubChem CID: 224246 	pKa (strongest acidic): 12.57 pKa (strongest basic): - Partition coefficient (Log P): 1.758 Intrinsic solubility (mg mL^{-1}): -3.834 (High)					
Flumetasone CAS registration number: 2135-17-3 ChemSpider ID: 15632	Molecular formula: $C_{22}H_{28}F_2O_5$ Monoisotopic mass (Da): 410.1899 pKa (strongest acidic):	$[M+H]^+$	411.1978	121.0648; 253.1223; 91.0542; 391.1915; 95.0491		

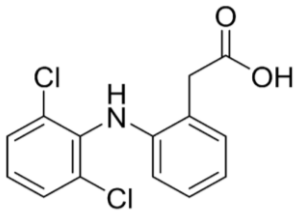
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
	12.42					
PubChem CID: 16490	pKa (strongest basic): -					
	Partition coefficient (Log P): 1.342					
	Intrinsic solubility (mg mL^{-1}): -3.918 (Moderate)					
Anti-Inflammatory/Non-Steroidal						
Mefenamic acid	Molecular formula: $C_{15}H_{15}NO_2$	$[M+H]^+$; $[M-H]^-$	242.1176; 240.1030	224.1070; 209.0835; 180.0808;	196.1132; 192.0819; 180.0819;	
CAS registration number: 61-68-7	Monoisotopic mass (Da): 241.1097			208.0757; 181.0886	194.0975; 179.0866	
ChemSpider ID:						

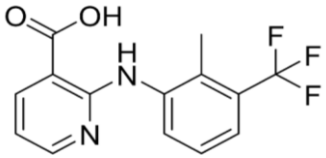
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
3904 PubChem CID: 4044 	pKa (strongest acidic): 2.47 pKa (strongest basic): 5.04 Partition coefficient (Log P): 4.402 Intrinsic solubility (mg mL^{-1}): -4.068 (Moderate)					
Tolfenamic acid CAS registration number: 13710-19-5 ChemSpider ID: 3904	Molecular formula: $C_{14}H_{12}ClNO_2$ Monoisotopic mass (Da): 261.0551 pKa (strongest acidic): 4.17	$[M+H]^+$; $[M-H]^-$	262.0629; 260.0484	180.0804; 229.0281; 244.0517; 209.0837; 208.0763	216.0575; 228.0211; 242.0367; 107.0496	

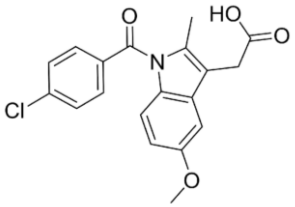
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 610479 	pKa (strongest basic): 1.8 Partition coefficient (Log P): 5.488 Intrinsic solubility (mg mL^{-1}): -4.301 (Moderate)					
Carprofen CAS registration number: 53716-49-7 ChemSpider ID: 2483	Molecular formula: $C_{15}H_{12}ClNO_2$ Monoisotopic mass (Da): 273.0551 pKa (strongest acidic): 4.11	$[M-H]^-$	272.0484		228.0586; 226.0429; 190.0662; 188.0506; 162.0349	

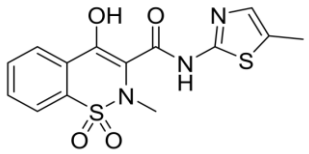
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 2581  	pKa (strongest basic): - Partition coefficient (Log P): 3.876 Intrinsic solubility (mg mL^{-1}): -4.876 (Low)					
Ketoprofen CAS registration number: 22071-15-4 ChemSpider ID: 3693	Molecular formula: $C_{16}H_{14}O_3$ Monoisotopic mass (Da): 254.0938 pKa (strongest acidic): 4	$[M+H]^+$; $[M-H]^-$	255.1016; 253.0870	105.0335; 209.0961; 95.0491; 255.1016; 105.0447	197.0608; 185.0608; 169.0660; 209.0961; 194.0726	

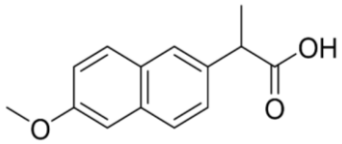
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 3825  	pKa (strongest basic): - Partition coefficient (Log P): 3.613 Intrinsic solubility (mg mL^{-1}): -3.854 (Moderate)					
Diclofenac CAS registration number: 15307-86-5 ChemSpider ID: 2925	Molecular formula: $C_{14}H_{11}Cl_2NO_2$ Monoisotopic mass (Da): 295.0161 pKa (strongest acidic): 4.01	$[M+H]^+$; $[M-H]^-$	296.0240; 294.0094	214.0418; 215.0496; 250.0185; 169.0648; 278.0134	250.0185; 214.0418; 178.0651	

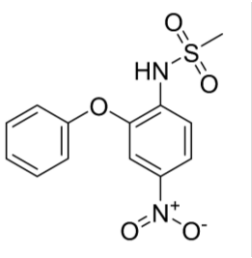
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 3033 	pKa (strongest basic): -1.08 Partition coefficient (Log P): 4.259 Intrinsic solubility (mg mL^{-1}): -4.298 (Moderate)					
Flunixin CAS registration number: 38677-85-9 ChemSpider ID: 34911	Molecular formula: $C_{14}H_{11}F_3N_2O_2$ Monoisotopic mass (Da): 296.0767 pKa (strongest acidic): 0.89	$[M+H]^+$; $[M-H]^-$	297.0845; 295.0700	279.0737; 277.0782; 264.0505; 259.0675; 236.0556	251.0802; 209.0520; 189.0458; 138.0349; 74.0037	

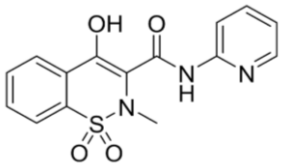
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 38081 	pKa (strongest basic): 5.37 Partition coefficient (Log P): 3.458 Intrinsic solubility (mg mL^{-1}): -3.995 (Moderate)					
Indomethacin CAS registration number: 53-86-1 ChemSpider ID: 3584	Molecular formula: $C_{19}H_{16}ClNO_4$ Monoisotopic mass (Da): 357.0762 pKa (strongest acidic): 4.38	$[M+H]^+$; $[M-H]^-$	358.0841; 356.0695	138.9945; 139.0053; 75.0229; 74.0151; 174.0913	312.0797; 297.0562; 282.0328; 158.0611; 252.0222	

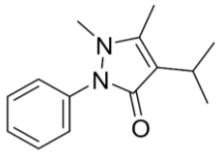
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 3715  	pKa (strongest basic): - Partition coefficient (Log P): 3.53 Intrinsic solubility (mg mL^{-1}): -4.252 (Moderate)					
Meloxicam CAS registration number: 71125-38-7 ChemSpider ID: 10442740	Molecular formula: $C_{14}H_{13}N_3O_4S_2$ Monoisotopic mass (Da): 351.0342 pKa (strongest acidic): 4.87	$[M+H]^+$; $[M-H]^-$	352.0420; 350.0275	115.0324; 68.9793; 73.0106; 141.0117; 88.0215	146.0610; 286.0656; 113.0179; 119.0502; 97.9944	

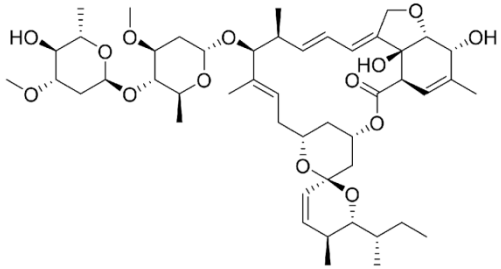
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 54677470 	pKa (strongest basic): 0.47 Partition coefficient (Log P): 1.329 Intrinsic solubility (mg mL^{-1}): -3.947 (Moderate)					
Naproxen CAS registration number: 22204-53-1 ChemSpider ID: 137720	Molecular formula: $C_{14}H_{14}O_3$ Monoisotopic mass (Da): 230.0938 pKa (strongest acidic): 4.24	$[M+H]^+$; $[M-H]^-$	231.1016; 229.0870	185.0961; 170.0726; 141.0699; 154.0777; 153.0699	169.0659; 170.0737; 139.0553; 141.0710; 115.0553	

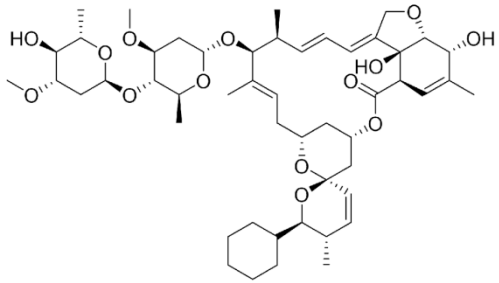
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 156391  	pKa (strongest basic): - Partition coefficient (Log P): 2.986 Intrinsic solubility (mg mL^{-1}): -3.447 (High)					
Nimesulide CAS registration number: 51803-78-2 ChemSpider ID: 4339	Molecular formula: $C_{13}H_{12}N_2O_5S$ Monoisotopic mass (Da): 308.0461 pKa (strongest acidic): 6.56	$[M-H]^-$	307.0394		307.0394; 229.0619; 198.0561; 122.0248; 78.9859	

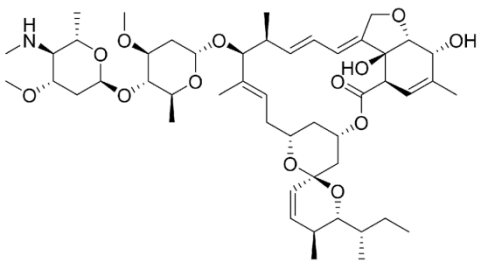
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 4495 	pKa (strongest basic): - Partition coefficient (Log P): 1.787 Intrinsic solubility (mg mL^{-1}): -3.654 (High)					
Piroxycam CAS registration number: 36322-90-4 ChemSpider ID: 10442653	Molecular formula: $C_{15}H_{13}N_3O_4S$ Monoisotopic mass (Da): 331.0621 pKa (strongest acidic): 5.06	$[M+H]^+$	332.0700	96.0444; 95.0604; 136.0867; 121.0396; 78.0338		

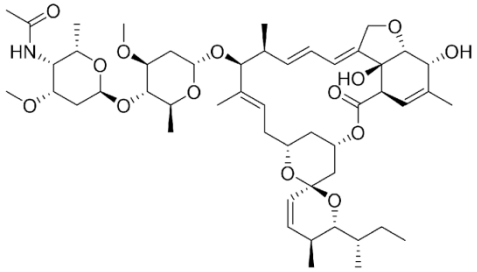
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 54676228 	pKa (strongest basic): 3.89 Partition coefficient (Log P): 0.39 Intrinsic solubility (mg mL^{-1}): -3.269 (High)					
Propyphenazone CAS registration number: 479-92-5 ChemSpider ID: 3646 PubChem CID:	Molecular formula: $C_{14}H_{18}N_2O$ Monoisotopic mass (Da): 230.1414 pKa (strongest acidic): -	$[M+H]^+$	231.1492	146.0964; 189.1022; 112.1121; 95.0491; 82.0651		

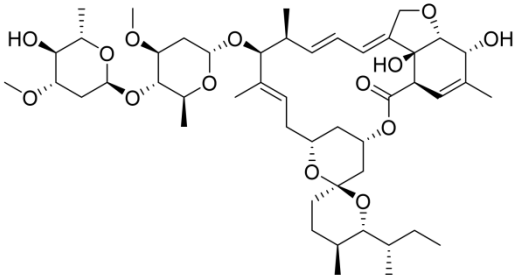
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
3778 	pKa (strongest basic): 0.67 Partition coefficient (Log P): 2.074 Intrinsic solubility (mg mL^{-1}): -2.757 (High)					
Antiparasitic *Avermectin B_{1a}/Abamectin B_{1a}* CAS registration number: 65195-55-3 ChemSpider ID:	Molecular formula: $C_{48}H_{72}O_{14}$ Monoisotopic mass (Da): 872.4917	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$; $[M+NH_4]^+$	873.4995; 871.4849; 895.4814; 890.5260	69.0335; 145.0859; 113.0597; 305.2111; 193.1587	229.1081; 85.0295; 84.0217; 67.0189; 835.4638	$[M+Na]^+$ 69.0335; 145.0859; 113.0597; 305.2111; 193.1587

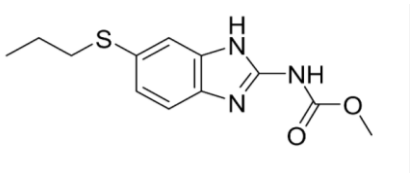
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
10286553 PubChem CID: 66434889 	pKa (strongest acidic): 12.47 pKa (strongest basic): - Partition coefficient (Log P): 5.848 Intrinsic solubility (mg mL^{-1}): -4.844 (Moderate)					$[M+NH_4]^+$ 305.2111; 113.0597; 69.0335; 95.0491; 145.0859
Doramectin CAS registration number: 117704-25-3 ChemSpider ID: 8008478	Molecular formula: $C_{50}H_{74}O_{14}$ Monoisotopic mass (Da): 898.5073 pKa (strongest acidic): 12.47	$[M+H]^+$; $[M+Na]^+$; $[M+NH_4]^+$	899.5151; 921.4971; 916.5417	331.2268; 593.3473; 67.0542		

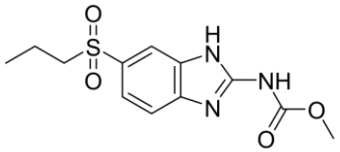
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 9832750 	pKa (strongest basic): - Partition coefficient (Log P): 6.274 Intrinsic solubility (mg mL^{-1}): -5.467 (Low)					
Emamectin (Emamectin B_{1a}) CAS registration number: 119791-41-2 ChemSpider ID: 9311801	Molecular formula: $C_{49}H_{75}NO_{13}$ Monoisotopic mass (Da): 885.5233 pKa (strongest acidic): 12.47	$[M+H]^+$; $[M-H]^-$	886.5311; 884.5166	158.1176; 82.0651; 67.0417; 126.0913; 91.0542	242.1398; 84.0217; 97.0659; 848.4954; 840.5267	

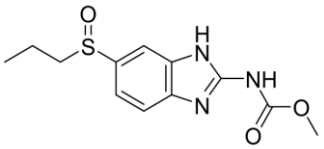
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 11549937 	pKa (strongest basic): - Partition coefficient (Log P): 6.724 Intrinsic solubility (mg mL^{-1}): -0.079 (High)					
Eprinomectin (Eprinomectin B_{1a}) CAS registration number: 133305-88-1 ChemSpider ID: 16736607 PubChem CID:	Molecular formula: $C_{50}H_{75}NO_{14}$ Monoisotopic mass (Da): 913.5182 pKa (strongest acidic): 12.49	$[M+H]^+$; $[M+Na]^+$	914.5260; 936.5080	186.1125; 112.0757; 154.0863; 68.0495; 67.0542		$[M+Na]^+$ 186.1125; 112.0757; 154.0863; 68.0495; 67.0542

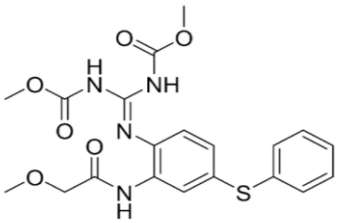
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
6444397 	pKa (strongest basic): -1.34 Partition coefficient (Log P): 5.56 Intrinsic solubility (mg mL^{-1}): -4.915 (Moderate)					
Ivermectin B_{1a}/22,23-Dihydroavermectin B_1 CAS registration number: 70288-86-7 ChemSpider ID: 7988461	Molecular formula: $C_{48}H_{74}O_{14}$ Monoisotopic mass (Da): 874.5073 pKa (strongest acidic): 12.47	$[M+H]^+$; $[M+Na]^+$; $[M+NH_4]^+$	875.5151; 897.4971; 892.5417	569.3473; 307.2268; 714.4337; 570.3551		$[M+Na]^+$ 713.4259; 569.3473; 307.2268; 714.4337; 570.3551 $[M+NH_4]^+$

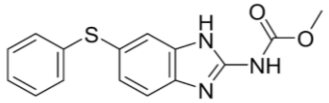
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 6321424 	pKa (strongest basic): - Partition coefficient (Log P): 5.826 Intrinsic solubility (mg mL^{-1}): 1.957 (High)					569.3473; 307.2268; 95.0491; 113.0597; 69.0335
Albendazole CAS registration number: 54965-21-8 ChemSpider ID: 1998 PubChem CID: 2082	Molecular formula: $C_{12}H_{15}N_3O_2S$ Monoisotopic mass (Da): 265.0880 pKa (strongest acidic): 9.68	$[M+H]^+$; $[M-H]^-$	266.0958; 264.0812	234.0692; 192.0224; 159.0427; 191.0148; 131.0478	189.0002; 232.0550; 159.9975; 161.0053; 81.9757	

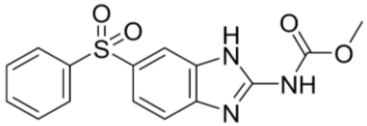
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
	pKa (strongest basic): 4.21 Partition coefficient (Log P): 3.205 Intrinsic solubility (mg mL^{-1}): -4.382 (Moderate)					
Albendazole metabolite (Albendazole sulfone) CAS registration number: 75184-71-3 ChemSpider ID: 48031	Molecular formula: $C_{12}H_{15}N_3O_4S$ Monoisotopic mass (Da): 297.0778 pKa (strongest acidic): 8.72	$[M+H]^+$; $[M-H]^-$	298.0856; 296.0711	266.0591; 131.0478; 224.0122; 159.0424; 191.0325	264.0448; 157.0282; 129.0332; 115.0301; 133.0282	

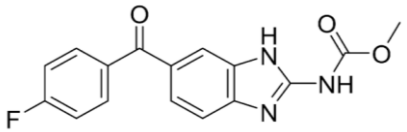
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 53174 	pKa (strongest basic): 2.74 Partition coefficient (Log P): 1.673 Intrinsic solubility (mg mL^{-1}): -3.437 (High)					
Albendazole metabolite (Albendazole sulfoxide) CAS registration number: 54029-12-8 ChemSpider ID: 75767	Molecular formula: $C_{12}H_{15}N_3O_3S$ Monoisotopic mass (Da): 281.0829 pKa (strongest acidic): 9.26	$[M+H]^+$; $[M-H]^-$	282.0907; 280.0761	240.0435; 208.0174; 191.0688; 159.0427; 191.0148	204.9951; 248.0499; 173.0231; 129.0332; 65.0145	

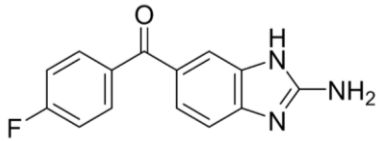
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 83969 	pKa (strongest basic): 3.58 Partition coefficient (Log P): 1.566 Intrinsic solubility (mg mL^{-1}): -3.389 (High)					
Febantel CAS registration number: 58306-30-2 ChemSpider ID: 4514715 PubChem CID:	Molecular formula: $C_{20}H_{22}N_4O_6S$ Monoisotopic mass (Da): 446.1255 pKa (strongest acidic): 9.48	$[M+H]^+$; $[M-H]^-$	447.1333; 445.1187	415.1071; 383.0809; 280.0539; 116.0369; 109.0106	298.0643; 266.0393; 189.0001; 159.9975; 161.0053	

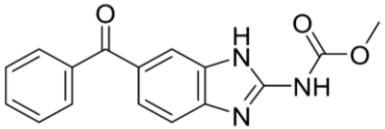
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
135449328 	pKa (strongest basic): - Partition coefficient (Log P): 3.166 Intrinsic solubility (mg mL^{-1}): -4.682 (Low)					
Fenbendazole CAS registration number: 43210-67-9 ChemSpider ID: 3217 PubChem CID:	Molecular formula: $C_{15}H_{13}N_3O_2S$ Monoisotopic mass (Da): 299.0723 pKa (strongest acidic): 9.59	$[M+H]^+$; $[M-H]^-$	300.0801; 298.0656	268.0536; 190.0068; 159.0426; 109.0106; 131.0478	266.0394; 189.0002; 159.9975; 161.0053; 81.9757	

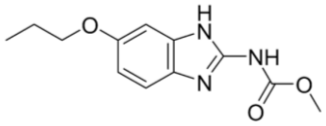
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
3334 	pKa (strongest basic): 4.06 Partition coefficient (Log P): 3.99 Intrinsic solubility (mg mL^{-1}): -5.36 (Low)					
Fenbendazole metabolite (Fenbendazole sulfone) CAS registration number: 54029-20-8 ChemSpider ID: 142389 PubChem CID:	Molecular formula: $C_{15}H_{13}N_3O_4S$ Monoisotopic mass (Da): 331.0621 pKa (strongest acidic): 8.79	$[M+H]^+$; $[M-H]^-$	332.0700; 330.0554	300.0437; 159.0427; 131.0478; 104.0369; 77.0260	298.0292; 160.0152; 129.0332; 115.0301; 106.0173	

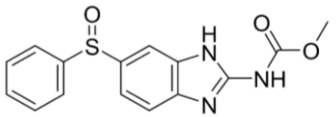
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
162136 	pKa (strongest basic): 2.82 Partition coefficient (Log P): 2.756 Intrinsic solubility (mg mL^{-1}): -4.397 (Moderate)					
Flubendazole CAS registration number: 31430-15-6 ChemSpider ID: 32932 PubChem CID:	Molecular formula: $C_{16}H_{12}FN_3O_3$ Monoisotopic mass (Da): 313.0857 pKa (strongest acidic): 9.17	$[M+H]^+$	314.0936	74.0150; 282.0673; 123.0241; 123.0353; 75.0229		

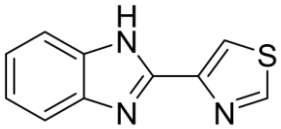
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
35802 	pKa (strongest basic): 3.42 Partition coefficient (Log P): 3.403 Intrinsic solubility (mg mL^{-1}): -5.207 (Low)					
Flubendazole metabolite (2-Aminoflubendazole) CAS registration number: 82050-13-3 ChemSpider ID: 22797878	Molecular formula: $C_{14}H_{10}FN_3O$ Monoisotopic mass (Da): 255.0802 pKa (strongest acidic): 12.01	$[M+H]^+$	256.0881	256.0881; 123.0241; 113.0396; 123.0353; 75.0229		

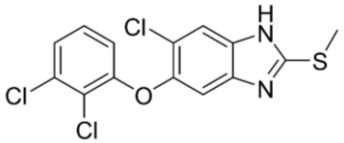
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 57358774 	pKa (strongest basic): 6.35 Partition coefficient (Log P): 2.717 Intrinsic solubility (mg mL^{-1}): -4.857 (Low)					
Mebendazole CAS registration number: 31431-39-7 ChemSpider ID: 3890 PubChem CID:	Molecular formula: $C_{16}H_{13}N_3O_3$ Monoisotopic mass (Da): 295.0951 pKa (strongest acidic): 9.17	$[M+H]^+$; $[M-H]^-$	296.1030; 294.0884	264.0768; 130.0400; 104.0369; 95.0491; 105.0447	262.0622; 129.0332; 115.0302; 160.0152; 106.0173	

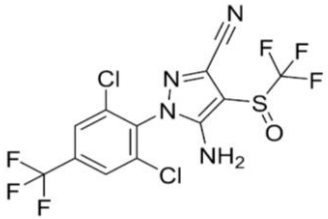
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
4030 	pKa (strongest basic): 3.42 Partition coefficient (Log P): 3.26 Intrinsic solubility (mg mL^{-1}): -4.937 (Low)					
Oxibendazole CAS registration number: 20559-55-1 ChemSpider ID: 4461 PubChem CID:	Molecular formula: $C_{12}H_{15}N_3O_3$ Monoisotopic mass (Da): 249.1108 pKa (strongest acidic): 10	$[M+H]^+$	250.1186	218.0924; 176.0455; 148.0505; 81.0335; 80.0495		

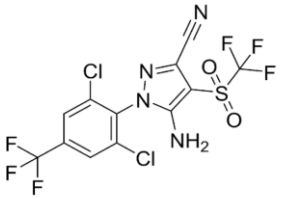
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
4622 	pKa (strongest basic): 4.73 Partition coefficient (Log P): 2.522 Intrinsic solubility (mg mL^{-1}): -3.412 (High)					
Oxfendazole CAS registration number: 53716-50-0 ChemSpider ID: 37316 PubChem CID:	Molecular formula: $C_{15}H_{13}N_3O_3S$ Monoisotopic mass (Da): 315.0672 pKa (strongest acidic): 9.26	$[M+H]^+$; $[M-H]^-$	316.0750; 314.0605	284.0488; 191.0689; 223.0576; 299.0723; 159.0427	282.0332; 204.9954; 237.0203; 173.0233	

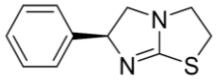
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
40854 	pKa (strongest basic): 3.57 Partition coefficient (Log P): 2.615 Intrinsic solubility (mg mL^{-1}): -4.359 (Moderate)					
Thiabendazole CAS registration number: 148-79-8 ChemSpider ID: 5237 PubChem CID:	Molecular formula: $C_{10}H_7N_3S$ Monoisotopic mass (Da): 201.0355 pKa (strongest acidic): 10.28	$[M+H]^+$	202.0433	175.0324; 131.0604; 65.0386; 92.0495; 104.0495		

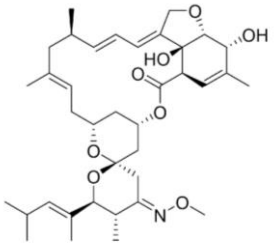
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
5430 	pKa (strongest basic): 4.08 Partition coefficient (Log P): 2.329 Intrinsic solubility (mg mL^{-1}): -3.097 (High)					
Triclabendazole CAS registration number: 68786-66-3 ChemSpider ID: 45565 PubChem CID: 50248	Molecular formula: $C_{14}H_9Cl_3N_2OS$ Monoisotopic mass (Da): 357.9496 pKa (strongest acidic): 10.46	$[M+H]^+$; $[M-H]^-$	358.9574; 356.9428	343.9339; 273.9962; 198.9727; 170.9779; 242.0241	196.9582; 65.9986; 341.9194; 211.9817; 152.9861	

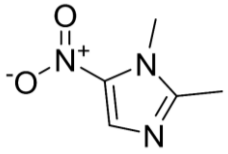
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
	pKa (strongest basic): 4.54 Partition coefficient (Log P): 5.884 Intrinsic solubility (mg mL^{-1}): -7.325 (Low)					
Fipronil CAS registration number: 120068-37-3 ChemSpider ID: 3235 PubChem CID:	Molecular formula: $C_{12}H_4Cl_2F_6N_4OS$ Monoisotopic mass (Da): 435.9382 pKa (strongest acidic): -	$[M-H]^-$	434.9314		329.9596; 349.9585; 183.0176; 163.0113; 143.0051	

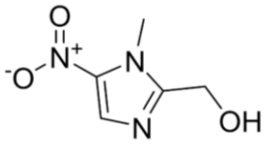
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
3352 	pKa (strongest basic): 0.18 Partition coefficient (Log P): 4.489 Intrinsic solubility (mg mL^{-1}): -5.959 (Low)					
Fipronil metabolite (Fipronil sulfone) CAS registration number: 120068-36-2 ChemSpider ID: 2336427	Molecular formula: $C_{12}H_4Cl_2F_6N_4O_2S$ Monoisotopic mass (Da): 451.9331 pKa (strongest acidic): -	$[M-H]^-$	450.9263		414.9497; 281.9923; 243.9894; 218.0097; 148.0077	

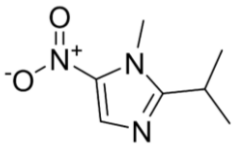
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 3078139 	pKa (strongest basic): -0.45 Partition coefficient (Log P): 4.596 Intrinsic solubility (mg mL^{-1}): -5.967 (Low)					
Levamisole CAS registration number: 14769-73-4 ChemSpider ID: 25037	Molecular formula: $C_{11}H_{12}N_2S$ Monoisotopic mass (Da): 204.0716 pKa (strongest acidic): -	$[M+H]^+$	205.0794	178.0685; 91.0542; 123.0263; 118.0651; 117.0699		

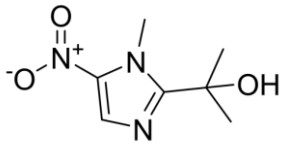
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 26879 	pKa (strongest basic): 11.58 Partition coefficient (Log P): 2.358 Intrinsic solubility (mg mL^{-1}): -3.223 (High)					
Moxidectin CAS registration number: 113507-06-5 ChemSpider ID: 22901017	Molecular formula: $C_{37}H_{53}NO_8$ Monoisotopic mass (Da): 639.3766 pKa (strongest acidic): 12.55	$[M+H]^+$; $[M-H]^-$; $[M+Na]^+$	640.3844; 638.3698; 662.3663	91.0542; 528.2956; 98.0600; 199.1117; 498.2847	528.2956	

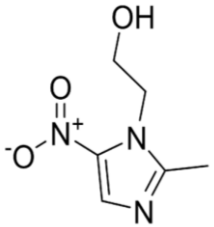
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 16760141 	pKa (strongest basic): 2.01 Partition coefficient (Log P): 5.67 Intrinsic solubility (mg mL^{-1}): -6.539 (Low)					
Dimetridazole CAS registration number: 551-92-8 ChemSpider ID: 2980	Molecular formula: $C_5H_7N_3O_2$ Monoisotopic mass (Da): 141.0533 pKa (strongest acidic): -	$[M+H]^+$	142.0611	112.0631; 95.0604; 81.0447; 97.0396; 96.0682		

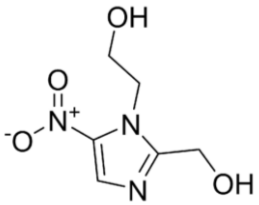
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 3090 	pKa (strongest basic): 2.9 Partition coefficient (Log P): 0.231 Intrinsic solubility (mg mL^{-1}): -0.286 (High)					
Dimetridazole metabolite (Hydroxydimetridazole/HMMNI) CAS registration number: 936-05-0 ChemSpider ID:	Molecular formula: $C_5H_7N_3O_3$ Monoisotopic mass (Da): 157.0482 pKa (strongest acidic): 13.8	$[M+H]^+$	158.0560	140.0455; 66.0338; 69.0447; 67.0417; 94.0525		

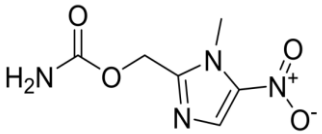
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
484517 PubChem CID: 557356 	pKa (strongest basic): 1.36 Partition coefficient (Log P): -0.586 Intrinsic solubility (mg mL^{-1}): 0.103 (High)					
Ipronidazole CAS registration number: 14885-29-1 ChemSpider ID: 25097 PubChem CID:	Molecular formula: $C_7H_{11}N_3O_2$ Monoisotopic mass (Da): 169.0846 pKa (strongest acidic): -	$[M+H]^+$	170.0924	109.0760; 84.0808; 124.0995; 96.0682; 125.0709		

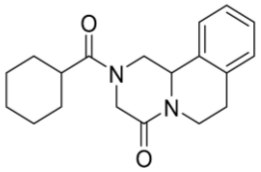
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
26951 	pKa (strongest basic): 2.66 Partition coefficient (Log P): 1.474 Intrinsic solubility (mg mL^{-1}): -1.173 (High)					
Ipronidazole metabolite (Hydroxy Ipronidazole) CAS registration number: 35175-14-5 ChemSpider ID: 520172	Molecular formula: $C_7H_{11}N_3O_3$ Monoisotopic mass (Da): 185.0795 pKa (strongest acidic): 13.54	$[M+H]^+$	186.0873	168.0767; 82.0651; 186.0873; 121.0760; 138.0788		

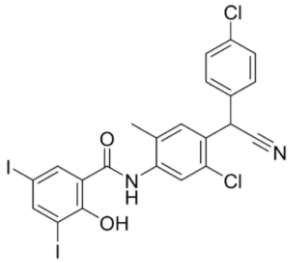
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 598402  	pKa (strongest basic): 1.4 Partition coefficient (Log P): 0.415 Intrinsic solubility (mg mL^{-1}): -0.751 (High)					
Metronidazole CAS registration number: 443-48-1 ChemSpider ID: 4029	Molecular formula: $C_6H_9N_3O_3$ Monoisotopic mass (Da): 171.0638 pKa (strongest acidic): 15.42	$[M+H]^+$	172.0717	128.0455; 82.0525; 81.0447; 111.0427; 98.0475		

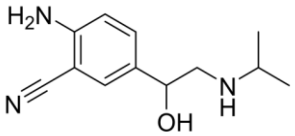
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 4173  	pKa (strongest basic): 2.81 Partition coefficient (Log P): -0.459 Intrinsic solubility (mg mL^{-1}): -0.16 (High)					
Metronidazole metabolite (Hydroxymetronidazole) CAS registration number: 4812-40-2 ChemSpider ID: 108713	Molecular formula: $C_6H_9N_3O_4$ Monoisotopic mass (Da): 187.0588 pKa (strongest acidic): 13.77	$[M+H]^+$	188.0666	144.0405; 126.0298; 123.0554; 68.0495; 80.0369		

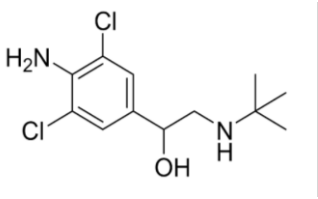
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 121858  	pKa (strongest basic): 1.27 Partition coefficient (Log P): -1.277 Intrinsic solubility (mg mL^{-1}): 0.237 (High)					
Ronidazole/1-Methyl-2-carbamoyloxymethyl-5-nitroimidazole CAS registration number: 7681-76-7 ChemSpider ID: 4915	Molecular formula: $C_6H_8N_4O_4$ Monoisotopic mass (Da): 200.0540 pKa (strongest acidic): 13.97	$[M+H]^+$; $[M+Na]^+$	201.0618; 223.0438	140.0455; 67.0417; 66.0338; 110.0475; 94.0525		$[M+Na]^+$ 199.9941; 144.9883; 162.9988

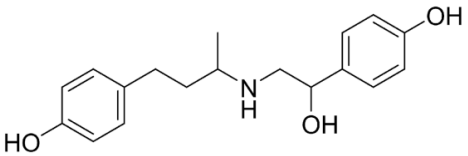
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 5094 	pKa (strongest basic): 1.34 Partition coefficient (Log P): -0.479 Intrinsic solubility (mg mL^{-1}): -0.46 (High)					
Praziquantel CAS registration number: 55268-74-1 ChemSpider ID: 4722 PubChem CID: 4891	Molecular formula: $C_{19}H_{24}N_2O_2$ Monoisotopic mass (Da): 312.1832 pKa (strongest acidic): - pKa (strongest basic): -0.6	$[M+H]^+$	313.1911	203.1179; 174.0913; 132.0808; 129.0699; 83.0855		

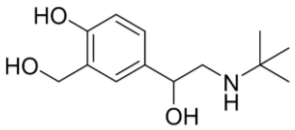
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
	Partition coefficient (Log P): 2.302 Intrinsic solubility (mg mL^{-1}): -4.586 (Low)					
Closantel CAS registration number: 57808-65-8 ChemSpider ID: 38827 PubChem CID: 42574	Molecular formula: $C_{22}H_{14}Cl_2I_2N_2O_2$ Monoisotopic mass (Da): 661.8516 pKa (strongest acidic): 6.41 pKa (strongest basic): -	$[M+H]^+$; $[M-H]^-$	662.8595; 660.8449	264.0339; 194.0964; 635.8485; 214.0418; 534.8094	126.9050; 344.8279; 532.9315; 315.0086; 279.0320	

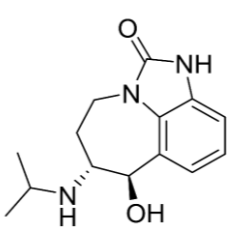
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
	Partition coefficient (Log P): 7.713 Intrinsic solubility (mg mL^{-1}): -6.977 (Low)					
Beta-Agonists						
Cimaterol CAS registration number: 54239-37-1 ChemSpider ID: 2653	Molecular formula: $C_{12}H_{17}N_3O$ Monoisotopic mass (Da): 219.1366 pKa (strongest acidic): 14.11	$[M+H]^+$	220.1444	202.1331; 160.0863; 116.0495; 143.0599; 89.0386		

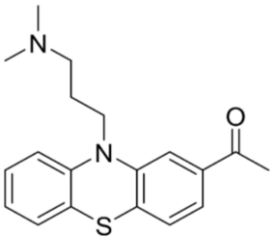
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 2755 	pKa (strongest basic): 9.57 Partition coefficient (Log P): 0.702 Intrinsic solubility (mg mL^{-1}): -1.605 (High)					
Clenbuterol CAS registration number: 37148-27-9 ChemSpider ID: 2681 PubChem CID: 2783	Molecular formula: $C_{12}H_{18}Cl_2N_2O$ Monoisotopic mass (Da): 276.0791 pKa (strongest acidic): 14.06	$[M+H]^+$	277.0869	203.0135; 132.0682; 259.0763; 168.0449; 205.0118		

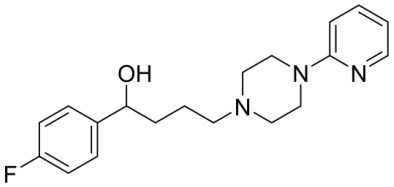
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
	pKa (strongest basic): 9.63 Partition coefficient (Log P): 2.334 Intrinsic solubility (mg mL^{-1}): -2.992 (High)					
Ractopamine CAS registration number: 97825-25-7 ChemSpider ID: 50604 PubChem CID:	Molecular formula: $C_{18}H_{23}NO_3$ Monoisotopic mass (Da): 301.1673 pKa (strongest acidic): 9.19	$[M+H]^+$	302.1751	107.0491; 284.1645; 164.1070; 121.0648; 136.0757		

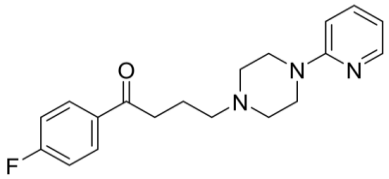
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
56052  	pKa (strongest basic): 9.89 Partition coefficient (Log P): 2.204 Intrinsic solubility (mg mL^{-1}): -2.46 (High)					
Salbutamol CAS registration number: 18559-94-9 ChemSpider ID: 1999 PubChem CID: 2083	Molecular formula: $C_{13}H_{21}NO_3$ Monoisotopic mass (Da): 239.1516 pKa (strongest acidic): 10.12	$[M+H]^+$; $[M-H]^-$	240.1594; 238.1449	222.1489; 166.0864; 148.0758; 121.0648; 91.0542	218.1187; 220.1343; 190.1237; 144.0455; 134.0373	

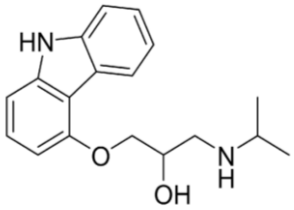
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
	pKa (strongest basic): 9.4 Partition coefficient (Log P): 0.344 Intrinsic solubility (mg mL^{-1}): -0.796 (High)					
Zilpaterol CAS registration number: 117827-79-9 ChemSpider ID: 2343170 PubChem CID:	Molecular formula: $C_{14}H_{19}N_3O_2$ Monoisotopic mass (Da): 261.1472 pKa (strongest acidic): 12.97	$[M+H]^+$	262.1550	244.1442; 202.0974; 185.0709; 157.0760; 130.0651		

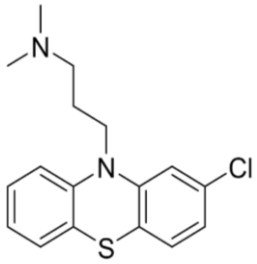
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
25218684 	pKa (strongest basic): 9.14 Partition coefficient (Log P): 0.84 Intrinsic solubility (mg mL^{-1}): -2.459 (High)					
Sedatives						
Acepromazine CAS registration number: 61-00-7 ChemSpider ID: 5852	Molecular formula: $C_{19}H_{22}N_2OS$ Monoisotopic mass (Da): 326.1447 pKa (strongest acidic): -	$[M+H]^+$	327.1526	254.0627; 239.0757; 86.0968; 178.0651; 150.0464		

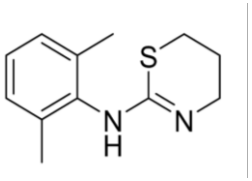
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 6077 	pKa (strongest basic): 9.11 Partition coefficient (Log P): 3.489 Intrinsic solubility (mg mL^{-1}): -4.437 (Moderate)					
Azaperol CAS registration number: 2804-05-9 ChemSpider ID: 2338342 PubChem CID: 3080589	Molecular formula: $C_{19}H_{24}FN_3O$ Monoisotopic mass (Da): 329.1898 pKa (strongest acidic): 14.44	$[M+H]^+$	330.1976	312.1869; 192.1183; 149.1074; 147.0917; 121.0762		

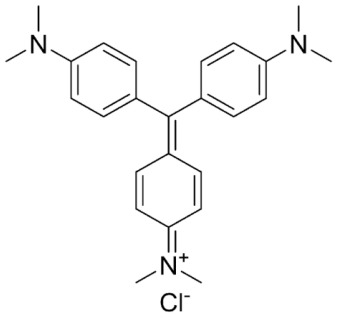
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
	pKa (strongest basic): 8.75 Partition coefficient (Log P): 3.119 Intrinsic solubility (mg mL^{-1}): -2.692 (High)					
Azaperone CAS registration number: 1649-18-9 ChemSpider ID: 14695 PubChem CID:	Molecular formula: $C_{19}H_{22}FN_3O$ Monoisotopic mass (Da): 327.1741 pKa (strongest acidic): -	$[M+H]^+$	328.1820	165.0710; 149.1073; 147.0917; 121.0762; 123.0241		

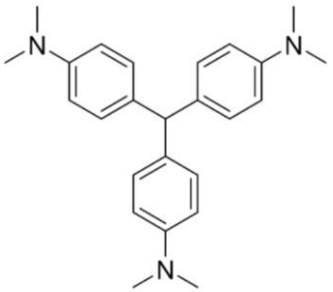
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
15443 	pKa (strongest basic): 8.31 Partition coefficient (Log P): 3.206 Intrinsic solubility (mg mL^{-1}): -3.149 (High)					
Carazolol CAS registration number: 57775-29-8 ChemSpider ID: 64783 PubChem CID:	Molecular formula: $C_{18}H_{22}N_2O_2$ Monoisotopic mass (Da): 298.1676 pKa (strongest acidic): 14.03	$[M+H]^+$	299.1754	194.0964; 139.0542; 116.1070; 89.0386; 74.0600		

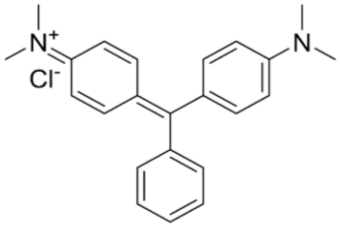
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
71739  	pKa (strongest basic): 9.27 Partition coefficient (Log P): 2.712 Intrinsic solubility (mg mL^{-1}): -4.379 (Moderate)					
Chlorpromazine CAS registration number: 50-53-3 ChemSpider ID: 2625 PubChem CID:	Molecular formula: $C_{17}H_{19}ClN_2S$ Monoisotopic mass (Da): 318.0952 pKa (strongest acidic): -	$[M+H]^+$	319.1030	86.0964; 246.0139; 319.1030; 214.0418; 239.0763		

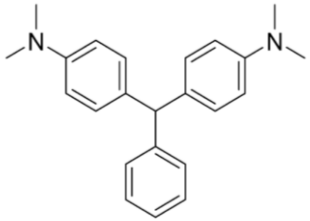
Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
2726 	pKa (strongest basic): 9.2 Partition coefficient (Log P): 4.535 Intrinsic solubility (mg mL^{-1}): -4.848 (Low)					
Prospecting sedatives						
Xylazine CAS registration number: 7361-61-7 ChemSpider ID:	Molecular formula: $C_{12}H_{16}N_2S$ Monoisotopic mass (Da): 220.1029	$[M+H]^+$	221.1107	164.0528; 105.0699; 95.0491; 90.0372; 71.9902		

Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
5505 PubChem CID: 5707 	pKa (strongest acidic): - pKa (strongest basic): 9.54 Partition coefficient (Log P): 3.633 Intrinsic solubility (mg mL^{-1}): -3.572 (Moderate)					
Corants						
Gentian violet/Crystal violet CAS registration number: 548-62-9 ChemSpider ID:	Molecular formula: $C_{25}H_{30}N_3$ Monoisotopic mass (Da): 372.2434	$[M]^+$	372.2434			$[M]^+$ 356.2121; 328.1934; 239.0855; 340.1808; 268.1121

Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
10588 PubChem CID: 11057 	pKa (strongest acidic): - pKa (strongest basic): 4.83 Partition coefficient (Log P): 1.396 Intrinsic solubility (mg mL^{-1}): The molecule cannot be neutralized and the calculation is not defined for molecules with non-zero charge					
Gentian violet/Crystal violet metabolite (Leucocrystal Violet) CAS registration number: 603-48-5 ChemSpider ID:	Molecular formula: $C_{25}H_{31}N_3$ Monoisotopic mass (Da): 373.2513 pKa (strongest acidic): -	$[M+H]^+$	374.2591	358.2278; 239.1543; 237.1386; 165.0699; 152.0621		

Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
62270 PubChem CID: 69048 	pKa (strongest basic): 5.36 Partition coefficient (Log P): 5.81 Intrinsic solubility (mg mL^{-1}): -4.153 (Moderate)					
Malachite green CAS registration number: 569-64-2 ChemSpider ID: 10820	Molecular formula: $C_{23}H_{25}N_2$ Monoisotopic mass (Da): 329.2012 pKa (strongest acidic):	$[M]^+$	329.2012			$[M]^+$ 313.1699; 208.1121; 165.0699; 239.0855; 163.0542

Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
PubChem CID: 11294  	pKa (strongest basic): 4.52 Partition coefficient (Log P): 1.287 Intrinsic solubility (mg mL^{-1}): The molecule cannot be neutralized and the calculation is not defined for molecules with non-zero charge					
Malachite green metabolite (Leucomalachite green) CAS registration number: 129-73-7 ChemSpider ID:	Molecular formula: $C_{23}H_{26}N_2$ Monoisotopic mass (Da): 330.2091 pKa (strongest acidic): -	$[M+H]^+$	331.2169	239.1543; 223.1230; 165.0699; 153.0699; 152.0621		

Group/Class - Pharmacologically active Substance	Physicochemical properties	Monitored ion	Theoretical exact mass MS (*m/z*)	Fragment ions (*m/z*) MS^2		
				$[M+H]^+$	$[M-H]^-$	Others
60551 PubChem CID: 67215 	pKa (strongest basic): 5.17 Partition coefficient (Log P): 5.702 Intrinsic solubility (mg mL^{-1}): -4.376 (Moderate)					

Values were calculated using online Data taken from Chemicalize: log P: octanol/water partition coefficient [107]; pKa: acid/base dissociation constants data taken from computational predictions from [108]; solubility information: low: if < 0.01 mg mL^{-1}; moderate: if is between 0.01 and 0.06 mg mL^{-1} and high if > 0.06 mg mL^{-1} [109]. Chemical structures were drawn using Chemdraw version 18.1 [110]. Identification numbers were taken from Chemspider [111] and PubChem [112].

Table S5. Retention time of veterinary drugs and their metabolites evaluated by Q-Exactive Orbitrap HRMS.

Group/Class - Pharmacologically active Substance	Retention time (min)					
	Method A		Method B*			
			Aqueous extract (Tube 1)		Organic extract (Tube 2)	
	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$
Antimicrobials/Aminoglycosides						
Amikacin						
Apramycin						
Dihydrostreptomycin						
Spectinomycin						
Streptomycin						
Gentamicin (Gentamicin C_1)						
Gentamicin (Gentamicin C_{1a})						
Gentamicin (Gentamicin C_2-C_{2a})						
Hygromycin (Hygromycin B)						
Kanamycin (Kanamycin A)						
Neomycin (Neomycin B)						
Tobramycin						
Antimicrobials/Amphenicols						
Chloramphenicol				8.53		
Florfenicol		7.19	7.27			
Thiamphenicol		6.47		4.92		
Antimicrobials/Betalactams						
Amoxicillin						
Ampicillin	6.85		7.39			
Cephalexin	6.62		5.07			
Cefalonium			4.89			
Cephapirin	5.78		3.82			
Cefazolin			6.26			
Cefoperazone			8.15			
Cefquinome	6.17		5.32			
Cloxacillin	9.55[a]		11.08[b]			
Dicloxacillin	9.85[b]		11.36			
Nafcillin	9.84[c]		9.20			
Oxacillin	9.38[a]		9.79[c]			
Benzylpenicillin	7.26		9.96			
Phenoxymethylpenicillin/Phenoxymethyl V penicillin	9.45[a]		10.48[c]			
Antimicrobials/Lincosamides						
Clindamycin	8.47		9.41			

Group/Class - Pharmacologically active Substance	Retention time (min)					
	Method A		Method B*			
			Aqueous extract (Tube 1)		Organic extract (Tube 2)	
	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$
Lincomycin		6.31	4.54			
Antimicrobials/Macrolides						
Azithromycin			9.34			
Erythromycin (Erythromycin A-H_2O)	9.20		10.58[d]			
Spiramycin (Spiramycin I)	7.35[e]		9.34			
Tilmicosin		6.30	9.92			
Tylosin (Tylosin A)	8.84		10.39			
Antimicrobials/Quinolones-Fluoroquinolones						
Nalidixic acid	8.89		10.09			
Oxolinic acid	8.12		8.90			
Ciprofloxacin	6.62		6.29			
Danofloxacin	6.63		6.78			
Difloxacin	6.83		7.72			
Enrofloxacin	6.62		6.94			
Flumequine	9.11		10.40			
Norfloxacin	6.56		6.07			
Sarafloxacin	6.94		7.62			
Antimicrobials/Sulphonamides						
Sulfachlorpyridazine	6.99		6.49			
Sulfadiazine	5.54		2.41			
Sulfadimethoxine	7.94		9.52			
Sulfadoxine	7.15			7.21		
Sulfisoxazole/Sulfafurazole	7.25		8.03			
Sulfamerazine		6.19	3.97			
Sulfamethazine/Sulfadimidine	6.68		5.19			
Sulfathiazole	5.86		3.65			
Sulfamethoxazole	7.07		7.19			
Sulfaquinoxaline	8.09		9.67			
Antimicrobials/Tetracyclines						
Chlortetracycline	7.82		8.51			
Doxycycline	6.80		6.21			
Oxytetracycline		6.93				
Tetracycline	8.35		6.21			
Antimicrobials/Others						
Bromhexine	9.06		10.41			
Dapsone	6.47		6.12			

Group/Class - Pharmacologically active Substance	Retention time (min)					
	Method A		Method B*			
			Aqueous extract (Tube 1)		Organic extract (Tube 2)	
	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$
Rifampicin		9.90		11.47		
Tiamulin	8.86		10.64			
Antimicrobials Prospect/Quinolones-Fluoroquinolones						
Marbofloxacin	6.23		5.60			
Antimicrobials Prospect/Macrolides						
Josamycin/Leucomycin A_3			11.04			
Leucomycin/Leucomycin A_5	8.98		10.61			
Tildipirosin	5.43				9.23	
Tulathromycin (Tulathromycin A)	6.30		5.44			
Antimicrobials Prospect/ Sulfonamides						
Phthalylsulfathiazole		7.48	8.62			
Sulfacetamide/*N*-Sulfanilylacetamide	5.62			1.46		
Sulfamethoxypyridazine	6.78		5.75			
Antimicrobials Prospect/Others						
Diminazene	5.39					
Fosfomycin						
Isoniazid	1.35					
Novobiocin					10.58	
Rifaximin		10.35		11.75		
Antibiotic Growth Promoters						
Avilamycin (Dichloroisoeverninic acid)		7.99		7.06		
Halquinol/Chlorhydroxyquinoline (7-Chloro-8-quinolinol)					9.98	
Halquinol/Chlorhydroxyquinoline (5,7-Dichloro-8-quinolinol/Chloroxine)					10.58	
Halquinol/Chlorhydroxyquinoline (5-Chloro-8-hydroxyquinoline)					10.16	
Virginiamycin (Virginiamycin M_1)	9.60[a]		10.96			
Anticoccidials						
Amprolium						
Clopidol	6.40		2.94			
Diaveridine	6.12		4.68			
Decoquinate		13.46	13.49			
Diclazuril		11.02				10.55
Ethopabate	8.65[a]		9.33			
Lasalocid (Lasalocid A)						13.12
Maduramicin						

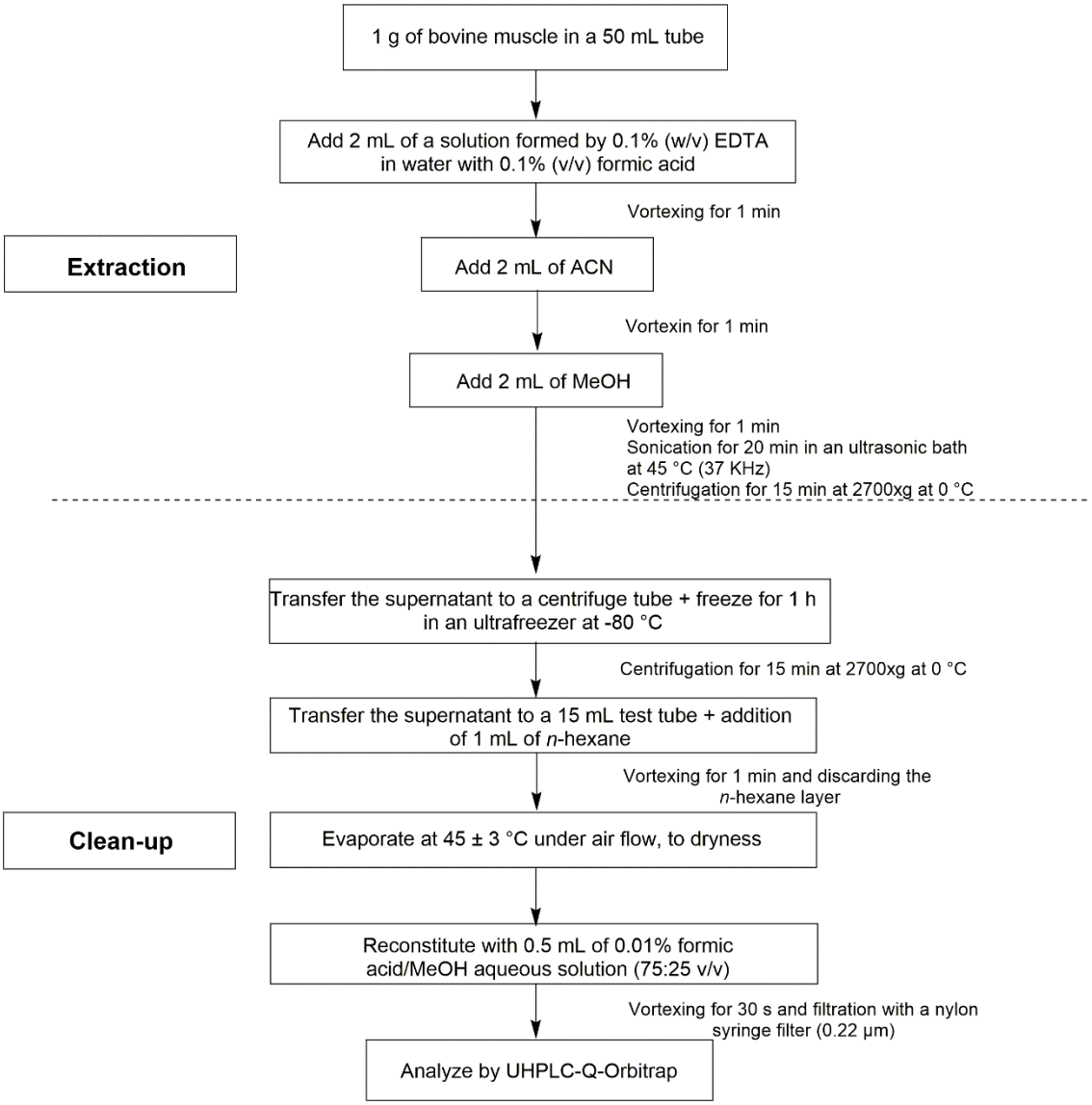
Group/Class - Pharmacologically active Substance	Retention time (min)					
	Method A		Method B*			
			Aqueous extract (Tube 1)		Organic extract (Tube 2)	
	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$
Monensin (Monensin A)						
Narasin (Narasin A)						
Nicarbazin (4,4′-Dinitrocarbanilide - DNC)		10.69				10.37
Robenidine	9.87				10.18	
Salinomycin	13.08[a]			13.84		
Toltrazuril						
Trimethoprim	6.28				9.35	
Anti-inflammatories/Steroidal						
Prednisolone			10.03			
Prednisone			10.02			
Anti-inflammatories Prospect/Steroidal						
Isoflupredone acetate/9-Fluoroprednisolone acetate						
Flumetasone						
Anti-Inflammatory/Non-Steroidal						
Mefenamic acid		11.99				10.70
Tolfenamic acid		11.06				10.41
Carprofen		11.08		11.93		
Ketoprofen		9.96	11.22			
Diclofenac				12.11		
Flunixin		11.05		11.13		
Indomethacin				12.12		
Meloxicam		9.74	11.24			
Naproxen						
Nimesulide		9.82		11.63		
Piroxycam	8.66		10.16			
Propyphenazone	9.19		10.38			
Antiparasitic/Avermectins						
Avermectin B_{1a}/Abamectin B_{1a}						
Doramectin						
Emamectin (Emamectin B_{1a})	11.48					
Eprinomectin (Eprinomectin B_{1a})						
Ivermectin B_{1a}/22,23-Dihydroavermectin B_1						
Moxidectin					11.73	
Antiparasitic/Benzimidazoles						
Albendazole	10.04		10.48			

Group/Class - Pharmacologically active Substance	Retention time (min)					
	Method A		Method B*			
			Aqueous extract (Tube 1)		Organic extract (Tube 2)	
	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$
Albendazole metabolite (Albendazole sulfone)	8.07		8.57			
Albendazole metabolite (Albendazole sulfoxide)	7.95		7.01			
Closantel		11.06		14.64		
Febantel	10.80		12.18			
Fenbendazole	10.57		11.24			
Fenbendazole metabolite (Fenbendazole sulfone)	8.66		10.16			
Flubendazole	9.68		10.58			
Flubendazole metabolite (2-Aminoflubendazole)	8.07		8.79			
Levamisole	5.83		3.52			
Mebendazole	9.44		10.34			
Oxibendazole	8.96		9.11			
Oxfendazole	8.85		9.21			
Thiabendazole	7.10		4.53			
Triclabendazole		11.84			10.67	
Antiparasitic/Phenylpyrazoles						
Fipronil		10.90		12.65		
Fipronil metabolite (Fipronil sulfone)		11.14		13.04		
Antiparasitic/Nitroimidazoles						
Dimetridazole						
Dimetridazole metabolite (Hydroxydimetridazole/HMMNI)						
Ipronidazole	7.87		6.70			
Ipronidazole metabolite (Hydroxy Ipronidazole)	7.28					
Metronidazole						
Metronidazole metabolite (Hydroxymetronidazole)						
Ronidazole/1-Methyl-2-carbamoyloxymethyl-5-nitroimidazole						
Antiparasitic/Isoquinoline-pyrazines						
Praziquantel	10.16		11.24			
Beta-Agonists						
Cimaterol						
Clenbuterol						
Ractopamine						
Salbutamol	5.26					
Zilpaterol						
Sedatives						

Group/Class - Pharmacologically active Substance	Retention time (min)					
	Method A		Method B*			
			Aqueous extract (Tube 1)		Organic extract (Tube 2)	
	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$	$HESI^+$	$HESI^-$
Acepromazine	8.88		10.39			
Azaperol	7.04		6.12			
Azaperone	7.44		7.10			
Carazolol	7.58		9.19			
Chlorpromazine	9.61		10.94			
Prospecting sedatives						
Xylazine	7.01		6.51			
Corants						
Gentian violet/Crystal violet	9.68[f]		11.87[f]			
Gentian violet/Crystal violet metabolite (Leucocrystal Violet)			10.13			
Malachite green	9.12[f]					
Malachite green metabolite (Leucomalachite green)	12.56		12.17			

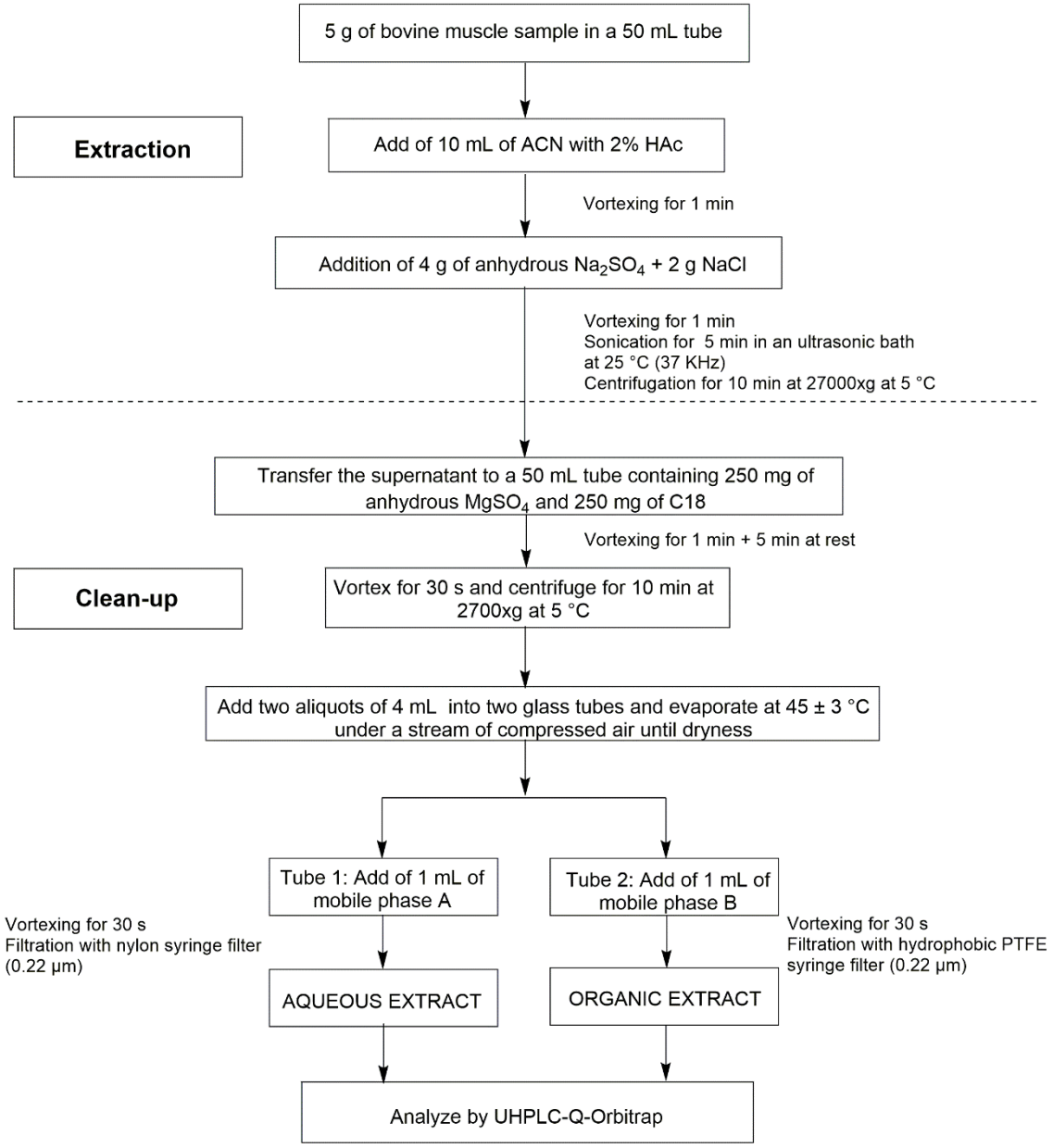
Adducts: [a]$[M+Na]^+$; [b]$[(M-H-CH_3OH)]^+$; [c]$[(M+H_2-CO)+H]^+$; [d]$[M-H_2O+H]^+$; [e]$[M+2H]^{2+}$; [f]$[M]^+$. Abbreviations: $HESI^+$: heated electrospray ionization source operated in positive ion mode; $HESI^-$: heated electrospray ionization source operated in negative ion mode; min: minute. *In method B, the analytes marked in gray were analyzed by the organic extract.

Figure S1. General flowchart of the sample preparation procedure according to method A.



Prepared according to the modified method described by Dasenaki et al. [57].

Figure S2. General flowchart of the sample preparation procedure according to method B.



Prepared according to the modified method described by Silva et al. [22].

Figure S3. Analyte identification criteria [22,57].

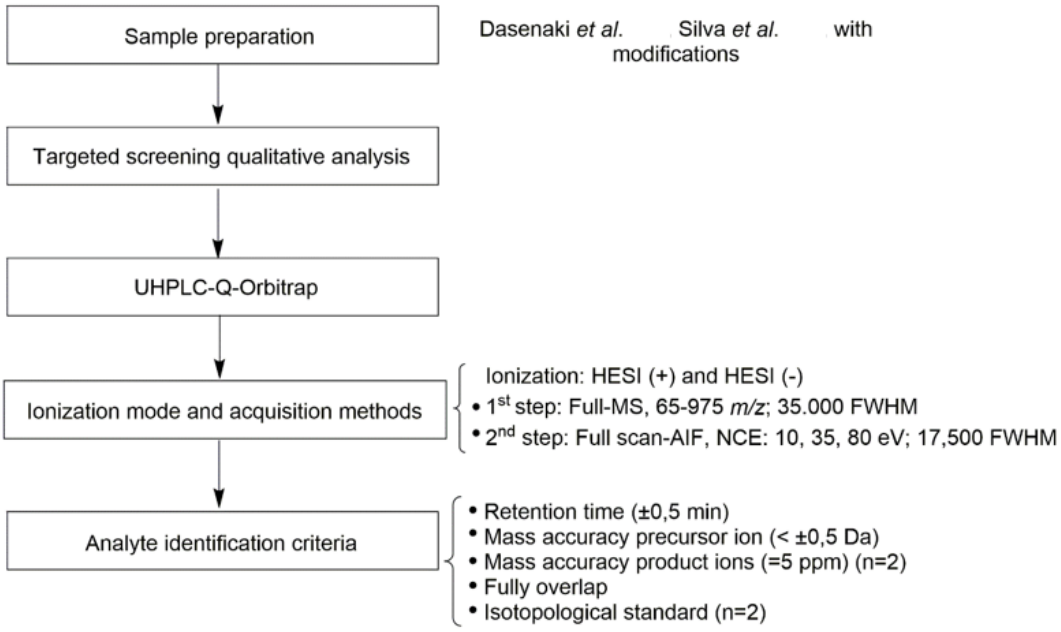
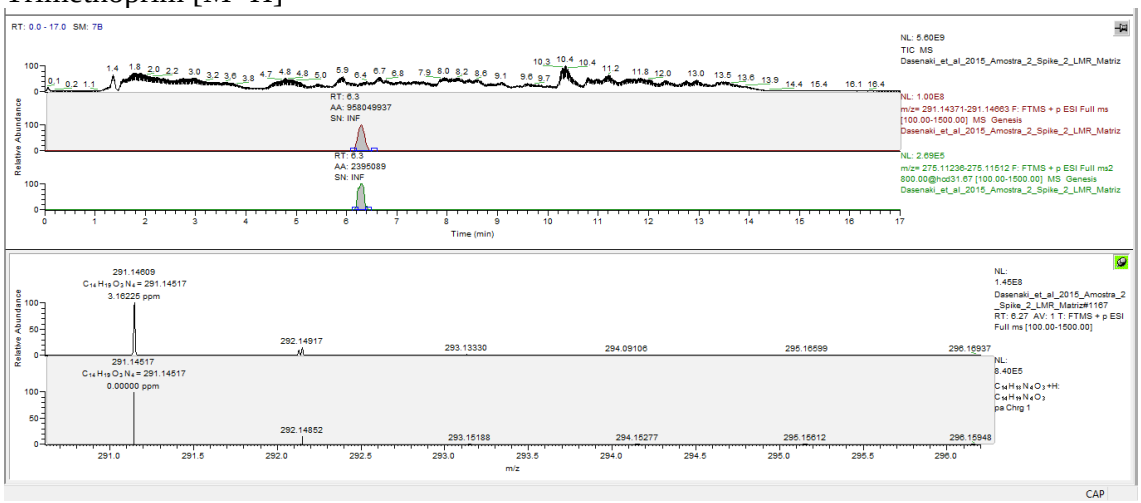
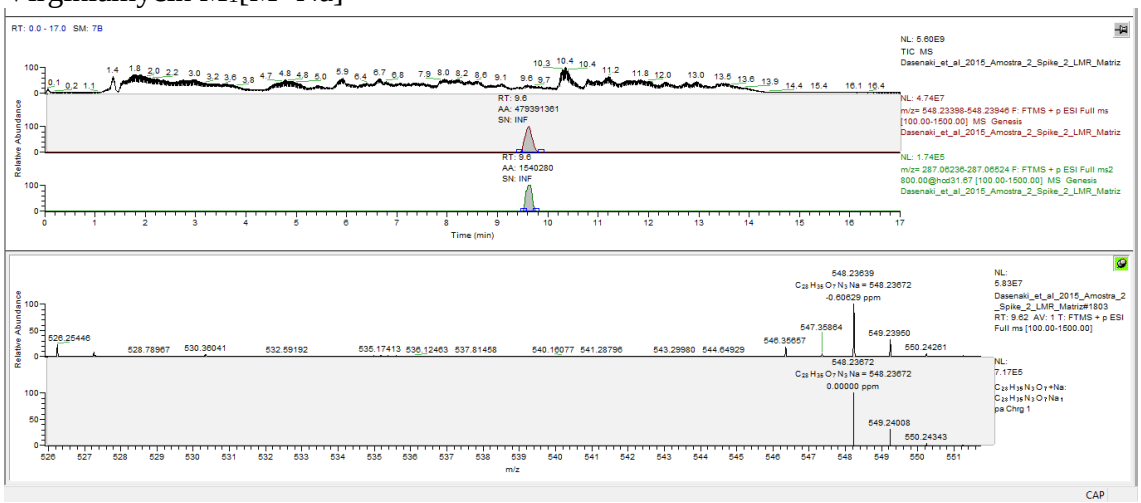


Figure S4. Examples of extracted mass traces of a spiked bovine muscle tissue at 2 MRL according to the established criteria for analyte identification.

Trimethoprim $[M+H]^+$



Virginiamycin $M_1[M+Na]^+$



Dichloroisoeverninic acid $[M-H]^-$